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PROCESS INTEGRATION FOR WATER MINIMISATION IN OIL PROCESSING AND PETROCHEMISTRY

A Thesis submitted to the
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by

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under the supervision of
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CHAPTER 1

Introduction

1.1. Objective

This work is intended to tackle process integration for water minimisation in oil processing and petrochemistry creating an original methodology including formulation of physical/mathematical model for water network as oriented graph, solution of optimisation problem with original variant of hybrid genetic algorithm (GA) and finally topology visualisation in a new graphical format, facilitating also relevant water balance representation for industrial applications. In literature different approaches for water networks are presented but mainly two problems can be formulated

- *Water minimisation problem* – when the analysis is concentrated on water using units transferring contaminants from process streams to water streams, involving a variety of basic processes not only mass transfer.
- *Mass exchange network approach* – when mainly mass transfer is taken into account and alternative mass transfer agents can be concurrent to water network.

I consider in my Thesis that water minimisation problem is more relevant for the application field focused (oil processing and petrochemistry). This determine me to dedicate the objective of this Thesis to develop a methodology tackling this problem. Chosen approach belongs to the category of source reduction design/retrofit methodologies, involving identification and implementation of plant modifications based on water streams reuse and (partial) regeneration. The target is to minimise supply water flowrate and/or to improve several indexes related to water network topology and/or economic aspects with a systematic approach.

1.2. Context of research work

This work is the result of more than 15 years expertise in research and more than 12 years expertise in industrial water systems analysis as responsible for the concerned working team in the Centre for Technology Transfer in the Process Industries (CTTIP) at University Politehnica of Bucharest (UPB). This period was a good opportunity to collaborate with Centre for Process Integration (CPI) at University of Manchester and Romanian professionals from oil processing industry and petrochemistry. In the last five years research collaboration was performed with colleagues in the Department of Chemical Engineering at UPB to develop present methodology.

The software for application of GA in optimisation was not developed in the frame of this work, being used as an optimisation tool. However the methodology proved to be very useful to tackle in original way complex industrial problems of water minimisation, of a magnitude not yet reported in literature both as number of contaminants and as number of water-using units. Case studies developed in my Thesis used data from Romanian industrial partners, which were not reported in literature until now by other research groups in their work on water network analysis.

From the beginning the approach has many difficult aspects:

- The problem is very complex.
- Plant data is difficult to formulate and harvest from industrial sites.
- The mathematical model is highly non-linear with dimension exceeding current approaches, GA solving procedure allowing to obtain reasonable solutions.
- Literature does not present relevant solution to extended industrial problems (more than ten water using operations and more than four contaminants).

However, some benefice factors allowed to tackle with success the objective proposed:

- Collaboration with CPI at The University of Manchester enabled me to get expertise in using water systems analysis tool WATER dedicated to Process Integration Research Consortium (PIRC) members.
- Collaboration with Romanian oil processing and petrochemistry companies as PETROM and ASTRA ROMANA to solve industrial problems during some year in interesting projects.
- The work developed in some research projects funded by the Romanian Ministry of Education, Research and Youth in the last seven years.
- The collaboration inside the research groups of CTTIP at University Politehnica of Bucharest.
- The collaboration inside the Department of Chemical Engineering at University Politehnica of Bucharest where I am registered as PhD student.

Some results of this work are already published in the last years in 15 publications mentioned in this Thesis.

Main elements of originality are tracing all the stages of the research work:

- Physical and mathematical models present original approach for water networks based on oriented graph representation.

- Solving algorithm for Non-Linear Programming (NLP) problems formulated in this Thesis is based on original modified hybrid GA.
- Original graphical representation enable water network topology and water mass balance to be visualised easily.
- Complex industrial case studies support each development of proposed methodology, being published by the author in different international conferences, mainly ESCAPE and PRES.

1.3. Summary

The Thesis is structured on five chapters

Chapter 1 presents the objective, the context and the summary of the research work.

Chapter 2 is a systematic literature survey on significant results publishes in at least last 15 years.

Chapter 3 is dedicated to water network optimisation for multiple supply water sources.

Chapter 4 presents water network optimisation with economic aspects consideration.

Chapter 5 is dedicated to water network optimisation considering regeneration both in design and retrofit.

In Annex I detailed algorithm calculation of dependent variables for supply water flowrate optimisation is presented.

In Annex II user's interface for computer tool based on GA is presented.

All notations used in Thesis development are grouped in two lists : one for Chapter 2 for literature survey and one dedicated to the work developed in this Thesis in Chapters 3-5.

A list of more than hundred literature references ordered alphabetically reveal main published work in this field, used during the Thesis development to correlate the approach of personal work with results published by other researchers. A list of 15 personal publications is completing the references section. These publications are setup with colleagues from CTTIP, Department of Chemical Engineering at UPB and professionals from Romanian oil processing industry and petrochemistry.

Literature survey is systematically presented in Chapter 2 on following subjects:

- Process integration concepts and applications based either on graphical and optimisation approaches
- Mathematical models for problems related to water networks
- Algorithms for water networks optimisation.

Finally in Chapter 2 conclusions on literature survey and scope for present work are underlined.

Chapter 3 represents the core of the Thesis having following structure:

- Introduction and motivation
- Problem statement-Physical model
- Mathematical model
- Design criteria
- Optimisation algorithm
- Water network graphical representation
- Case studies to illustrate and support the methodology
- Conclusions.

Original approach for chosen problem – water minimisation-, for physical/mathematical models, for optimisation algorithm and water network graphical representation are analysed and presented in detail. Case studies illustrate and support the methodology, allowing to obtain better results compared to other published approaches and to tackle bigger size problems, closer to industrial demands. In this chapter the objective function for optimisation problem is water supply flowrate.

Continuing the work developed in Chapter 3, economic aspects are analysed in detail in Chapter 4, following similar approach as in Chapter 3. Main parts of this chapter are:

- Introduction
- Physical/mathematical model with emphasis on objective function formulation, based on pipes optimal diameter calculation, to diminish frictional losses.
- Design criteria based on total annualised cost and water network topological index, introduction of weighted objective function
- The new form of optimisation algorithm
- Case studies with relevance for oil refining industry are presented for minimisation of total annualised cost
- Case study to illustrate water network design with topological index minimisation or weighted objective function as a linear combination between supply water flowrate and topological index.
- Conclusions on results for water network optimisation based on economical indexes are comparatively presented.

Consideration of regeneration for water network optimisation is developed in Chapter 5 following a similar scheme:

- Introduction on relevance of regeneration for water networks optimisation
- New concepts to formulate and illustrate the new methodology
- Water minimisation problem statement based on supply water flowrate objective function
- An original approach to retrofit strategy
- Detailed mathematical models for water-using unit with regeneration and regeneration unit
- Design criteria for methodology formulation
- Based on previous chapters results, solving strategy and optimisation algorithm are presented to complete the new methodology
- Original contribution to water network graphical representation is extended to the case of regeneration
- Methodology illustration for two case studies using data from petrochemical plants for design with regeneration respectively for retrofit by introducing regeneration confirm the relevance of original work tacking the proposed subjects
- Conclusions reveal the significance of the work developed in this chapter.

Finally the Thesis has a General conclusions chapter underlying the originality of results and relevance of results as Thesis objectives are fulfilled.

CHAPTER 2

Process integration tools for wastewater minimisation

2.1 Process integration concepts

Process integration is a systematic and general approach used to design integrated process systems, from individual processes to overall site using different criteria. Based on first concepts introduced by Linnhoff et al., 1982, it developed to identify global insights and synthesise strategies for efficient use of energy or reduction of pollution effects on environment (Dunn & El-Halwagi, 2003).

In the past, the industrial goal from environmental point of view was to identify a recovery system that would allow reducing of the contamination of streams in order to reuse or recycle in the system. From a variety of process system configurations and operating conditions it was individually selected the best economic solution for the company (operating cost, capital investment, etc).

Recently, system design methodologies were oriented towards identifying a system that accomplishes not only the waste reduction tasks, but also a system that represents the most effective cost approach (Taal et al., 2003). These methodologies can be implemented within a variety of process industries: oil refining (Takama et al., 1980; Bagajewicz&Savelski 1999), petrochemistry (Mann & Liu, 1999), pulp and paper manufacturing (Yang et al., 2000; Mann et al., 2007), plastics production, food production (Hufendiek & Klemeš, 1997; Klemeš et al., 1999; Thevendiraraj et al., 2003), pharmaceuticals, industrial laundries and fibre drying industries (Wenzel et al., 2002).

During the late 1970s and 1980s, the efforts were oriented to develop process integration tools to identify energy savings in heat exchanger networks (Linnhoff&Flower, 1978, Townsend&Linnhoff, 1983, Smith et al., 2000, Klemes et al., 1997, Klemes &Perry, 2007). Over the last two decades, the research was oriented also to identify process integration tools for evaluation of environmental impact (El-Halwagi&Manousiouthakis 1989, Wang&Smith 1994, Klemeš et al., 1997; Bagajewicz&Savelski 1999, Smith 2005, Karuppiah&Grossmann 2006, Klemeš&Perry, 2007) or for retrofit (Hassan et al., 1999; Zhu et al., 2000).

Process integration methodologies used to design/retrofit water networks from environmental point of view can be classified in two categories:

- End-of-pipe design methodologies and tools (applied to remove contaminants by identifying new mass transfer agents, new reactive direct contact agents, using stream pressurisation and depressurisation, using membranes, etc)

- Source reduction design methodologies and tools (applied to identify and implement in the plant modifications based on stream reusing and stream partial regeneration).

Waste minimisation is one of the source reduction methodologies for environmental process design. It is used for design/retrofit a water network by reuse, regeneration reuse or regeneration recycling of water streams to minimise the supply water flowrate and also the wastewater flowrate.

The five steps of applying this systematic approach to industrial water minimisation are:

1. Establish the boundary limits for the site
2. Identify and evaluate the water-reuse study issues relative to costs
3. Evaluate the technical opportunities and water-reuse techniques
4. Implement the new water-reuse model or design
5. Review and update the model or design as needed

For a water network, the process integration methodologies give answers to several questions including:

- Which water streams should be reused?
- What is the optimal load of each water stream to be reused?
- What is the optimal streams allocation that is routed to the processes?
- What is the optimal system configuration?
- What is the maximal out concentrations of contaminants in the streams?

Typically a process integration study includes following elements:

- Process mapping and data acquisition
- Setting up a model of the processing plant and process simulation, amongst others for providing better and lacking data
- A pinch analysis to determine the scope for energy/water savings
- Process simulation for investigation of the consequences of various scenarios for process modification
- Detailed optimisation of the plant design, analyses and the simulation model
- Verification/validation of integrated topology.

The process integration tools cover a variety of techniques, ranging between two limits:

a. Graphical techniques based on “pinch analysis”
b. Mathematical optimisation-based approaches.

a. Graphical techniques

Main features are presented below.

- Based on first and second laws of thermodynamics.
- Based on mass load transferred between process streams and water streams.

- Two step methods: targeting the freshwater consumption of the whole water network and then designing the topology of the network for this target.
- Interactive methods, the engineer can take decision in a sequential manner.
- Can be extended to other concepts (Hydrogen Pinch, Total Site Pinch, etc.)

b. Mathematical optimisation-based approaches

Design and analysis optimisation methods use specialised algorithms to iteratively investigate the design space for the best values of input variables to achieve a specified goal. In many cases, optimisation can be applied to everyday design problems to improve product performance/quality while simultaneously reducing manufacturing cost, weight, environmental impact, etc.

There is a vast range of optimisation methods, the most of which can be categorised according to Fig. 2.1. Every method has a set of problems to which is more appropriated. This depends on a series of problem characteristics, especially the function describing it, not usually easily to obtain (Garcia et al., 2005).

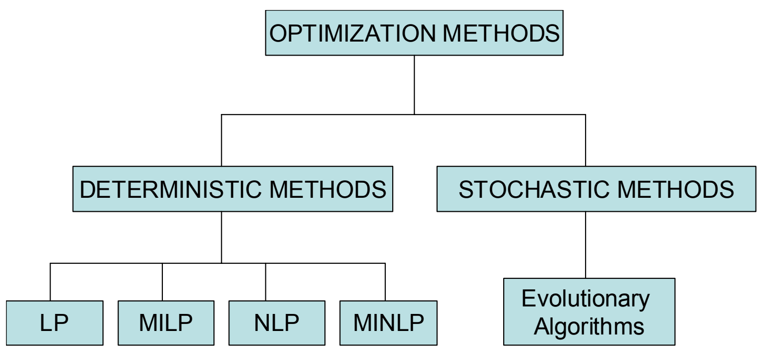


Figure 2. 1 Mathematical programming techniques (Garcia et al., 2005)

Linear programming (LP) is used to obtain the optimal solution to problems perfectly represented by a set of linear equations.

Non-Linear programming (NLP) is used for problems described by non-linear equations. It can be divided in two large method groups: deterministic and stochastic methods.

Deterministic methods include gradient-based and simplex algorithms. Gradient-based algorithms search the optimum by exploring along the direction of steepest descent of the objective function, until some convergence criterion is met. Some gradient-based methods are designed to handle constraints. If used properly for right kinds of problems, gradient-based algorithms usually require fewest evaluations to find a solution. However, these algorithms are susceptible to find a local (rather than global) optimum, if a poor start point is selected. Also, gradient-based methods are ill-suited for problems with discrete variables or noisy objective functions.

Stochastic methods have, as their main characteristic, the search for the optimal value through probability rules, working in an “oriented random” manner. Among the stochastic techniques, Evolutionary Strategies (ESs), Genetic Algorithms (GAs) and Simulated Annealing (SA) are widely used. Genetic algorithms, for example, are very useful for engineering problems with multiple optima, a noisy objective function, multiple objectives, and/or discrete design variables. Genetic algorithms start with a more global search and eventually converge to an optimal population of designs. However, they have the disadvantage of requiring more evaluations to converge, compared to gradient-based methods. In addition, many genetic algorithm implementations do not handle constraints.

In conclusion, process integration is a systematic approach used for linking process units and equipment in order to achieve better solutions/conditions for design and functionality. This approach can be applied on different process networks using process integration methodologies and tools based on developing a mathematical model for process network and than founding the best algorithms to solve this model.

2.2. Mathematical models for water networks

2.2.1. Introduction

Using mathematical programming approach to process design, operation, integration ie in wider sense for process synthesis, consists of three major steps (Grossmann et al., 2000):

1. Representation of all alternatives from which the optimum solution will be selected (superstructure)
2. Mathematical model formulation, involving generally discrete and continuous variables for selecting the configuration and operation alternatives. The main components of the model are:
    a) Criterion to be optimised expressed as mathematical function (objective function) of like economic index (cost minimisation) or performance index (flowrate minimisation).
    b) Constraints as inequalities (performance or operational indicators) and/or equalities (balance equations) embedding all stipulated requirements, restrictions and limitations specific to the problem.
3. Solution the optimisation model to find the optimal solution.

2.2.2. Superstructures

In application of mathematical programming techniques, it is necessary to formulate a superstructure of all possible alternatives. There are two major issues to postulate a superstructure:

- Given a set of alternatives that are to be analysed, what are the major types of representations that can be used and what are the implications for modelling.
- For a given representation that is selected, what are all the feasible alternatives that must be included to guarantee that the global optimum is not overlooked.

For water networks can be identified the following elements for a superstructure (Grossmann, 2005):

- *Mixing unit*: a set of inlet streams can be mixed to create a new stream (Fig. 2.2).
- *Separation unit*: one inlet stream is split in many outlet streams (Fig. 2.3).

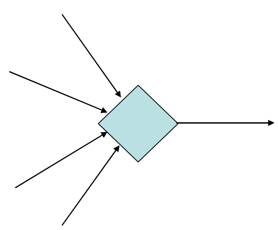


Figure 2. 2 Mixing unit (Grossmann, 2005)

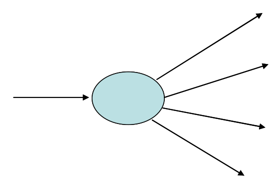


Figure 2. 3 Separation unit (Grossmann, 2005)

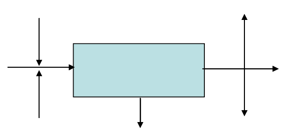


Figure 2. 4 Process unit (Grossmann,2005)

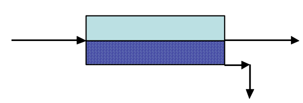


Figure 2. 5 Treatment unit (Grossmann, 2005)

- *Process unit*: a set of inlet streams and a set of outlet streams. For each contaminant internal mass load is considered constant (Fig.2.4).
- *Treatment unit*: a set of inlet streams and a set of outlet streams. Mass load of each contaminant at the exit is reduced (Fig. 2.5).

2.2.3. Mathematical model

Optimisation problem can be defined in the following form:

a. *Objective function f(x,y),*

$$\min(\max): f(x,y) \tag{2. 1}$$

b. *Model constraints:*

$$h(x,y) = 0 \tag{2. 2}$$

$$g(x, y) \leq 0 \quad (2.3)$$

$$x \in X, y \in \{0,1\} \quad (2.4)$$

Where:

$f(x, y)$ Objective function (freshwater flow rate, wastewater flow rate, total cost)

$h(x, y) = 0$ Equations that describe the performance of the system (mass and heat balance, design equations)

$g(x, y) \leq 0$ Inequalities that define the specifications or constraints for feasible choices

x – Continuous variables which correspond to the state or design variables

y – Discrete variables which are restricted to take 0 or 1 values to define the selection of an item or an action.

Optimisation problems can be classified in terms of continuous and discrete variables as (Grossmann, 2005):

- *Linear Problem* (LP) - the model has functions that are linear and there are no binary variables.
- *Mixed Integer Linear Problem* (MILP) – the model has linear functions and the discrete variables are presented.
- *Non Linear Problem* (NLP) – the model has functions that are nonlinear and there are no binary variables.
- *Mixed Integer Non Linear Problem* (MINLP) – the model has nonlinear functions and the discrete variables are present.

Generally, mathematical models can be classified as presented below.

- *Aggregated models* – high level representation in which the optimisation problem is greatly simplified by an aspect or objective (transhipment models for predicting the minimum number of mass exchanger network units).
- *Short cut models* – fairly detailed superstructures that involve cost optimisation but the performance of units is predicted with relatively simple nonlinear models in order to reduce the number of algebraic equations (synthesis model for heat exchanger).
- *Rigorous models* – detailed superstructures but involve rigorous and complex models for predicting the performance of the units (synthesis of distillation sequences).

2.2.4. Synthesis strategies

There are two major strategies that can be used to solve mathematical models for design and synthesis:

- *Simultaneous strategies* - a single model is optimised at once and all trade-offs are taken simultaneous into account.
- *Sequential strategies* – solving a sequence of sub-problems at an increasing level of detail to avoid solving a large single problem.

2.2.5. Mathematical models for water networks

A number of efforts for the clean production technology have been increasingly made to formulate a corresponding mathematical model to achieve the goal of fundamental structural changes that allow extensive water reuse or decreasing wastewater generation. Given a set of water-using units it is desired to determine a network of interconnections of water streams between units so that the overall supply water consumption is minimised while the units receive water of adequate quality. This defines a superstructure incorporating all relevant water streams within the process under investigation together with all units that introduce or remove waterborne contaminants. There are numerous optimisation models of various complexity and scale that have been developed to give optimal solutions for problems in water resources management. Historically, a list of mathematical models formulated by different authors is presented.

2.2.5.1. Transhipment model (Takama et al., 1980)

To formulate this model, Takama et al., presumed that an entity (contaminant mass) can be transported between a source ("rich" process streams) to a sink ("lean" water streams) (Figs. 2.6,and 2.7), by analogy with transhipment model.

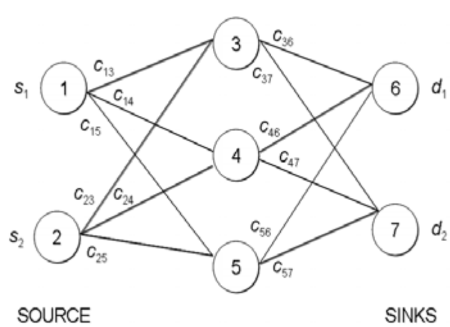


Figure 2. 6 Transhipment model (Takama et al., 1980)

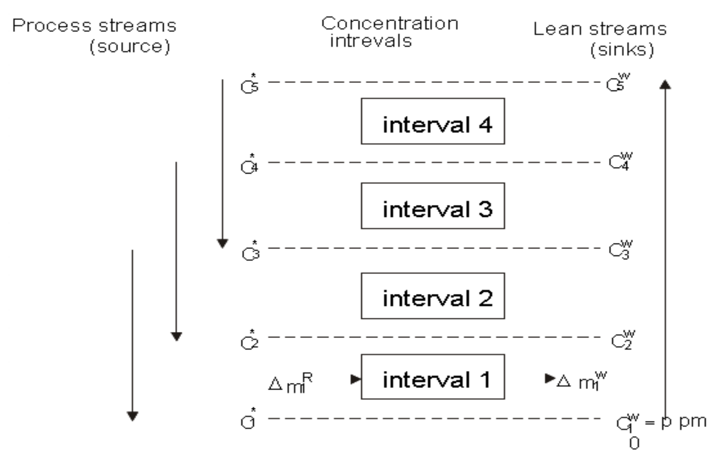


Figure 2. 7 Concentration intervals (Takama et al., 1980)

Hypotheses:

- Process streams are always sources of contaminants and are placed in the left side of the graphical representation.

- Concentration intervals (deposits of contaminant) are represented by horizontal lines.

There are two concentrations scales:

- C_i^* (ppm) - levels of concentration for operation data
- C_i^w (ppm) - inlet and outlet concentration of contaminant from “deposits”

Always lean water streams represent the final destination for contaminant and they are represented in the right side. The solution for this model is to find the minimum flow rate of lean water stream used to transfer the contaminant from process streams to water streams.

Objective function: the minimum flow rate of lean stream

$$y = f_{min}(x) \tag{2. 5}$$

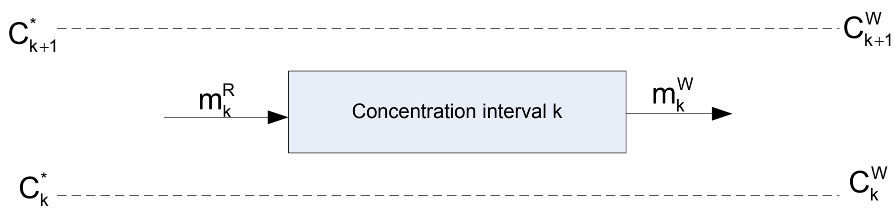


Figure 2. 8 Concentration interval for transhipment model (Takama et al., 1980)

Mathematical model:

- mass balance of contaminant around concentration interval k (Fig.2.8)

$$m_k^R = m_k^W = f_{min}(C_{k+1}^w - C_k^w) \qquad k = 1,2,\dots,n_{int} \tag{2. 6}$$

Constraints:

- contaminant concentration of each process stream cannot be over the contaminant concentration of each water stream

$$\begin{aligned} &C_k^S = 0 && k = 1 \\ &C_k^S \le C_i^* && k = 2,\dots,n_{int+1} \quad i=1,2,\dots,int \end{aligned} \tag{2. 7}$$

2.2.5.2. Concentration interval model (El-Halwagi & Manousiouthakis, 1990)

They formulated a LP model to determine the required flow rate of each lean stream and minimum total cost of lean streams. The network was represented as a set of rich streams (process streams) and a set of lean streams (agent streams) that can transfer certain species from rich streams to the lean streams at minimum cost. Based on transhipment model, the author built a concentration interval diagram using limiting compositions of rich and lean streams. Interval of concentration k^{th}, delimited by contaminant concentrations Y_k and Y_{k-1} is presented in Fig.2.9.

For each concentration interval, the contaminant load of i[th] rich stream passing through the k[th] interval was calculated through the following expressions:

$$W_{i,k} = G_i(Y_{k-1} - Y_k) \qquad (2.\ 8)$$

If a process stream is not passing the interval k, values of $W_{i,k}$ are 0.

Similarly, contaminant load of j[th] lean stream passing through the k[th] interval was given by:

$$W_{j,k} = L_j(X_{k-1} - X_k) \qquad (2.\ 9)$$

From each concentration interval a residual mass load δ_k was transported to the next interval.

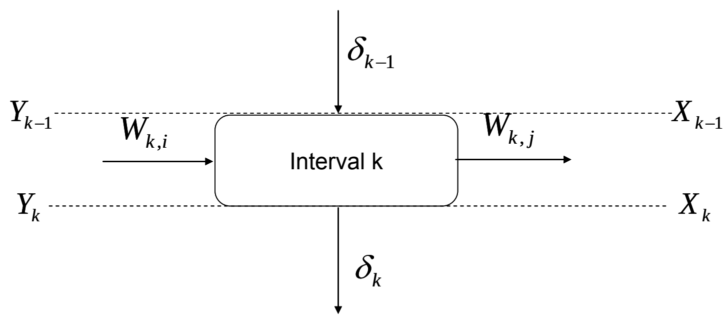


Figure 2. 9 Concentration interval k (El-Halwagi & Manousiouthakis,1990)

Hypotheses :

- The flowrate of each stream is constant as it passes through the network
- All the required separation duties are based on single contaminant
- Streams recycling and mixing are not allowed within the network
- The equilibrium relation governing the distribution of contaminant between rich and lean streams is linear and independent of the presence of other soluble components

Mathematical model:

- Objective function : the minimum lean stream cost

$$\min \sum_j c_j L_j \qquad (2.\ 10)$$

Subject to:

- Overall mass balance around the interval k

$$\sum_i W_{k,i} + \delta_{k-1} = \sum_j W_{k,j} + \delta_k \qquad k=1,2,\ldots,N \qquad (2.\ 11)$$

- Constraints
  - Mass residual loads are positive

$$\delta_k \geq 0$$
$$\delta_0 = 0 \quad \text{k=1,2,...,N-1} \tag{2. 12}$$
$$\delta_N = 0$$

- Flowrate of lean streams are positive

$$L_j \geq 0 \text{ j= 1,2,...N}_S \tag{2. 13}$$

2.2.5.3. NLP model for oil refinery (Rossiter & Ravi, 1995)

Rossiter and Ravi model was developed to identify all possible recycle and reuse options for each water stream. The model included two alternative contaminant pickup modes (equilibrium or fixed quantity) and two regeneration modes (fixed percentage removal and fixed outlet concentration).

The superstructure for this model is presented in Fig. 2.10 and Fig. 2.11.

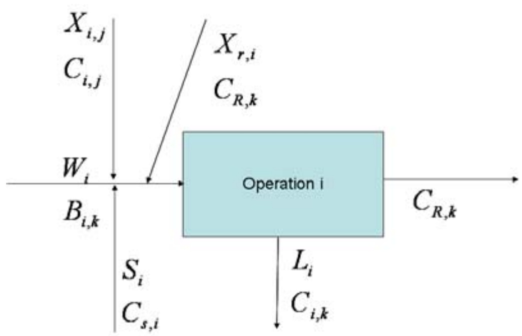


Figure 2. 10 Superstructure of process units (Rossiter & Ravi, 1995)

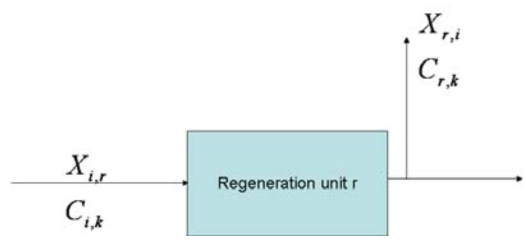


Figure 2. 11 Superstructure of regeneration units (Rossiter & Ravi, 1995)

Hypotheses:

- The network has n process units
- Each unit i can be handle with water process stream, with water from source, with re-used water streams or regenerated water streams
- Simultaneous multi-component mass transfer is considered
- Each operation can haves losses
- To remove contaminant composition there are r regeneration units considered

Mathematical model:

- Objective functions
  - Minimum Flow Rate Of Freshwater

$$\min \sum_i W_i + \sum_r \left[(k1_r + k2_r - 1) \times \sum_i X_{i,r} \right] \tag{2. 14}$$

- Minimum Flow Rate Of Regenerated Water

$$\min \sum_i W_i + \sum_r \left[(k1_r + k2_r - 1) \times \sum_i X_{i,r} \right] + \sum_s smax_s - \sum_i L_i \tag{2. 15}$$

Subject to:

- Overall mass balance over operation i :

$$\sum_s S_i + W_i + \sum_{j \neq i} X_{j,i} + \sum_r X_{r,i} = \sum_{j \neq i} X_{i,j} + \sum_r X_{i,r} + L_i \tag{2. 16}$$

- Partial mass balance over operation i :

$$\sum_s S_i (C_{i,k} - C_{S,k}) + W_i C_{i,k} + \sum_{j \neq i} X_{j,i} (C_{i,k} - C_{j,k}) + \sum_r X_{r,i} (C_{i,k} - C_{r,k}) - L_i C_{i,k} = m_{i,k} \tag{2. 17}$$

- Partial mass balance of component k over operation i :

$$\sum_s S_i C_{S,k} + \sum_{j \neq i} X_{j,i} C_{j,k} + \sum_r X_{r,i} C_{r,k}) = \left(\sum_s S_i + W_i + \sum_{j \neq i} X_{j,i} + \sum_r X_{r,i} \right) B_{i,k} \tag{2. 18}$$

- Partial mass balance of component k over regeneration unit r :
    - If outlet concentration of contaminant $rspec_{r,k}$ from regenerator k is known

$$C_{r,k} = rspec_{r,k} \tag{2. 19}$$

    - If removal ratio of contaminant from regenerator k is fixed :

$$(1 - grd_{r,k}) \sum_i C_{i,k} X_{i,r} = \sum_i C_{r,k} X_{r,i} \tag{2. 20}$$

- Overall mass balance over regenerator r :
    - If regenerated water stream is return to process

$$\sum_i X_{r,i} = k1_r \sum_i X_{i,r} \tag{2. 21}$$

    - If regenerated water stream is direct to treatment unit

$$X_{r,T} = k2_r \sum_i X_{i,r} \tag{2. 22}$$

Model constraints:

- Freshwater limit

$$\sum_i S_i \leq Smax \tag{2. 23}$$

2.2.5.4. Model of concentration intervals (Alva-Argaez et al., 1999)

This model combines insights from Water Pinch with mathematical programming. It was formulated based on transhipment model for transfer of contaminants between process streams and water streams on concentration intervals (Fig.2.12.).

Hypotheses:

- The water network can be described as a set of process units : $I = \{i \mid i = 1,2,...,N)$
- The quality specifications are expressed by contaminant concentrations : $C = \{c \mid c = 1,2,...,K)$
- There are a number of freshwater sources available : $S = \{s \mid s = 1,2,...,NS)$
- The contaminant concentration in water sources are : C_k^s
- Inlet maximum contaminant concentration of each operation: $C_{ki}^{in,max}$
- Outlet maximum contaminant concentration of each operation: $C_{ki}^{out,max}$
- Mass load of contaminant which is transferred from each operation : m_{ki}

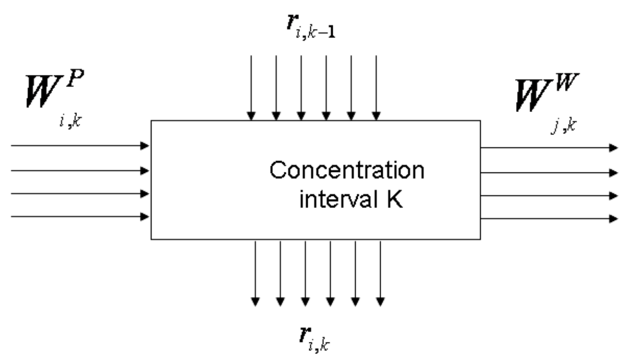


Figure 2. 12 Concentration interval for transfer of single contaminant (Alga-Algaez et al.,1999)

The authors developed mathematical models for single and multiple contaminants considering as objective function the operating costs:

a) LP model for single contaminant

- *Objective function :*

$$\min F = \sum_s c_s F^s \tag{2. 24}$$

- *Mass balance of contaminant on k^{th} interval around each unit u_i*

$$\sum_i m_{ki} + r_{i,k} - r_{i,k-1} = W_{i,k}^P \qquad k=1,2,\ldots,K \;\; i=1,2,\ldots,I \tag{2. 25}$$

$$\sum_i W_{i,j,k} = L_j(C_k - C_{k+1}) \tag{2. 26}$$

- *Constraints:*
  - No negativity for water flowrate

$$0 \le L_j \le L_j^U \tag{2. 27}$$

- Condition for existing of residual mass transferred between concentration intervals

$$r_{i,0} = r_{i,k} = 0 \quad r_{i,k} \geq 0 \qquad k=1,2,\ldots,K\text{-}1 \tag{2. 28}$$

b) MILP model for multiple contaminants

For each contaminant was build concentration intervals diagram (Fig. 2.13) and there was considered that each contaminant was transferred proportionally.

- *Objective function*: the same as (2.24)
- *Mass balance for component c on interval k and operation i*

$$\sum_i W_{c,i,j,k} + r_{c,i,k} - r_{c,i,k-1} \geq W^P_{c,i,k} \qquad k=1,2,\ldots,K \;\; i=1,2,\ldots,I \;\; c=1,2,\ldots C \tag{2. 29}$$

$$\sum_i W_{c,i,j,k} = L_j(C_{c,k} - C_{c,k+1}) \qquad k=1,2,\ldots,K \;\; i=1,2,\ldots,I \;\; c=1,2,\ldots C \tag{2. 30}$$

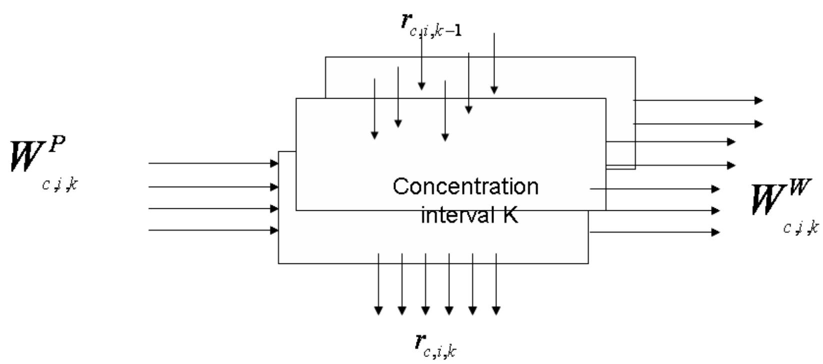


Figure 2. 13 Concentration intervals for transfer of multiple contaminants (Alga-Algaez et al.,1999)

- *Constraints:*
  - Non negativity condition for water flowrate

$$0 \leq L_j \leq L^U_j \tag{2. 31}$$

  - Total mass load of contaminant c exchanged between water-using unit i and freshwater source j is the sum of mass load of contaminant which is transferred over each interval

$$\sum_i W^{TOT}_{c,i,j} = \sum_k W_{c,i,j,k} \tag{2. 32}$$

  - Condition for existing of residual mass of each interval

$$r_{i,0} = r_{i,k} = 0 \quad r_{i,k} \geq 0 \qquad k=1, 2,\ldots, K\text{-}1 \tag{2. 33}$$

  - Condition for existing a match between unit i and source j

$$Y_{i,j} = \{0,1\} \tag{2. 34}$$

2.2.5.5. Model for reused water network (Yang et al., 2000)

Yang and co-workers introduced a mathematical approach to design an optimal network when multiple contaminants are contained in water streams. They formulated a superstructure as in Fig.2.14. To remove M contaminants, the fresh water stream was mixed with two types of recycles streams named internal and external streams. The internal streams came back from the same unit (with a greater contaminant concentration) and the external streams came from other processes. Combining these elements the superstructure of the system was defined as in Fig. 2.15.

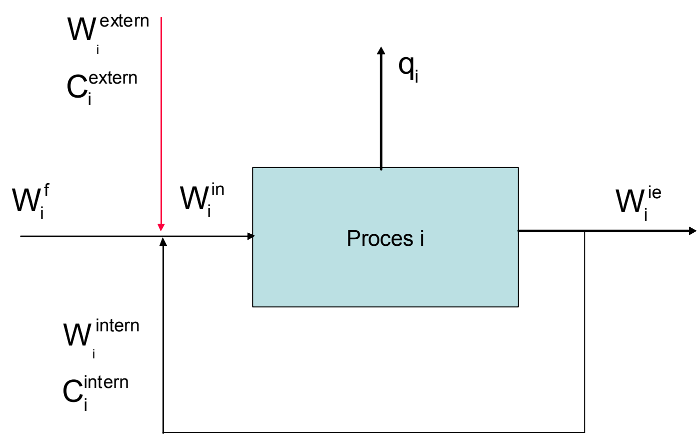


Figure 2. 14 The element of superstructure (Yang et al., 2000)

Hypotheses:

- The network contains N units ($i \in N$)
- There are M contaminants in the system ($j \in M$)
- $q_{i,j}$ mass load of contaminant j removed from unit i
- $(C_{i,j}^{in})_{\max}$ maximum limiting inlet concentration for contaminant j in unit i
- $(C_{i,j}^{ie})_{\max}$ maximum limiting outlet concentration for contaminant j in unit i

Mathematical model

- Objective function: optimum configuration of water network that consumes the minimum amount of freshwater while the operating quality can be ensured.

$$\min \sum_{i=1}^{N} W_i^f \qquad (2.35)$$

Subject to:

- Total mass balance at the entrance of each unit i (mixer)

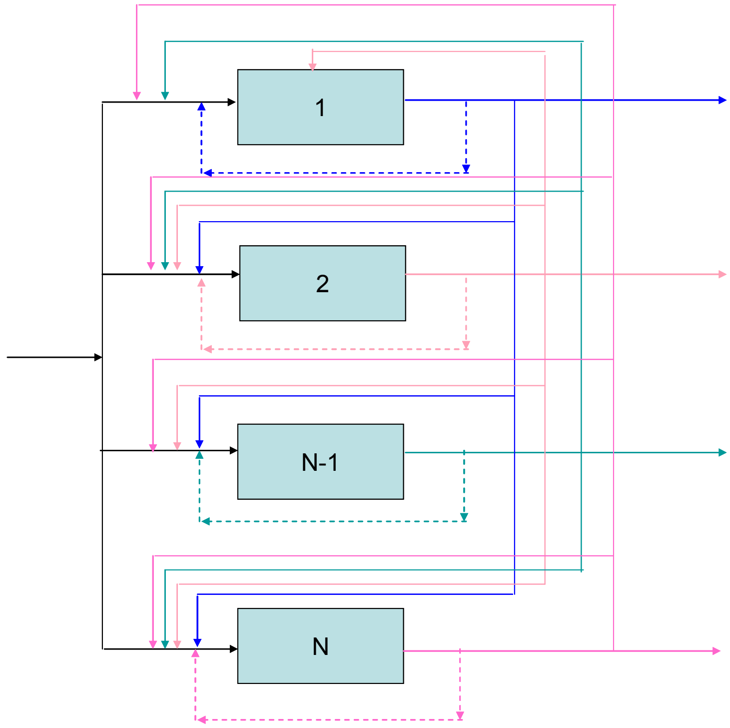


Figure 2. 15 Superstructure of model (Yang et al., 2000)

$$W_i^{in} = W_i^f + \sum_{j=1}^{N} W_{j,i}^r \tag{2. 36}$$

- Total mass balance at the exit of each unit i (splitter)

$$W_i^{ie} = W_i^w + \sum_{j=1}^{N} W_{j,i}^r \tag{2. 37}$$

- Contaminant mass balance at the entrance of each unit i (mixer)

$$C_{i,k}^{in} W_i^{in} = \sum_{j=1}^{N} C_{j,k}^{ie} W_{j,i}^r \tag{2. 38}$$

- Contaminant mass balance at the exit of each unit i (splitter)

$$q_{i,k} = C_{ik}^{ie} W_i^{ie} - C_{ik}^{in} W_i^{in} \tag{2. 39}$$

- Constraints
  - outlet contaminant concentration can not be over maximum limit

$$0 \le C_{i,k}^{ie} \le (C_{i,k}^{ie})_{max} \tag{2. 40}$$

  - inlet contaminant concentration can not be over maximum limit

$$0 \le C_{i,k}^{in} \le (C_{i,k}^{in})_{max} \tag{2. 41}$$

  - Condition for positive flowrates

$$W_i^{in}, W_i^f \ge 0 \tag{2. 42}$$

$$W_{i,j}^{r} \geq 0 \qquad (2.43)$$

2.2.5.6. Uncertainty parameters model (Suh & Lee, 2002)

In 2002, Suh and Lee proposed a method which provides robust design results both economic and technical aspects, for designing water network under parameter uncertainty. The parameter uncertainty can be quantitatively represented by several scenarios and their probabilities. The robust optimal design problem was considered as a multi-objective optimisation problem in which the expected costs, the economic robustness alternatives and the technical robustness are the three objectives.

The design problem can be formulated as multi-scenarios NLP problems which minimise the Net Present Cost (which consists of the cost of piping and pumping and freshwater costs).

Hypotheses:

- Multi-contaminant wastewater
- Multiple operations network
- Steady-state mass balance

The superstructure of the model is the same as (Yang et al., 2000).

Objective function:

$$C_S = P_C + Oc_S(1-tx)\text{prcoef} - \left(\frac{Pc}{Ny}\right)\text{tx prcoef} \qquad s=1,2,\ldots,S \qquad (2.44)$$

Mathematical model:

- Mass balance for stream mixing before entering the unit

$$W_{is}^{f} + \sum_{j=1}^{N} W_{jis}^{r} = W_{is}^{in} \qquad i=1,2,\ldots N, \quad s=1,2,\ldots,S \qquad (2.45)$$

- Component mass balance for stream mixing before entering the unit

$$C_{jks}^{ie} \sum_{j=1}^{N} W_{jis}^{r} = C_{jks}^{in} W_{is}^{in} \qquad i=1,2,\ldots N, \quad s=1,2,\ldots,S \quad k=1,2,\ldots,M \qquad (2.46)$$

- Mass balance around the unit

$$W_{is}^{in} = W_{is}^{ie} \qquad i=1,2,\ldots N, \quad s=1,2,\ldots,S \quad k=1,2,\ldots,M \qquad (2.47)$$

$$D_{is}^{ie} = D_{is}^{in} \qquad i=1,2,\ldots N, \quad s=1,2,\ldots,S \quad k=1,2,\ldots,M \qquad (2.48)$$

- Component mass balance around the unit

$$W_{is}^{in}C_{iks}^{in} + D_{is}^{in}C_{iks}^{in} = W_{is}^{ie}C_{iks}^{ie} + D_{is}^{ie}C_{iks}^{ie} \quad i=1,2,\ldots N, \quad s=1,2,\ldots,S \; k=1,2,\ldots,M \qquad (2.49)$$

- Mass balance for stream splitting after leaving the unit

$$W_{is}^{ie} = \sum_{i=1}^{N} W_{ijs}^{r} + W_{is}^{w} \qquad i=1,2,\ldots N, \quad s=1,2,\ldots,S \tag{2. 50}$$

Constraints

- Capacity constraints

$$X_i \geq W_{is}^{f} \qquad i=1,2,\ldots N, \quad s=1,2,\ldots,S \tag{2. 51}$$

$$Y_{ij} \geq W_{ijs}^{r} \quad i=1,2,\ldots N, \quad j=1,2,\ldots N \quad s=1,2,\ldots,S \tag{2. 52}$$

$$Z_i \geq W_{is}^{W} \quad i=1,2,\ldots N, \quad s=1,2,\ldots,S \tag{2. 53}$$

- Unit constraints

$$C_{iks}^{in} \leq C_{ik}^{in,max} \quad i=1,2,\ldots N, \quad s=1,2,\ldots,S \quad k=1,2,\ldots,M \tag{2. 54}$$

$$C_{iks}^{ie} \leq C_{ik}^{ie,max} \quad i=1,2,\ldots N, \quad s=1,2,\ldots,S \quad k=1,2,\ldots,M \tag{2. 55}$$

- Variable constraints

$$W_{is}^{f}, W_{is}^{in}, W_{is}^{ie}, W_{is}^{w} \geq 0 \qquad i=1,2,\ldots N, \quad s=1,2,\ldots,S \tag{2. 56}$$

$$W_{ijs}^{r} \geq 0 \quad i=1,2,\ldots N, \quad j=1,2,\ldots N \quad s=1,2,\ldots,S \tag{2. 57}$$

$$C_{iks}^{in}, C_{iks}^{ie} \geq 0 \qquad i=1,2,\ldots N, \quad s=1,2,\ldots,S \quad k=1,2,\ldots,M \tag{2. 58}$$

Capital cost is calculated as function of capacity of freshwater pipe line into unit i, capacity of recycled r discharged wastewater flow pipe line from unit i (Eq.2.59).

$$P_C = \alpha\left(\sum_{i=1}^{N} X_i + \sum_{i=1}^{N}\sum_{j=1}^{N} Y_{i,j} + \sum_{i=1}^{N} Z_i\right) \tag{2. 59}$$

For each scenario, operating cost is a function of freshwater flow rate to unit i in scenario s and unit capital cost of piping and pumping (Eg.2.60).

$$Oc_S = 8000\alpha \sum_{i=1}^{N} W_{is}^{f} \qquad s=1,2,\ldots,S \tag{2. 60}$$

To solve this model the authors propose compositions of contaminants at the entrance of process in different scenarios, flow rates and limiting compositions for each contaminant. These compositions are the uncertainty parameters for the process.

2.2.5.7. Linear models for water network (Koppol et al., 2003)

In the paper, Koppol et al., 2003 the authors proposed some linearised models for optimisation of water network considering also regeneration/treatment units and single contaminant. They formulated this model in four stages:

P1. Minimum flow rate for process water network (Fig.2.16)

Objective function

$$\min \sum_{j} F_j^{W} \tag{2. 61}$$

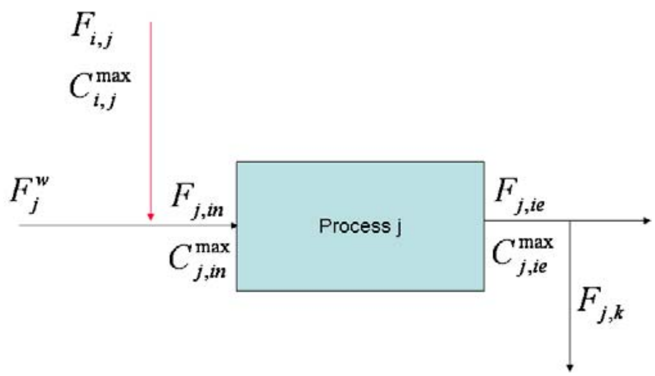


Figure 2. 16 Superstructure model P1 (Koppol et al.,2003)

Mathematical model:

- Total mass balance

$$F_j^W + \sum_i F_{i,j} - \sum_k F_{j,k} - F_{j,ie} = 0 \tag{2. 62}$$

- Component mass balance:

$$\sum_i F_{i,j}(C_{i,ie}^{max} - C_{j,ie}^{max}) - F_j^W C_{j,ie}^{max} + L_j = 0 \tag{2. 63}$$

Constraints:

- Compositions constraints :

$$\sum_i F_{i,j}(C_{i,ie}^{max} - C_{j,ie}^{max}) - F_j^W C_{j,in}^{max} \leq 0 \tag{2. 64}$$

- Flow rates constraints :

$$F_j^W, F_{i,j}, F_{j,k}, F_{j,ie} \geq 0 \tag{2. 65}$$

P2. Minimum flow rate for process water network and regeneration/treatment (Fig.2.17)

If decentralised treatment units were incorporated, the model remained also linear. Linearity was achieved by fixing the treated water concentration at the lowest possible value, which minimised the freshwater flow rate. The lower bounds of treated water concentration were obtained from treatment technology limitations.

Objective function:

$$\min \sum_j F_j^W \tag{2. 66}$$

Mathematical model:

- Total mass balance

$$F_j^W + \sum_i F_{i,j} + \sum_k F_{k,j} - \sum_j F_{j,h} - \sum_k F_{j,k} - F_{j,ie} = 0 \tag{2. 67}$$

- Contaminant mass balance:

$$\sum_i F_{i,j}(C_{i,ie}^{max} - C_{j,ie}^{max}) + \sum_k F_{k,j}(C_{k,ie}^{max} - C_{j,ie}^{max}) - F_j^W C_{j,ie}^{max} + L_j = 0 \tag{2. 68}$$

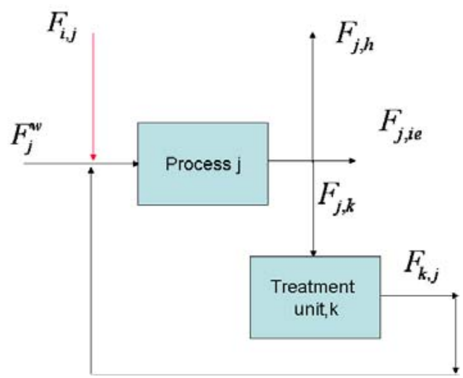


Figure 2. 17 Superstructure model P2 (Koppol et al.,2003)

Constraints

- Concentrations constraints

$$\sum_i F_{i,j}(C_{i,ie}^{max} - C_{j,in}^{max}) + \sum_k F_{k,j}(C_{k,ie}^{max} - C_{j,in}^{max}) - F_j^W C_{j,in}^{max} \le 0 \tag{2. 69}$$

- Flowrate constraints

$$F_j^w, F_{i,j}, F_{j,k}, F_{j,ie} \ge 0 \tag{2. 70}$$

P3. Minimum regeneration cost for process water network

Because multiple solutions for freshwater flowrate were possible, another model was formulated to minimise the regeneration cost for a target freshwater obtained from model P1 (Fig.2.16). The regeneration cost was related to total flowrate or to the total load removed.

P4. Minimum capital cost for process water network

In the fourth step, the capital cost was minimised, considering binary variables for possible interconnections and the freshwater flowrate and regeneration cost provided by the optimisation of models from step 1 and 3. The mathematical model was formulated as the follow:

Objective function:

Minimise the number of inlet, outlet and interconnections between the processes

$$\min \sum_{i,j} Y_{i,j} + \sum_{w,j} Y_{w,j} + \sum_{j,o} Y_{j,o} \tag{2. 71}$$

Mathematical model:

b) Mass and component mass balance (eqs.2.79,2.80)

c) Freshwater flowrate is provided by solution of model P1 :

$$\sum_j F_j^W = \alpha \tag{2. 72}$$

d) Regeneration cost provided by solution of P3,

$$\min a_R \sum_k \sum_j F_{j,k} = \beta \tag{2. 73}$$

Constraints:

$$\begin{aligned} &F_{i,j} - UY_{i,j} \le 0 \\ &F_j^w - UY_{w,j} \le 0 \\ &F_{j,ie} - UY_{j,o} \le 0 \end{aligned} \tag{2. 74}$$

2.2.5.8. Regeneration/Treatment model (Feng &Chu, 2004)

Feng and Chu proposed a decomposition of water network into three subsystems: water utilisation system, water regeneration system and wastewater treatment system, as in Fig. (2.18). Wastewater stream is split it into stream to regeneration system for reuse and wastewater stream with higher contaminant concentrations to be treated for discharge.

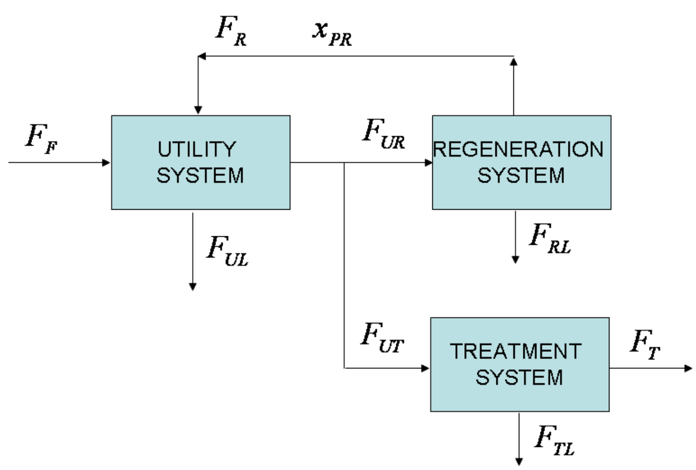


Figure 2. 18 Elements of water network system for model (Feng&Chu ,2004)

Hypotheses:

- The Total Cost of whole water system network included the freshwater costs, regenerated water costs and wastewater treatment costs.

$$C_{TW} = C_F + C_R + C_T \tag{2. 75}$$

- The cost of each type of water was given as a product between flow rate and unit cost (for freshwater can be taken constant, but for regeneration and treatment units cost were dependent of regeneration\treatment process, quality and volume of wastewater)

$$C_F = c_F \cdot F_F \qquad C_R = c_R \cdot F_R \qquad C_T = c_T \cdot F_T \tag{2. 76}$$

- Dependence of cost of regeneration\treatment over contaminant removal efficiency was expressed as:

$$c_R = \alpha F_R^{\beta} \left(\frac{x_{PR,max}}{x_{PR}} \right)^{\gamma} \quad (2.77)$$

Objective function:

$$\min C_{TW} = c_F \cdot F_F + c_R \cdot F_R + c_T \cdot F_T \quad (2.78)$$

Mathematical model:

- Total mass balance around process units:

$$F_F + F_R = F_{UR} + F_{UT} + F_{EL} \quad (2.79)$$

- Total mass balance around regeneration units:

$$F_{UR} = F_R + F_{RL} \quad (2.80)$$

- Total mass balance around treatment units:

$$F_{UT} = F_T + F_{TL} \quad (2.81)$$

Constraints:

- Freshwater flow rate was function of the post-regeneration contaminant concentration which was governed by the water quality requirements:

$$F_F = f1(x_{PR}) \quad (2.82)$$

- Regenerated water flow rate was function of the post-regeneration contaminant concentration:

$$F_R = f2(x_{PR}) \quad (2.83)$$

- Treated water flow rate was function of the post-regeneration contaminant concentration:

$$F_T = f3(x_{PR}) \quad (2.84)$$

- Regeneration costs were function of x_{pR} and wastewater flow rate sent to regeneration :

$$c_R = f4(F_{R,} x_{PR}) \quad (2.85)$$

- Treatment cost depended only on wastewater flow rate sent to treatment because the disposal limit was constant :

$$c_T = f5(F_T) \quad (2.86)$$

2.2.5.9. Non-convex NLP model for integrated water network (Karuppiah & Grossmann, 2006)

These authors addressed the problem of optimal synthesis of an integrated water system, where water-using units and water treatment units were combined into single network.

Hypotheses:

- For formulation of mass balance equations they used individual component flows in a stream instead of total flows and the streams compositions; a superstructure which incorporates all feasible design alternatives for reuse, recycle and treatment was proposed.
- The water flow demand of the water processes are assumed to be fixed.
- A certain number of contaminants were picked up in the water using process.
- Upper bounds were specified on contaminant concentrations that were allowed for each system (based on consideration of minimum mass transfer driving force, solubility of the contaminants, fouling and corrosion limitations).
- Treatment units removed a fraction of selected contaminants, specified by a fixed removal ratio for each contaminant.
- The total flowrate of a stream was taken to be equal to that of pure water in that stream since the individual contaminant flows were negligible.
- The cost of pumping and the cost of pipeline are neglected.
- The network was operated under isothermal and isobaric conditions.

Objective function:

- To minimise the sum of freshwater flowrate into the network and the total flowrate of wastewater being treated inside the treatment units.

$$\min(FW + \sum_{\substack{t\in TU \\ i\in t_{out}}} F_i) \tag{2. 87}$$

- To minimise cost function

$$\min(HC_{FW}FW + AR\sum_{\substack{t\in TU \\ i\in t_{out}}} IC^t(F_i)^\alpha + H\sum_{\substack{t\in TU \\ i\in t_{out}}} OC^t F^i) \tag{2. 88}$$

Mathematical model:

The model is written from overall mass balances around mixer units, process units, splitter unit and treatment units (Fig. 2.19)a, b, c, d, as follows:

a) Around mixer units:

$$F^k = \sum_{i \in m_{in}} F^i \qquad \forall m \in MU,\ \forall k \in m_{out} \tag{2.89}$$

$$F^k C_j^k = \sum_{i \in m_{in}} F^i C_j^i \qquad \forall j,\ \forall m \in MU,\ \forall k \in m_{out} \tag{2.90}$$

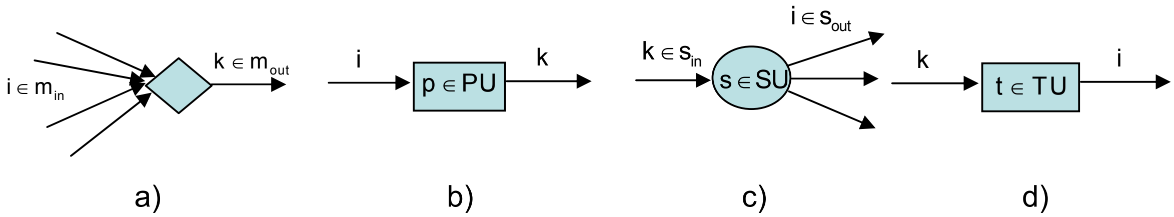


Figure 2. 19 Superstructure of non-convex model (Karuppiah & Grossmann,2006)
a) mixing unit b) water process unit c) splitter unit d) treatment unit

b) Around water-process units:

$$F^k = F^i = P^p \qquad \forall p \in PU,\ \forall i \in p_{in},\ \forall k \in p_{out} \tag{2.91}$$

$$P^p C_j^i + L_j^p = P^p C_j^k \qquad \forall j,\ \forall p \in PU,\ \forall i \in p_{in}, \forall k \in p_{out} \tag{2.92}$$

c) Around splitter units:

$$F^k = \sum_{i \in s_{out}} F^i \qquad \forall s \in SU,\ \forall k \in s_{in} \tag{2.93}$$

$$C_j^i = C_j^k \qquad \forall j,\ \forall s \in SU,\ \forall i \in s_{out}, \forall k \in s_{in} \tag{2.94}$$

d) Around treatment units:

$$F^k = F^i \qquad \forall t \in TU,\ \forall i \in t_{out}, \forall k \in t_{in} \tag{2.95}$$

$$C_j^i = \beta_j^t C_j^k \qquad \forall j,\ \forall t \in TU,\ \forall i \in t_{out}, \forall k \in t_{in} \tag{2.96}$$

2.3. Algorithms for optimisation of water networks

The goal to optimise the water network is to find the values of the variables in the process that yield the best value of the performance criterion (usually for water network there is a trade-off between flowrate and costs). To find the best solution, different techniques can be used.

- Graphical techniques, which are ease to use and better understood by engineers.
- Optimisation techniques (as a black box approach) where the engineer is provided little insight to understand how the water reuse network is constructed.

Graphical methods are used as an effective approach to discover the operational bottlenecks (pinch points) and to design a new network or to revamp an existing one.

In the last few years there are two distinct types of optimisation algorithms used for water network design:

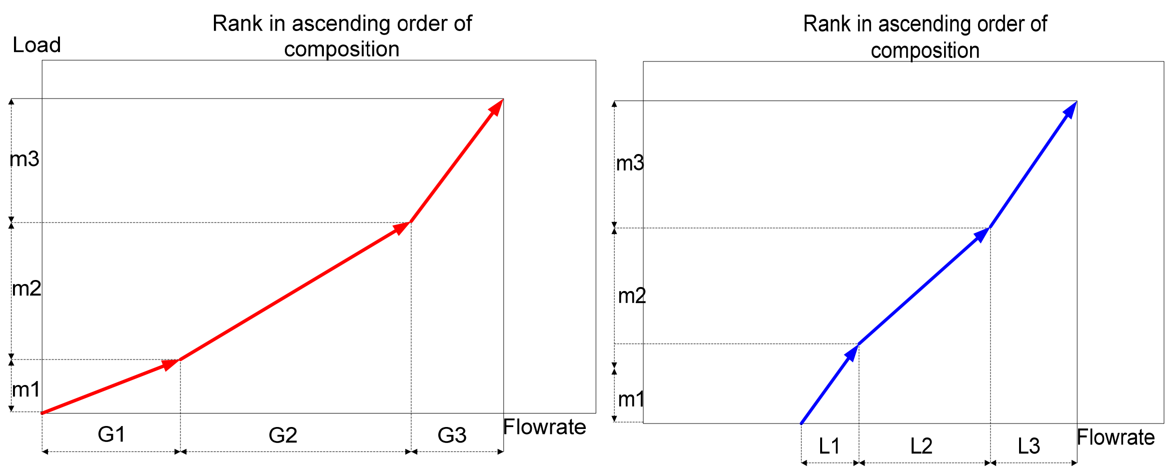
a) *Deterministic algorithms*, with specific rules for moving from one solution to the other; based on gradient methods have the possibility of getting trapped at local optimum depending upon the degree of non-linearity and initial guess, but not guarantee the global optimal solution

b) *Stochastic algorithms* (as Genetic Algorithm or Simulated Annealing), which are stochastic in nature with probabilistic transition rules, based on the principle of evolution (survival of the fittest). Simulated Annealing (SA) is a probabilistic non-traditional optimisation technique, which mimics the cooling phenomenon of molten metals to constitute a search procedure. Genetic Algorithms (GAs) are computerised search and optimisation algorithms based on the mechanics of natural genetics and natural selection.

2.3.1. Graphical methods

Used as better understanding tools for wastewater minimisation, the graphical representations were developed in very high manner. Many authors proposed different graphical representations which can be used for driving the freshwater targets considering single contaminant or multiple contaminants cases.

2.3.1.1. Composite curve (El-Halwagi & Manousiouthakis, 1989)



a) sink composite curve *b) Source composite curve*

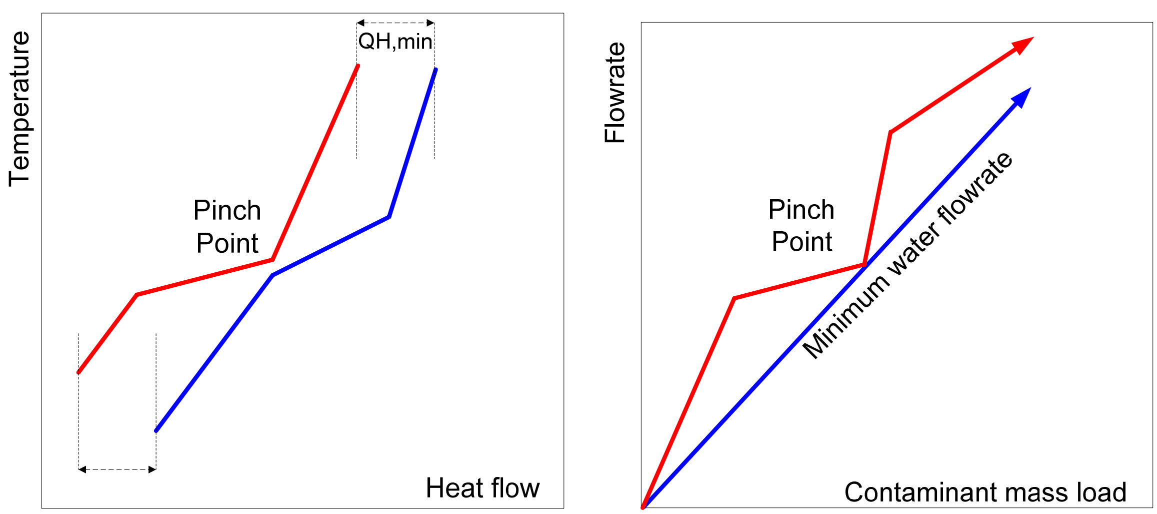
Figure 2. 20 Composite curves (El-Halwagi & Manousiouthakis, 1989)

El-Halwagi introduced for the first time the concept of mass transfer operation where some species can be transferred between rich process streams and different agents of transport (lean streams). The rich streams had a mass flowrate G_i and had to bring from supply composition to a target composition for each contaminant.

Similarly, each lean stream had a mass flowrate L_j bounded in a way similar to the bounds of rich streams. Each stream was represented as an arrow line between bounded compositions and the slope was the flowrate of agent. This was a targeting method used to determine the minimum freshwater demand for single contaminant case study.

2.3.1.2. Water Pinch Diagram (Wang & Smith, 1994a, Smith 1995, Smith 2005)

Wang and Smith introduced *Composite curve diagram* to target the minimum water and wastewater flowrates, based on extension of the pinch analysis techniques from heat integration (Fig.2.21). Each water-using unit was considered as being described by the mass transfer of contaminant between process streams to the water streams. Specifying the limiting inlet and outlet concentration of contaminant for each operation, the composite curve could be constructed combining these streams on a concentration versus mass load of contaminant plot. Against this composite was drawn the limiting profile line which touch the composite in pinch point. The slope of limiting profile line was the targeting freshwater (Fig. 2.22). This targeting procedure for minimum freshwater consumption was modified to be applied for multiple contaminants case (Wang & Smith, 1994b). Modifying inlet and outlet concentrations and mass loads for each water-using units until all streams were placed on the diagram for all contaminants, they proposed a shifting strategy to achieve the feasible target.



a) Energy pinch *b) Water pinch*

Figure 2. 21 Composite curve diagram (Wang & Smith, 1994a)

A reference contaminant was selected to perform the shifting of the streams and proportional mass transfer was assumed in the calculus.

They also considered the possibility of regeneration of some streams to a environmental limit and the reuse them again in the water network. The slope of limiting water profile after regeneration was the minimum flowrate of regenerated water which could be reused (Fig. 2.23).

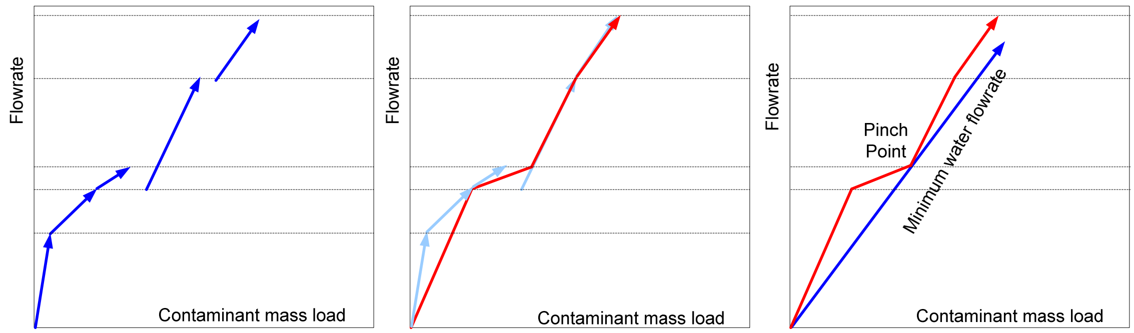


Figure 2. 22 Steps to obtain composite curve diagram (Wang & Smith, 1994a)

This method applicability was only limited to mass transfer-based operations. Water as cooling and heating media in cooling towers and boilers and as a reactant could not be appropriately represented as mass transfer operation. It is also difficult to model situations in which several aqueous streams enter and leave an operation at different concentrations, for example, as in the reactor system.

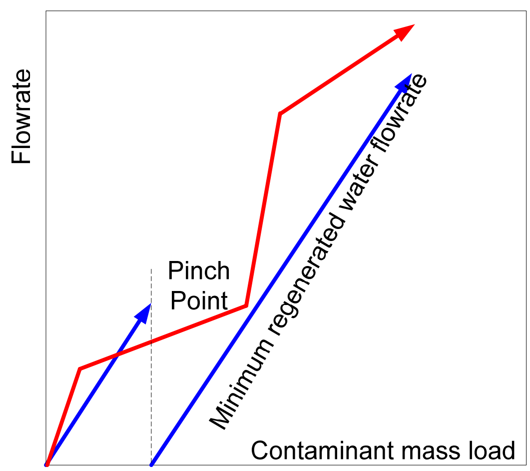


Figure 2. 23 Composite curve diagram for water network with regeneration (Wang & Smith, 1994a)

2.3.1.3. Pinch Diagram (Dhole et al., 1996)

Dhole and co-workers presented an alternative graphical method for targeting water network to eliminate the limitations of water pinch diagram (water losses, gains, etc). They also suggested process changes like mixing and bypassing to further reduce the fresh water consumption. Each operation was considered to have aqueous inlet and outlet streams with different flowrates and concentrations. All the input stream requirements were plotted together on a water flowrate (the numbers increase downwards) versus contaminant mass load diagram (Fig.2.24). This representation was also analogous to the original heat pinch diagram.

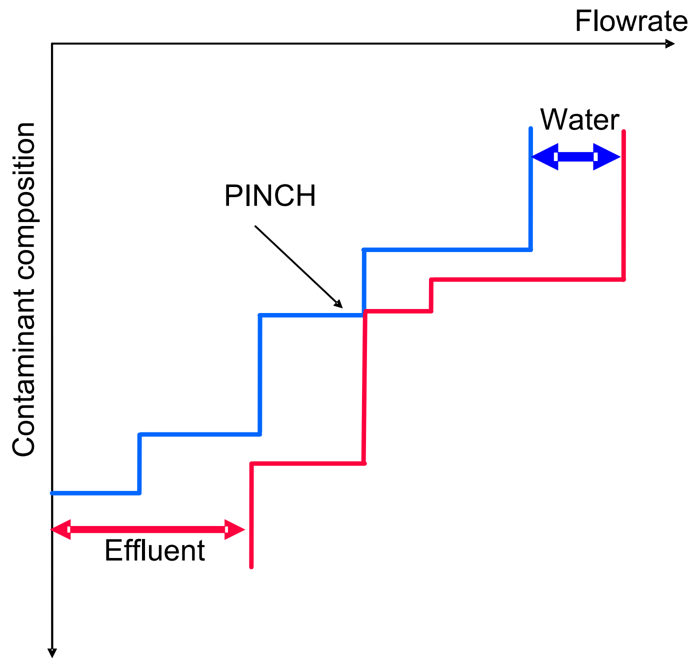


Figure 2. 24 Pinch Diagram (Dhole et al., 1996)

The pinch divides the problem into two regions: above and below the pinch. In order to achieve the target, freshwater should not be used below the pinch and sources above the pinch should not be discharged as wastewater. Distance between composite curves gave the minimum freshwater flowrate. Also this diagram had limitations because gave a graphical representation of a particular design. It did not give a clear picture of the situation, because mixing of water sources could change the shape of the source composite and hence the targets.

2.3.1.4. Source - Sink diagram (El-Halwagi et al., 1996)

El-Halwagi and co. defined the network as follows: for each species exists sources and sinks which can be also considered as sources (Fig. 2.25). For this reason the process integration can be made by segregation, mixing, interception, reusing and manipulation of source/sink units. On a flowrate - composition diagram (Fig. 2.26), El-Halwagi represented sources as blue circles and sinks as red squares. Limiting compositions for flowrates and compositions were also delimited on the diagram. The sources placed on intersection of these two limiting zones could be used to feed the corner process (the source a can feed unit S). All sources near source a could be mixed using lever rule to be used in the unit.

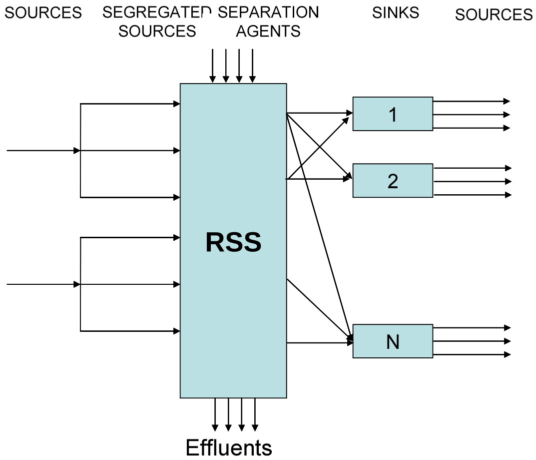


Figure 2. 25 Mass exchanger network, (El-Halwagi et al., 1996)

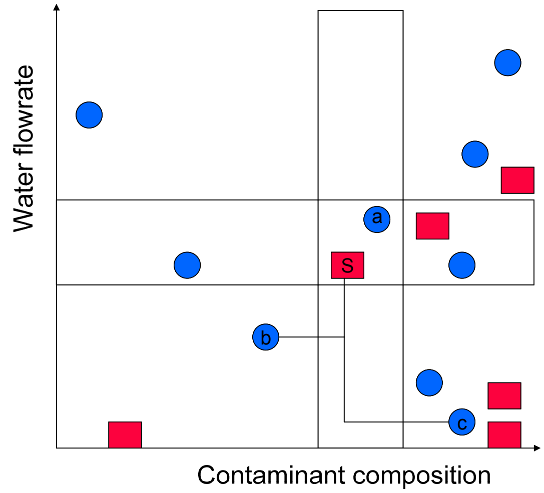


Figure 2. 26 Source - sink diagram (El-Halwagi et al., 1996)

2.3.1.5. Water surplus diagram (Hallale, 2002)

Another graphical representation for targeting freshwater and wastewater minimisation was presented by Hallale. He used a similar representation as (Dhole et al., 1996) and overcomes many of the limitations of mass transfer based approach. To obtain the demand and source composite curves, Hallale used the purity of water rather the contaminant concentration (Fig.2.27).

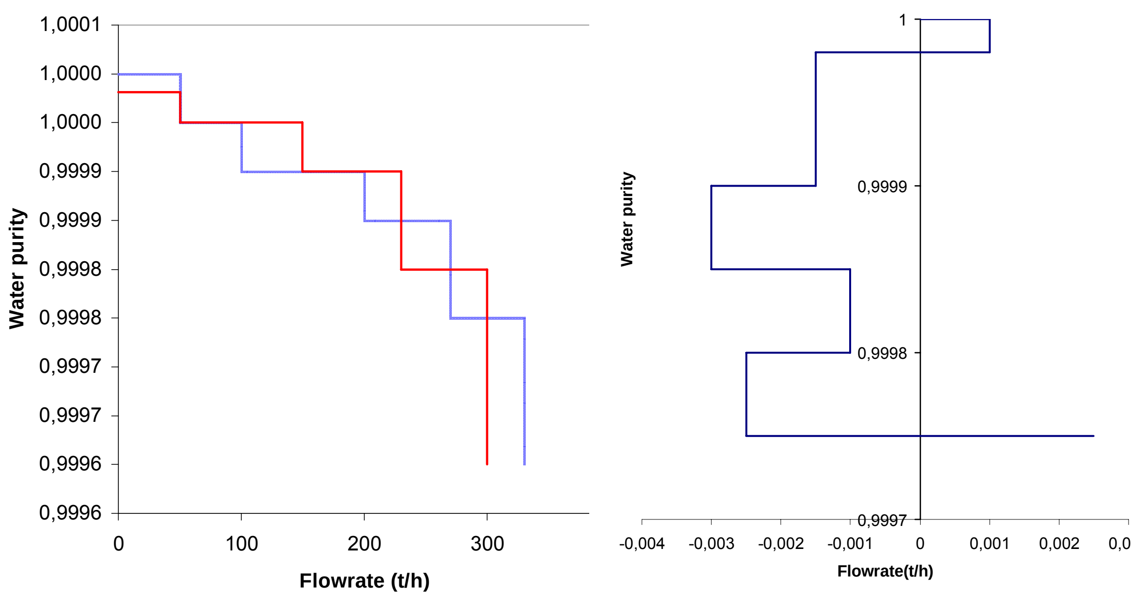


Figure 2. 27 Water surplus diagram (Hallale, 2002)

Purity was calculated as a ratio between composition of water without contaminant and the composition of pure water. By definition, the composition of pure water is 1 million ppm. Assuming an arbitrary freshwater initially, the demand and source compositions were plotted starting from zero flowrate. The composite curves were not totally overlapped, obtaining positive and negative rectangles which corresponded to the deficit of surpluses calculated. These cumulative surplus or deficit values were plotted on purity versus flowrate diagram (Surplus diagram). The procedure was repeated for different values of freshwater flowrates until the diagram was placed in the positive region. This flowrate which is determined by trial and error method is the minimum target.

2.3.1.6. Resources conservation diagram (El-Halwagi, et al., 2003)

Focusing on a mathematical formulation, El-Halwagi proposed in 2003 a new graphical representation to obtain the minimum freshwater for a water network using segregation, mixing and direct recycle/reuse strategies.

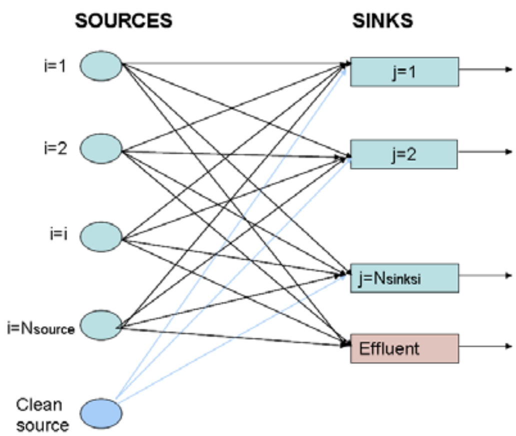


Figure 2. 28 Network structure (El-Halwagi et al., 2003)

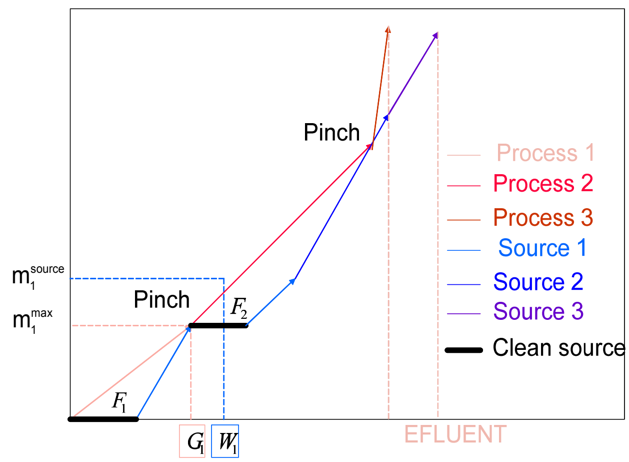


Figure 2. 29 Composite curves (El-Halwagi et al., 2003)

First, the problem was formulated mathematically to provide a systematic basis for solution. Then, dynamic programming techniques were employed to derive the mathematical conditions and characteristics of an optimal design strategy. These conditions and strategies were represented into a graphical form to identify rigorous targets for minimum usage of fresh source (Fig. 2.28). Also a pinch point can be identified which provide information about the use of fresh water resources, the discharge and relations between sources and sinks.

2.3.1.7. Nearest neighbours diagram (Prakash & Shenoy, 2005)

Prakash and Shenoy proposed a targeting method for fixed flowrate and fixed contaminant load operation. The method consisted of plotting separate source and demand composites with flowrate as horisontal axis and contaminant load as vertical axis (Fig. 2.30 and Fig. 2.31). To determine the minimum freshwater flowrate for fixed flowrate problems, a nearest neighbour principle was developed. This principle states that the source streams to be chosen must be the nearest available neighbours in terms of contaminant concentration. For fixed contaminant load problem, it was applied the nearest neighbours principle to process unit that lie across the pinch. Units that lied entirely on one side of the pinch point were satisfied by the cleanest source available.

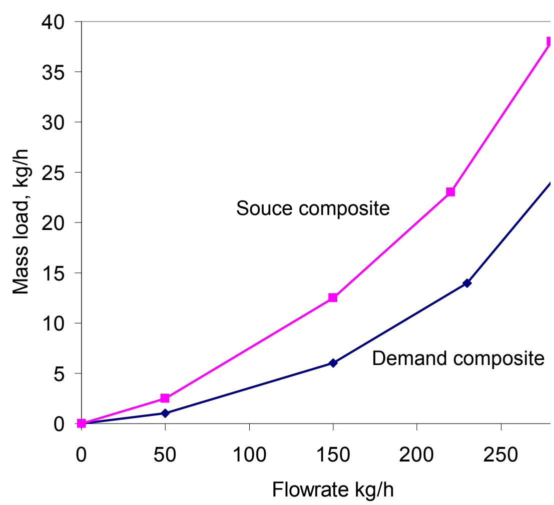


Figure 2. 30 Composite curves (Prakash& Shenoy, 2004)

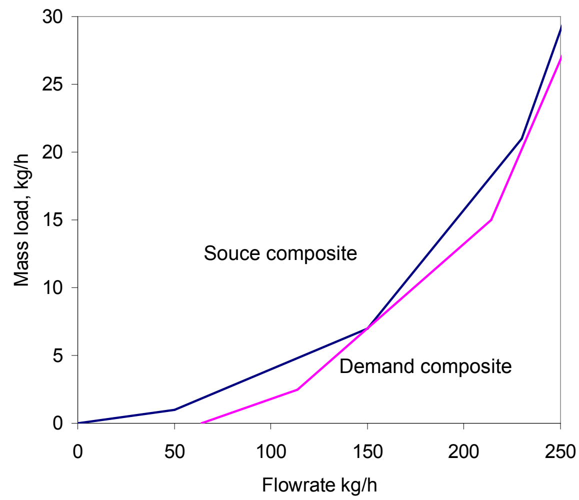


Figure 2. 31 Translated Composite curves (Prakash & Shenoy, 2004)

2.3.1.8. Property based composite curve (Kazantzi & El-Halwagi, 2005)

El-Halwagi introduced in 2005 a new property–based pinch analysis diagram to identify rigorous target for material reuse. Quality of components which were transferred between process streams and source streams were expressed in term of property (contaminants composition, volatility, solubility, PH, etc).

Using the flowrate for each source and calculating the value of a property load, El-Halwagi developed a representation tool for each source in ascending order to create a source composite curve as presented in Fig. 2.32. In the same manner it was drawn the fresh line using flowrate and property operator for fresh sources. Pushing the source composite to fresh line composite until the two composites touch at the pinch point, it was possible to determine the minimum consumption of fresh resource and the minimum discharge of the waste, as illustrated in Fig. 2.33.

2.3.1.9. Quality based composite curve (Bandyopadhyay, 2006)

The analysis proposed a process integration graphical tool based on pinch principle and established the minimum waste generation target prior to the detailed design procedure.

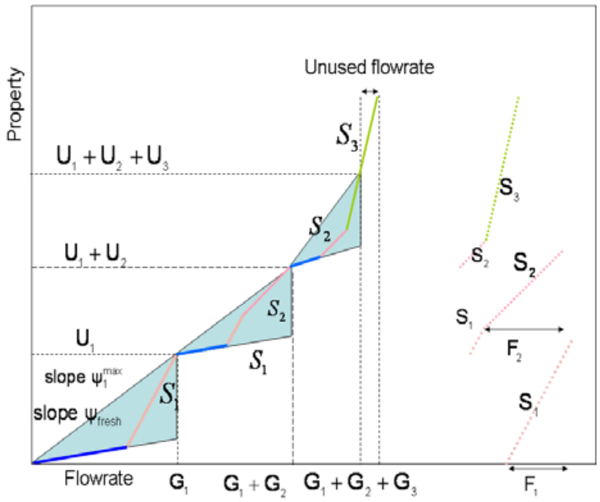


Figure 2. 32 Property-based composite curve (Kazantzi & El-Halwagi, 2005)

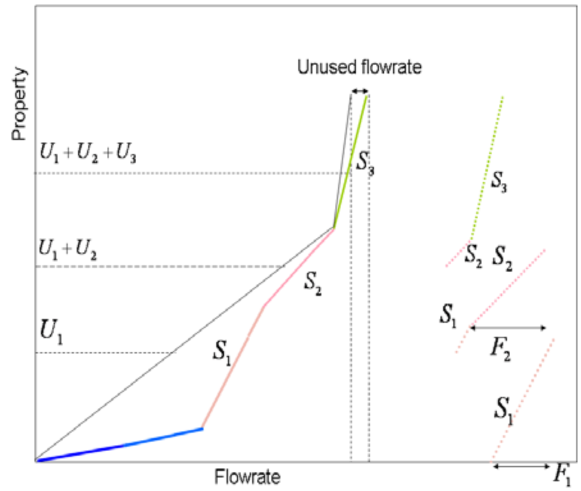


Figure 2. 33 Translated Property-based composite curve (Kazantzi & El-Halwagi, 2005)

Because this graphical representation was used not only for water minimisation but also for hydrogen management and material minimisation, the author used quality of a stream (contaminant composition, purity of hydrogen or vapour pressure), as a property represented on the plot. Source composite curve was obtained by plotting cumulative qualities of each source on a quality versus quality load diagram (Fig. 2.34).

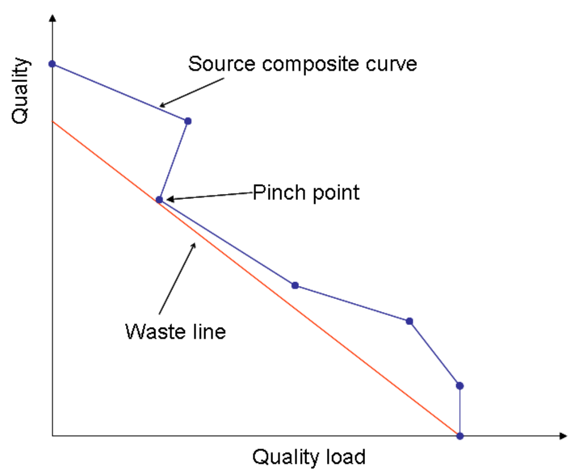


Figure 2. 34 Quality-based composite curve (Bandyopadhyay, 2006)

Also the waste line was plotted as a line with negative slope on this quality versus quality load diagram, its slope was inversely proportional to the waste flow. These two curves were touched at pinch point.

2.3.2. Superstructure - based algorithms

In the last years, design and synthesis of process networks using mathematical programming based on superstructure was an important engineering problem. It was necessary to develop a network of interconnections and than to optimise this network, to obtain the best alternative.

The synthesis problem based on superstructures was defined as follows: for input streams specifications and output streams then was desired to obtain an optimal network addressing to the performance criteria: operating costs, product quality, environmental issues, etc. The optimisation approach involved three steps: formulation of all possible alternatives into a superstructure, the mathematical formulation of the model and formulation of an algorithm to solve this model (Adjiman et al., 1998).

The last step of the optimisation approach was highly dependent on the properties of the mathematical model.

To solve the superstructure models, there are available the following mathematical algorithms (Grossmann & Biegler, 2004):

a) Lipschitzian algorithm (Hansen et al., 1992a)
b) Branch and bound algorithm (Al-Khayyal, 1992; Al-Khayyal & Falk, 1983; Horst & Tuy, 1987)
c) Cutting plane algorithm (Tuy et al., 1985)
d) Difference of convex (DC) and reverse convex algorithm (Tuy, 1987)
e) Outer-approximation (OA) algorithm (Horst et al., 1992)
f) Primal-dual algorithm (Ben-Tal et al., 1994; Floudas & Visweswaran, 1990)
g) Reformulation–linearisation algorithm (Sherali & Alameddine, 1992; Sherali & Tuncbilek, 1992)
h) Interval algorithm (Hansen, 1980).

Branch and Bound is a basic algorithm for solving integer and discrete problems. The method is based on enumeration of integer solutions as a tree structure. The structure starts with a root (all possible solutions) and many leaf nodes on the right which represent the actual solutions. Branch and Bound algorithm is based on concept of relaxations: sub-problems with one or more of the discrete variable relaxed to continuous variables.

This method has the following steps:

- Starting by considering the root problem (the original problem with the complete feasible region), the lower-bounding and upper-bounding procedures are applied to the root problem.
- If the bounds match, then an optimal solution has been found and the procedure terminates
- Otherwise, the feasible region is divided into two or more regions, these sub-problems divide the feasible region.

- The algorithm is applied recursively to sub-problems. If an optimal solution is found to a sub-problem, it is a feasible solution to the full problem, but not necessarily globally optimal.
- If the lower bound for a node exceeds the best known feasible solution, no globally optimal solution can exist in the subspace of the feasible region represented by that node. Therefore, the node can be removed from consideration.
- The search proceeds until all nodes have been solved or pruned, or until some specified threshold is met between the best solution found and the lower bounds on all unsolved sub-problems.

Outer approximation algorithm solves the MINLP by an iterative process. The problem is decomposed into a NLP sub-problem (which has the integer values fixed) and a MILP master problem. The NLP sub-problem optimise the continuous variables and provide an upper bound to the MINLP solution, while the MILP master problem has the role of predicting a new lower bound for the MINLP solution, as well as new integer variables for each iteration. The search terminates when the predicted lower bound equals or exceeds the current upper bound.

The logic-based approach is a cutting-plane method for solving convex MINLPs that uses an MIP master problem. In each iteration, cuts are generated by solving a separation problem that is defined by disjunctive constraints.

Most of the studies published in literature have dealt with the issue of minimising wastewater generation in water using units using a superstructure-based algorithm. The authors tried to improve these methods to obtain the best solution for different kind of water networks. Almost of chemical engineering problems are defined as MINLP or NLP.

Feng & Seider, 2001, proposed a novel network structure with internal water mains to reduce the water consumption and to simplify the piping network in a plant. This superstructure was extended for regeneration and multiple contaminants (Cao et al., 2004; Wang et al., 2003).

Alva-Argaez et al., 1998, formulated a MINLP model for water network as a superstructure which included water using units and treatment units. To approximate the optimal solution, they decompose this model into a sequence of MILP problems. In 2006, the authors proposed a new decomposition of NLP model to design a water-using system in petroleum refining (a complex network with seven water-using units and three contaminants) (Alva-Argaez et al., 2006).

Galan & Grossmann, 1998 suggested an effective heuristic mathematical programming procedure to solve the superstructure given by Wang & Smith (1994b).

Bagajewicz et al., 1999 have proposed a method to transform the formulation of a multi-contaminant large scale water system from a NLP problem to a LP problem and solved it to optimality. Later, the authors proposed necessary conditions for optimality considering one contaminant (Savelski & Bagajewicz, 2001) or multiple contaminants (Savelski & Bagajewicz, 2003), specific for oil refinery water network.

Lee & Grossmann, 2003, formulated the decentralised wastewater treatment network as a non-convex *Generalised Disjunctive Programming* (GDP) problem and solved the problem to global optimality.

A superstructure of water network for attending zero discharge option was proposed by Koppol et al., 2003. Zero liquid discharge possibilities in oil refineries was studied using a new iterative procedure as an extension of the procedure proposed by Bagajewicz & Rivas, 2000.

A real world design problem for synthesis of process water systems was solved by Ullmer et al., 2005. They solved the superstructure combining the advantages of heuristic rules and mathematical methods to generate a promising design.

Karuppiah & Grossmann, 2006, proposed a superstructure that incorporated all feasible design alternatives for water treatment, reuse and recycle, as a non-convex NLP problem, which was solved to global optimality. The problem took the form of a non-convex GDP problem if there was a flexibility of choosing different treatment technologies for the removal of the various contaminants in the wastewater streams. They obtained a convex relaxation of the original model using a new deterministic spatial branch and contract algorithm and applied on five water networks from literature.

These superstructures can be optimised using the existing standard methods for solving MINLPs (Grossmann, 2002), like Outer Approximation (OA) and Generalised Benders Decomposition (GBD). The authors developed an advanced logic-based optimisation approach as a way of facilitating the modelling of discrete/continuous problems, and of reducing the combinatorial search space. The power and scope of the techniques was demonstrated on a variety of process integration problems.

Turkay & Grossmann, 1996, modelled the MINLP problem for the optimal synthesis of process networks as a discrete optimisation problem involving logic disjunctions with nonlinear equations and pure logic relations.

Bergamini et al., 2005 proposed a deterministic algorithm, which did not rely on spatial branch-and-bound, but was based on the Logic-Based Outer Approximation that exploited the special structure of flowsheet synthesis models (demonstrated on 5 case studies from literature). The method was capable of considering non-convexities, while guaranteeing global solution for optimal synthesis of process network problem.

Deterministic algorithms for optimisation of nonlinear and mixed-integer nonlinear models for water networks got important advances in the past 10 years. Based mostly on spatial branch and bound concepts, these algorithms have been improved by the development of new tight convex relaxations for a variety of functions, and by more effective strategies for reducing the bounds of the variables.

The main disadvantages of these algorithms were presented by Garrard & Fraga, 1998:

- the need to simplify the nonlinear equations to guarantee global optimality or to provide a differentiable function for a nonlinear programming solver
- the need to find a good, feasible, starting guess and
- in some cases, a dramatic increase in size of the solution space as the problem expands.

2.3.3. Evolutionary algorithms - the approach for large scale water network optimisation

Evolutionary algorithms operate on a population of potential solutions applying the principle of survival of the fittest to produce better approximations to a solution. At each generation, a new set of approximations is created by the process of selecting individuals according to their level of fitness in the problem domain and breeding them together using operators borrowed from natural genetics. This process leads to the evolution of population of individuals that are better suited to their environment than the individuals that were created from, just as in natural adaptation (Pohlheim, 2005).

Evolutionary algorithms differ substantially from more traditional search and optimisation methods. The most significant differences are (Pohlheim, 2005):

a) search a population of points in parallel, not just a single point.
b) do not require derivative information or other auxiliary knowledge; only the objective function and corresponding fitness levels influence the directions of search.
c) use probabilistic transition rules, not deterministic ones.
d) are generally more straightforward to apply, because no restrictions for the definition of the objective function exist.
e) can provide a number of potential solutions to a given problem; the final choice is left to the user.

The various applications of evolutionary algorithms are (Babu, 2001):

a) process design and optimisation,

b) computer-aided molecular design,

c) heat integrated processes,

d) synthesis & optimisation of non-ideal distillation systems,

e) design of ammonia synthesis reactor,

f) online optimisation of culture temperature for ethanol fermentation,

g) generation initial parameter estimations for kinetic models of catalytic processes, molecular scale catalyst design,

h) estimation of heat transfer parameters in trickle bed reactors,

i) automated design of heat exchanger networks using artificial intelligence based optimisation, optimal design of heat exchangers, etc.

Several different types of evolutionary algorithms were developed independently:

- genetic programming - which evolve programs, evolutionary programming - which focuses on optimising continuous functions without recombination,
- evolutionary strategies - which focuses on optimising continuous functions with recombination
- genetic algorithms (GAs) - which focus on optimising general combinatorial problems.

GAs are based on biological principles of natural selection and are implemented as a computer simulator in which a population of abstract representations (called chromosomes) of candidate solutions (called individuals) to an optimisation problem, evolves towards better solutions (Pohlheim, 2005) (Fig. 2.35).

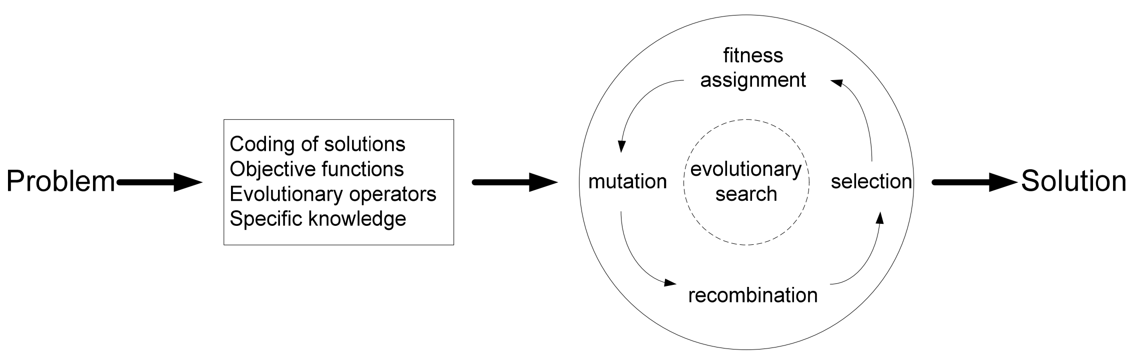


Figure 2. 35 Problem solution using genetic algorithms (Pohlheim, 2005)

Each parameter is mapped into a gene in the chromosome. Traditionally, parameters can be binary strings, real numbers, integers or complex data structures (graphs, trees). Parameters can have limits or can be set from a set of discrete values (Garrard, Fraga, 1998).

The evolution usually starts from a population of randomly generated individuals and happens in generations. A population of solutions (chromosomes, Fig.2.36) is created to start the genetic algorithm (Liao & Sun, 2001). The number of solutions in the population is often determined by the problem to solve and is usually in the range of 10-500 solutions (Fig 2.36.) In each generation, the fitness of every individual in the population is evaluated, multiple individuals are stochastically selected from the current population (based on their fitness) and modified (recombined and possibly mutated) to form a new population.

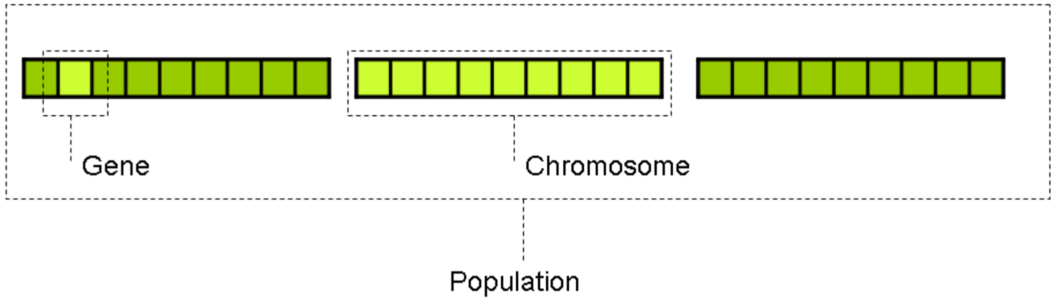


Figure 2. 36 The elements of a population of chromosomes, (Liao & Sun, 2001)

The solution domain is evaluated by a fitness function. The fitness function measures the *quality* of represented solution (how good or useful solution is). The fitness function is the value of objective function for given parameters or the solution generated by the chromosome. GA proceeds to initialise a population of solutions randomly, then, improve it through repetitive application of mutation, crossover and selection operators. The algorithm is stopped when user specified criteria (fitness function, number of generation or some threshold on the diversity in population) is met.

Selection

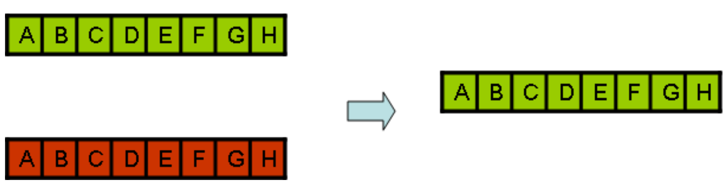


Figure 2. 37 Selection of chromosomes, (Liao & Sun, 2001)

Once all of the solutions were evaluated, two or more must be selected to be parents and therefore create offspring for the next generation. The selection process is usually a random process which is weighted towards those individuals with higher fitness (Fig.2.37).

Crossover

Once selected, the parents can then be "mated" or put through the cross-over process. In this operation, the chromosomes of the parents it "cut and spliced" to create one, two or more child solutions. This operation tries to combine the genetic material of the parents in such a way that those features which made the parents fit in the previous generation are carried through to the next.

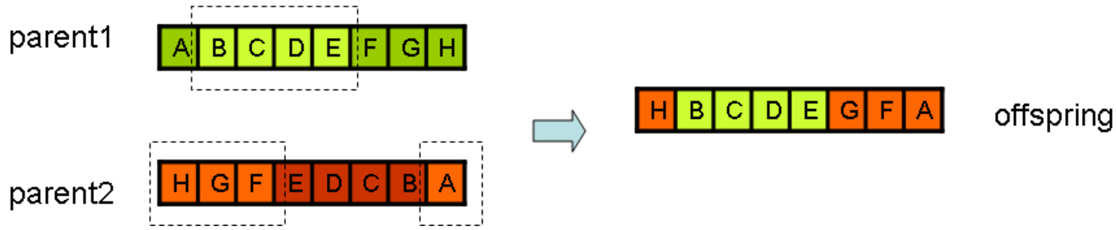


Figure 2. 38 Crossover of chromosomes, (Liao & Sun, 2001)

However, the point(s) at which the chromosomes are spliced are random, as is the execution of crossover itself (although in the range of 70-100%) (Fig.2.38).

Mutation

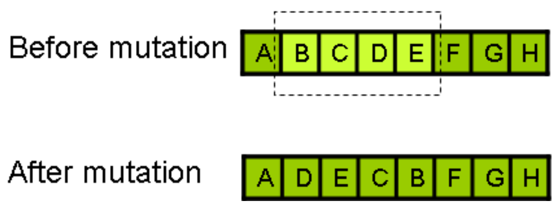


Figure 2. 39 Mutation of chromosomes, (Liao & Sun, 2001)

Without mutation, the genetic algorithm could only manipulate those genes which were present in the initial population. Therefore mutation provides a mechanism for adding random genetic material into the chromosome by changing one or more of the gene values at random. As this is a potentially destructive operation, this is typically performed with a low probability (1-10%) (Fig.2.39).

Evolution flow of GAs:

- *Initialise population*
    - create an initial random population and evaluate each member using the evaluation function
- *Evolve population*
    - Use selection operators to select parents from current population (current generation) based on fitness
    - Apply operators to parents to generate a number of children
    - Children provide or contribute to the next generation
- *Make the next generation current*
- *Continue evolution for a fixed number of generations or until best solution is found.*

The standard genetic algorithm can be summarised with the following pseudo code. Bold words imply variable names and comments are in italics (Kennedy, 1998):

Make a **population** of random genomes

while a good enough solution has not yet been found

Score the population

Build phenotypes from the genotypes in the population.

Score each phenotype using the fitness function.

Build a new population

Make a new empty population: **newPopulation**.

for each new offspring to breed

Select two **parents** from the **population**.

Crossover the **parents** to make a **child**.

Perhaps mutate the **child**.

Put the **child** in the **newPopulation**.

end for

population ← newPopulation

end while.

Application of genetic algorithms (GAs) in water engineering

Researchers, covering a wide range of water engineering-related topics tacked various applications of GAs. A number of fields in the water industry have been reviewed and the contributions of GAs can be summarised according to the following groupings:

- Runoff estimation
- Yield assessment of surface reservoirs
- Optimisation of the system components during the planning and design stage
- Operational optimisation
- Network rehabilitation
- Optimisation of operations of water purification plants and pump stations
- Optimisation of water network

Advantages of using GAs (Marczyk, A., 2004)

- Genetic algorithms are intrinsically parallel because explore the solution space in multiple directions at once. If one path turns out to be a dead end, GAs eliminate it and continue work on more promising avenues, giving them a greater chance each run of finding the optimal solution

- Due to the parallelism that allows them to implicitly evaluate many schema at once, genetic algorithms are particularly well-suited to solve problems where the space of all potential solutions is truly huge - too vast to search exhaustively in any reasonable amount of time
- Perform well in problems for which the fitness landscape is complex
- Have the ability to manipulate more parameters simultaneously.

For solving process engineering problems, the evolutionary algorithms were preferentially used by different authors. Lewin et al.,1998 presented an approach for synthesis of heat exchanger networks (HEN) using GAs. An efficient HEN structure representation was proposed which can be used by genetic operators and can be easily transformed into a form suitable for LP solver. This algorithm was modified also for solving NLP problems (Lewin, 1998).

Formulation of Lewin et al., 1998, Garrard & Fraga, 1998 suggested a new approach for mass exchange network synthesis without/with regeneration using GAs for single contaminant system. They defined encoding for mass exchange network synthesis problems that determines both the structure and the actual mass exchanges simultaneously, which did not require the solution of nonlinear program as part of the fitness evaluation.

Cisty, 2000 applied the genetic algorithm methodology to network rehabilitation optimisation considering both technical and economic aspects of the problem for a case study of the irrigation system.

Tsai & Chang, 2001 used GAs to identify the cost-optimal and least-consumption water usage and treatment networks.

Prakotpol & Srinophakun, 2004 developed a GA based program, GAPinch, to solve the wastewater minimisation problems. It covered both single and multiple contaminant systems, but for simple water networks (with 2 or 3 water-using units).

Cao et al., 2007, developed a new genetic algorithm, *pinch multi-agent genetic algorithm* (PMAGA) for water networks optimisation. PMAGA was more efficient for shorter computational time compared with other algorithms and could yield more water networks consuming the same minimum freshwater but with different configurations.

Zecchin et al., 2006 used a more recently evolutionary algorithm, *Ant Colony Optimisation Algorithm* (based on the analogy of the behaviour of a colony of searching ants and their ability to determine the shortest route between their nest and a food source) to obtain the best solution for a distribution water system.

Shopova & Vaklieva-Bancheva, 2006 presented BASIC - the genetic algorithm to exploit the benefit of the existing genetic schemes so as to be able to deal with various engineering problems. They used real schemes both for real and integer variables, included a number of selection, reproduction and mutation schemes in respective genetic operators, gave a replacement scheme and could easy fit to given problems.

2.4. Conclusions

On the based study of literature, following conclusions can be drawn. As a way to reduce the utilities and the environmental impact, process integration is a good and state-of-art tool used in last years. Water is an important utility which must be reduced in the future and huge amount of effluents discharged into the environment are be limited by legislation. Waste minimisation is one of source reduction methodologies for environmental process design. It is used for water networks design/retrofit by reuse, regeneration reuse or regeneration recycling of water streams to minimise supply water flowrate and also wastewater flowrate. Different techniques for water minimisation were developed in the last period. Some of them gave minimum flowrate of water supply before design based on graphical representation (Pinch Analysis), the others were based on mathematical programming techniques.

Graphical techniques are based on mass load transferred between process streams and water streams, are interactive methods, and are based on first and second laws of thermodynamics. The advantage of these techniques is that they provide valuable conceptual insight into the performance or behaviour of the system under consideration, but have some limitations when dealing with complex water networks. Graphical insights are of importance in practice because they allow the engineer to incorporate many factors that mathematical programming does not consider.

Mathematical programming techniques are based on formulation of mathematical models and solve with different optimisation algorithms (deterministic or stochastic). In many cases, these techniques were applied to obtain minimum freshwater consumption for water network or total cost or cost of investment, etc. These techniques considered the targeting and design stages being performed simultaneously. Using intensively the computer these methods can tackle problems of more complex nature. However, much of the conceptual insight available through the Pinch Analysis based approach is lost.

Many authors proposed different graphical representation which could be used to calculate the freshwater targets: composite curve diagram (El-Halwagi & Manousiou-thakis, 1989), Water Pinch Diagram (Wang & Smith, 1994a), Pinch Diagram (Dhole et al., 1996), Source - Sink diagram (El-Halwagi et al., 1996), Water surplus diagram (Hallale, 2002), Resources conservation diagram (El-Halwagi, et al., 2003), Nearest neighbors diagram (Prakash & Shenoy, 2005), Property based composite curves

(Kazantzi & El-Halwagi, 2005), Quality based composite curve (Bandyopadhyay, 2006),etc. These methods were used as better understanding tools for water minimisation, but had limitations (to handle multiple contaminants, no information about the topology of water network).

Since the graphical approach had limitations for complex systems and in particular when multiple contaminants are involved, the mathematical programming became most chosen technique to use for designing the water network. A number of efforts have been made to formulate a corresponding mathematical model to achieve the goal of fundamental structural changes that allow extensive water reuse or decreasing wastewater generation. State of art of mathematical models formulated for water network since 1990 is presented in this study. For each model the hypotheses, the equations, the constraints and the objective function specific for design an optimal water network are presented.

Takama et al., 1980 were the first authors who formulated a complete model for an oil refinery considering reusing and regeneration as strategy for minimisation of water usage. El- Halwagi & Manousiouthakis,1990 built a concentration interval diagram using limiting compositions of rich and lean streams and the equations are based on mass balance around this interval. Rossiter & Ravi, 1995 included in a model all possible recycle and reuse options for each water stream, Alga-Algaez et al.,1999 developed mathematical models for single and multiple contaminants based on concepts of El-Halwagi. Also, for multiple contaminants, Yang et al., 2000 formulated the model based on complex superstructure and Suh & Lee, 2002 for designing water network under parameter uncertainty or with internal water mains (Feng & Seider, 2001). Later, some authors considered treatment units as a part of water network, not only the water-using units (Koppol et al.,2003, Karuppiah & Grossmann, 2006) or internal regeneration of streams (Cao et al., 2004; Wang et al., 2003). Feng &Chu, 2004 decomposed the water network into three subsystems: water utilisation system, wastewater regeneration system and wastewater treatment system.

Depending on the nature of constraints and the types of variables involved in the model, different algorithms were required to solve the optimisation problem. Most of the optimisation problems were postulated as a superstructure which allowed a representation of all possibilities to reuse streams between water-using units, in a systematic way. The optimisation of superstructure was usually formulated as a NLP problem which involved or not discrete variables. The source of nonlinearities was contaminant material balance equations which involved bilinear terms from multiplication of water flowrate by contaminant concentration. A review of optimisation algorithms based on superstructure was presented also: Branch and Bound algorithm (Al-Khayyal, 1992; Al-Khayyal & Falk, 1983; Horst & Tuy, 1987), Outer-Approximation (OA) algorithm (Horst et al., 1992), Cutting Plane algorithm (Tuy et al., 1985), Difference of Convex (DC) and Reverse Convex algorithm (Tuy, 1987), Interval algorithm (Hansen, 1980), Outer Approximation (OA) and Generalised Benders Decomposition (GBD) (Grossmann, 2002). For water minimisation and design of water network, some authors suggested solving procedures for superstructure-based model by decomposing the NLP models (for a complex network with seven water-using units and three contaminants- Alva-Argaez et al., 2006, Bagajewicz et al., 1999) or used an effective heuristic procedure (Galan & Grossmann, 1998).

The superstructure-based algorithms have also disadvantages: no guarantees to find global optimality for complex optimisation problem and need a feasible starting guess. Some of these problems can be solved using Evolutionary algorithms which search a population of points in parallel, not just a single point, use probabilistic transition rules and can provide a number of potential solutions to a given problem.

The most popular evolutionary algorithm is Genetic Algorithm (GA). An overview about how chromosomes are computed and how is working this algorithm is presented. For different fields, the GA are used successfully: optimisation of heat exchanger network (Lewin et al.,1998; Lewin, 1998), synthesis of mass exchange network without/with regeneration for single contaminant system (Lewin et al., 1998, Garrard & Fraga, 1998), irrigation system rehabilitation (Cisty, 2000), to identify the cost-optimal and least-consumption water usage and treatment networks (Tsai & Chang, 2001), wastewater minimisation problem for single contaminant (Prakotpol & Srinophakun, 2004), pinch multi-agent genetic algorithm (PMAGA) for optimising water-using networks (Cao et al., 2007).

Design of an optimal water network using waste minimisation as an integration tool had a large interest in the last years. In Romania, is a large potential to apply process integration tools to reduce the amount of supply water used in industrial large sites (i.e. oil refinery site or petrochemical site) as we identified in previous reports to this work (Iancu, 2005a, Iancu, 2005b). GA algorithm is used as optimisation tools, in an original format, for an original formulation of water network model, as oriented graph.

NOMENCLATURE for CHAPTER 1

a_R	target freshwater consumption, [t/h]
AR	annualised factor for investment on treatment units, [\$/year]
$B_{i,k}$	inlet concentration of contaminant k in unit i, [ppm]
c_j	cost of lean stream per kg, [\$/kg]
$C = \{c \mid c = 1,2,...,Nc)$	a set of contaminant concentrations, [ppm]
C_i^*	levels of concentration for operation data, [ppm]
C_j^i	concentration of contaminant *j* in stream *i*, [ppm]
C_j^k	concentration of contaminant *j* in outlet stream *k*, [ppm]
C_k^S	contaminant concentration in supply water stream on interval k, [ppm]
C_i^w	inlet and outlet concentration of contaminant from “deposits”, [ppm]
C_k^w	contaminant concentration in water stream on interval k , [ppm]
C_{k+1}^w	contaminant concentration in water stream on interval k+1, [ppm]
$C_{i,k}$	outlet concentration of contaminant k in unit i , [ppm]
$C_{r,k}$	outlet concentration of contaminant k in regeneration unit r, [ppm]
$C_{S,j}$	contaminant concentration in water sources, [ppm]
$C_{i,ie}^{max}$	outlet limiting contaminant concentration for unit i, [ppm]
$C_{i,in}^{max}$	inlet limiting contaminant concentration for unit i, [ppm]
C_{jks}^{ie}	outlet contaminant composition for process j in scenario s, [ppm]
C_{jks}^{in}	inlet contaminant composition for process j in scenario s, [ppm]
$C_{in,c,i}^{max}$	inlet maximum contaminant concentration of each operation, [ppm]
$C_{ie,c,i}^{max}$	outlet maximum contaminant concentration of each operation, [ppm]
C_{FW}	cost of freshwater, [\$/kg]
D_{is}^{in}	drag in solution flow rate from unit i in scenario s,
D_{is}^{ie}	drag out solution flow rate from unit i in scenario s,
f_j^i	flow of contaminant *j* in stream *I*, [t/h]
f_{min}	minimum flow rate of water stream, [t/h]
F^i	total flow of stream i, [t/h]

F_j^w	freshwater demand to unit j, [t/h]
$F_{i,j}$	reused water flow rate from unit i to unit j, [t/h]
$F_{j,k}$	wastewater flow rate from unit j to treatment unit k, [t/h]
$F_{k,j}$	treated water flow rate from unit treatment k to unit j, [t/h]
$F_{j,ie}$	wastewater flow rate from unit j, [t/h]
FW	Freshwater intake into the system, [t/h]
$grd_{r,k}$	removal ratio of contaminant k in regeneration unit r, [%]
G_i	flowrate of rich streams, [t/h]
H	hours of plant operation per annum, [h]
i, j, h	number of unit
$I = \{i \mid i = 1,2,...,No\}$	a set of process units
$IC(F^i)^\alpha$	investment cost of treatment unit t, [$/year]
$J = \{j \mid j = 1,2,...,Ns\}$	a set of freshwater sources available
k	number of treatment units
$k1_r$	binary coefficient for existing streams between regeneration unit r and unit i, [-]
$k2_r$	binary coefficient for existing streams between regeneration unit r and treatment unit
kn_{int}	number of concentration intervals
L_i	mass flowrate of water loss from unit i, [t/h]
L_j	mass flowrate of lean streams (mass flow rate of freshwater stream j), [t/h]
L_J^p	contaminant load inside unit p for contaminant j, [g/h]
L_j^U	maximum availability of freshwater source j, [g/h]
$m_{C,i}$	mass load of contaminant which is transferred from each unit, [g/h]
$m_{i,k}$	mass load of contaminant k in unit i, [g/h]
m_{in}	set of inlet streams into mixer m
m_k^R	contaminant mass load of process stream on interval k, [g/h]
m_k^W	contaminant mass load which is transferred to water stream on interval k, [g/h]
m_{out}	outlet stream from mixer m
M	number of contaminants
MU	set of mixers

N	number of rich streams, number of unit, number of intervals
N_S	number of lean streams
No	number of process units
Ns	number of available sources
Ny	expected life of the plant, [years]
Oc_S	operating cost in scenario s, [$]
OCt	operating cost coefficient for treatment unit t
OC^iF^i	operating cost of a treatment unit t
P_C	capital cost, [$]
p_{in}	inlet stream into process unit p
p_{out}	outlet stream from process unit p
Pp	flow demand in process unit p, [t/h]
prcoef	present value coefficient for profit, [%]
PU	set of process units
$r_{i,k}$	residual mass from operation i in interval k, [t/h]
$rspec_{r,k}$	regeneration model specification, [%]
S	number of scenarios
s_{in}	inlet stream into splitter s
s_{out}	set of outlet streams from splitter s
$Smax_s$	maximum amount of available water source, [t/h]
S_i	flowrate of freshwater from source s to unit I, [t/h]
SU	set of splitters
t_{in}	inlet stream into treatment unit t
t_{out}	outlet stream from treatment unit t
TU	set of treatment units
Tx	taxation rate, [$]
X_i	capacity of freshwater pipe line into unit i, [t/h]
$X_{i,j}$	flowrate of reused water stream from unit i to unit j, [t/h]
$X_{i,r}$	flow rate of reused water stream from unit i to regeneration unit r, [t/h]
$X_{j,i}$	flow rate of reused water stream from unit j to unit i , [t/h]
X_k	contaminant composition of lean stream through interval k, [ppm]
X_{k-1}	contaminant composition of lean stream through interval k-1, [ppm]
$X_{r,i}$	flow rate of reused water stream from regeneration unit r to unit i

$X_{r,T}$	flow rate of regenerated water stream to treatment unit , [t/h]
$y_{i,j}, y_{w,j}, y_{j,o}$	binary variable for possible inlet, outlet and operations interconnections
$Y_{i,j}$	capacity of recycled wastewater flow pipe line from unit i to unit j, [t/h]
Y_{k-1}	contaminant composition of process stream in interval k-1, [ppm]
Y_k	contaminant composition of process stream in interval k, [ppm]
Z_i	capacity of discharged wastewater flow pipe line from unit i, [t/h]
W_i	flowrate of water to unit i, [t/h]
$W_{i,k}$	mass load of stream i in interval k, [g/h]
$W_{i,j,k}$	mass load transferred from unit i to freshwater j, [g/h]
$W_{i,k}^{P}$	mass load transferred from unit i in interval k, [g/h]
W_{is}^{f}	freshwater flowrate to unit i in scenario s, [t/h]
W_{jis}^{r}	recycle wastewater flowrate from unit i to unit j in scenario s, [t/h]
$W_{j,k}$	contaminant mass load that can be transferred to lean stream j through interval k, [g/h]
α	unit capital cost of piping and pumping, [$]
$\underline{\alpha}$	cost function exponent (0 < $\underline{\alpha}$≤1)
β	target regeneration cost, [$]

$\beta_j^t = 1 - (\text{removal ratio for contaminant j in unit t})$, [%]

δ_k	residual mass load from interval k, [g/h]

Chapter 3
Water network optimisation for multiple supply water sources

3.1. Introduction and Motivation

In the past the problem of environmental protection was approached through the enforcement of proper legislation aimed at the protection of the "quality" of the receiving waters. Attention was given more to the eventual effects caused by the wastes rather than to the characteristics of the wastes involved. The absence of damage to aquatic life or the specification of certain chemical and/or physical-chemical characteristics to be respected, are some typical examples of the meaning of "quality" of receiving waters. Subsequently, several legislations have adopted the concept of "standards" as a measure of the quality of the effluents. Such standards are to be satisfied (usually in terms of concentration limits) regardless of the origin of the wastes and of their volumes.

Today, water resources become more and more limited, industry being forced to look for water/wastewater minimisation strategies. On the other hand, to keep industry sustainability effluents must not harm the environment. Government authorities are imposing strict regulations in this respect. As a consequence attention is paid to water systems topology and treatment facilities. With an average of only 2660 m^3 water/inhabitant/year, comparatively with European average of 4000 m^3 water/ inhabitant/year, Romania is one of the relatively poor countries in water sources. Also, 71% of the wastewater are untreated or insufficiently treated and flows directly into natural receivers. To further improve the environment infrastructure, both in terms of quantity and quality, a future priority as "*Development of integrated waste management systems*" is proposed (Romanian Ministry of Environment and Water Management, 2006).

Oil refinery and petrochemical platforms represent typically example for large and fully integrated production sites. Oil refineries are industrial sites that manage huge amounts of raw materials, utilities and products. In this respect these sites are also intensive consumers of energy and water. In their storage and refining processes, oil refineries generate emissions to the atmosphere, produce effluents and pollute the soil, to the extent that environmental management became a major factor for oil refineries. Water is used intensively in a oil refinery as process water as well for cooling purposes. The main water contaminants are hydrocarbons, sulphides, ammonia and some metals.

In the context of the huge amount of raw material processed, oil refineries do not generate substantial quantities of waste (European Commission, 2003).

In Fig. 3.1, a typical oil refining and petrochemical platform is represented.

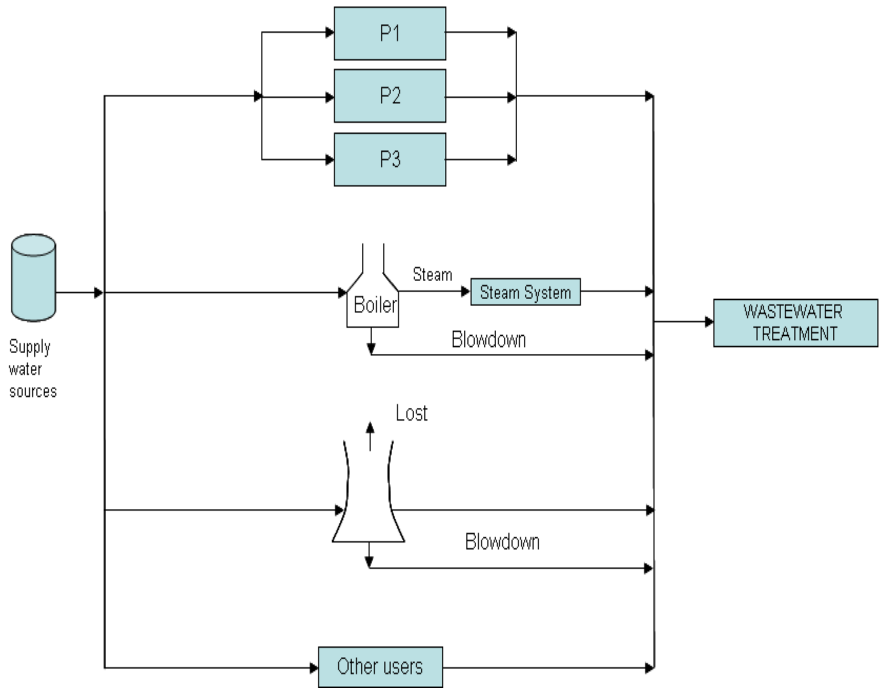


Figure 3. 1 A typical water network on a large site (Smith, 1997)

Water is used in different operations as a reaction medium, solvent in extraction processes, as stripping agent or for cleaning. Also, water is needed in boilers and in cooling towers as make-up for the evaporative losses. All the effluents tend to be mixed together and treated centrally in a wastewater treatment system and discharged into environment. These units produce huge amounts of wastewater streams containing numerous contaminants: salts, hydrocarbons, oil, organic compounds, ammonia, suspended solids, immiscible liquids, etc. (Smith 1995).

In my recent study (Iancu, 2005a), I noticed that oil refineries produce four types of wastewater: surface water runoff, cooling water, process water and sanitary wastewater. Wastewaters are treated in water treatment facilities and then discharged to public water treatment plants or surface waters. Surface water limits are based on the quantities of suspended solids, oil, greases, phenolic compounds, ammonia, sulphides, and chromium that may be present in the wastewater. Crude and product storage tank are also a source of surface water. Process wastewater contaminated by direct contact with oil accounts for a significant portion of total refinery wastewater. Main wastewater streams are from crude oil desalting, steam stripping, fractionator reflux drum drains and other sources. In oil refineries, steam stripping is specific to crude oil fractionation (atmospheric and vacuum towers) and to secondary processing plants as Fluid Catalytic Cracking (sour wastewater from the fractionator/gas concentration units and steam strippers with high levels of oil, suspended solids, phenols, cyanides, H_2S, NH_3), visbracking (wastewater from the fractionator hydrogen sulfide, ammonia, phenol, suspended solids, dissolved solids), sweetening, hydrotreating (sour wastewater from the fractionator and hydrogen separator (suspended solids, H_2S, NH_3, phenols), hydrocracking (sour wastewater from the fractionator) and hydrogen separator (with suspended solids, H_2S), catalytic reforming (process wastewater with high levels of oil, suspended solids, low H_2S), etc (Ionescu, 1999).

Petrochemical plants (Iancu, 2005b), as steam cracker, acrylonitrile plant, ethanol plant, polyolefines plant, maleic anhidride plant, etc. are also high water consumers and produce wastewater with different degrees of contamination.

In this respect, water network is a distinct entity of oil processing and petrochemical sites, with specific features. Characterisation of water networks includes water streams relating different sources/users-topology, streams flowrate and contaminants concentration.

Increased scientific and public awareness over the effects of oil refineries and petrochemical sites on the environment led the researchers/engineers to find ways of reducing the environmental impact of plant operation. In this context, the ideas of waste minimisation became everyday language in the process industry and chemical/process engineering literature. The possibilities for improvement of environmental performance through analysis of plant mass balances, improved housekeeping around the existing processes and finally process redesign, led to speculate that a zero-emission plant could be one day the norm. Many papers report successful water minimisation techniques (as a part of process integration techniques), illustrated with case studies. Several guides are available. A detailed study of literature from different water minimisation techniques for water network is presented in Chapter 2.

Different mathematical formulations (as LP, MILP, NLP, MINLP – depending on model complexity) were proposed for water networks (considering reuse/recycling strategies, regeneration strategies, treatment units included in water network), etc, as I presented in Chapter 2. Almost all formulations are based on considering water network as superstructure taking into account all possible connections between units, sources and treatment units. For simple water networks, the mathematical models are easily solved using different methods: graphical methods or mathematical optimisation methods. But, for complex water networks (like oil refinery and petrochemical water network), the model having a large number of variables, well known solving methods failed.

The aim of this work is to develop an efficient process integration methodology for process design that considers minimisation of technological utilities (supply water flowrate) and the environmental impact of a water network (wastewater flowrate) using an optimisation based framework. Water network in a plant is considered as a whole system allocating the quantity and quality of water to each water-using unit such as to maximise water-reusing and minimise wastewater discharge. It is desired to formulate a NLP mathematical model for a complex water network and to solve it with an optimisation tool able to tackle problems involving high number of variables. A problem with numerous contaminants is highly nonlinear. In literature, this problem is not solved yet as existing tools are not able to tackle directly (without simplifying assumptions) complex water networks with numerous contaminants.

In next paragraphs I develop in a systematic manner an original physical model for water network, stating the general problem to be solved, associated mathematical model, a solving algorithm based on Genetic Algorithm (GA) for optimisation of water network, a new graphical representation of topology of water network to allow easy and comprehensive visualisation. Several case studies demonstrate the applicability of developed methodology.

3.2. Problem statement – physical model

A water network is a set of **water-using units, streams** which interconnect these units, together with the **water supply sources** and the **links** to the **treatment system** (Fig.3.1). Sometimes, **treatment system** is included, also, in the *water network* structure, but in my approach I consider the treatment system outside the water network.

Water-using unit is generally (but not exclusively) a mass exchange unit between process streams/utility streams and water stream. But, there are units in which the transport of contaminants from process streams to water streams is determined by entrainment or mechanical mixing (filtration or washing equipment). The flowrate of contaminant transferred in a water-using unit to a water stream is called traditionally “mass load of contaminant”, denoted in my work as m_{ik} [kg/s]. It is to notice that the contaminant can be dissolved in water or can form solid-liquid suspension, liquid-liquid dispersion, emulsion, etc. Water streams leaving the water-using unit with increased level of contamination either is sent as wastewater stream to treatment units as effluent and discharged into the environment (if satisfies the environmental regulations) or is sent to other water-using unit as internal water streams. Each water using unit can be fed by only one water supply stream, freshwater (free of contaminants) or slightly contaminated water (having different degree of contamination), available on the site. In formulation of physical model, only water part of equipment is considered in modelling and optimisation.

Streams are defined as in each flowsheeting approach the information connection between supply water sources and water-using units, between water-using units, between water-using units and treatment units. From physical point of view streams are associated to the pipes transporting different types of water from/to and inside water network. As abstract concept, the stream is an element of water network topology representing the transfer of information between water-using units, supply water sources and units and between units and treatment unit characterised by flowrates, compositions and other physical-chemical properties.

The water supply source provides a water-using unit the needed water to transfer different contaminants. Due to the level of contamination, there more kinds of water sources: fresh water sources, slightly contaminated water sources, contaminated water sources, etc. Freshwater sources provide water free of contaminants, while slightly contaminated water sources could have low level of contamination. Water sources can be of different natural origin: surface sources (rivers, lakes) and groundwater wells. There are also artificial sources (desalination unit, by-product in chemical reactors, etc).

The treatment unit represents a facility where a set of physical, chemical and biochemical processes are used to remove the contaminants from wastewater streams generated by water-using units. Using different technologies the contaminants are removed up to a specific discharge limit, legally imposed.

Water network optimisation approach is driven to obtain the best water network topology from technological and economical point of view. Problem formulation involve to know data about water-using units (limiting contaminant compositions at the entrance and at the exit as well as mass load of each contaminant removed in water using units) and data for supply water sources - contaminant compositions (Takama et al., 1980; Wang & Smith, 1994a; Savelski & Bagajewicz, 2001).

In Fig. 3.2, as result of my research, I propose a schematic representation for water network handling one contaminant to define the physical model characterised by following elements:

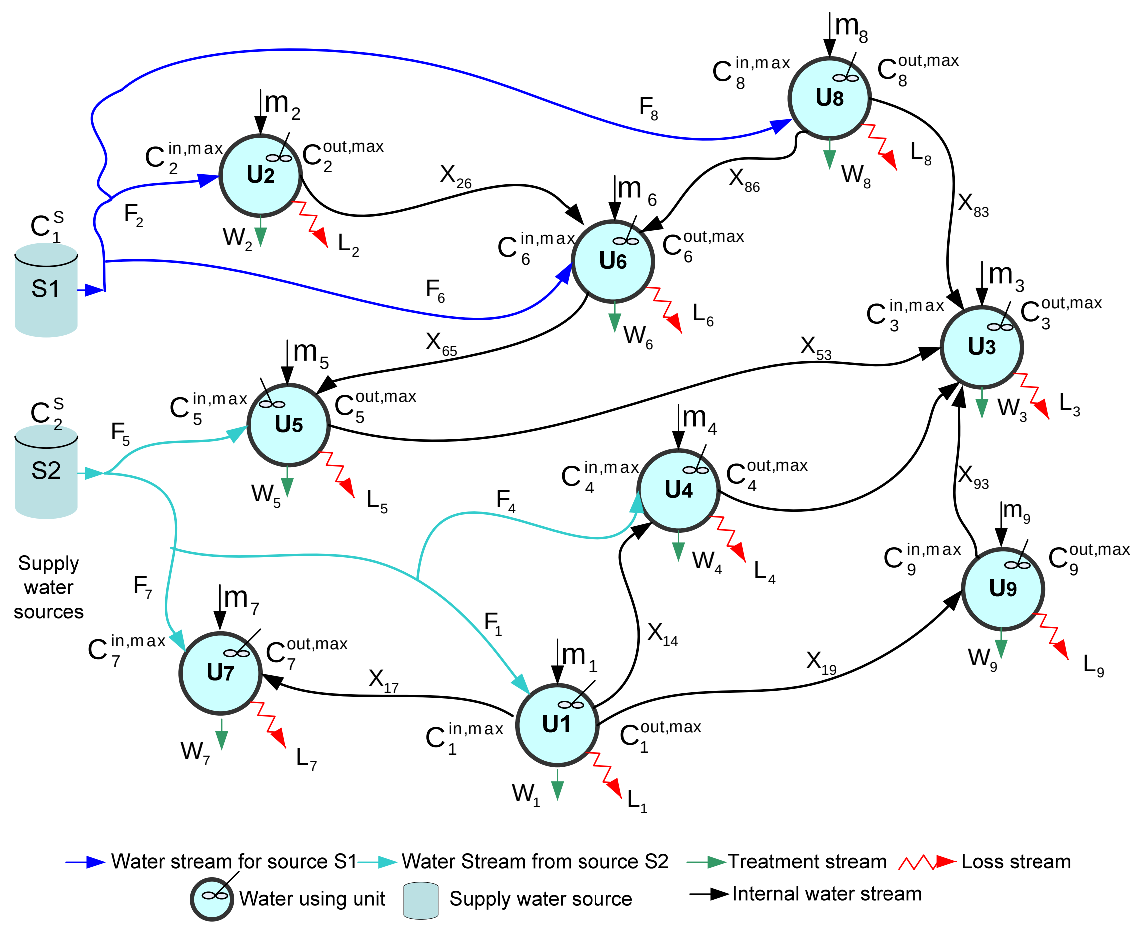


Figure 3. 2 A typical water network on a large site for water minimisation problem - one contaminant

$C_i^{in,max}$ limiting contaminant concentration [ppm] at the entrance of water-using unit u_i, i={1,2,…,9}

$C_i^{out,max}$ limiting contaminant concentration [ppm] at the exit of water-using unit u_i, i={1,2,…,9}

m_i mass load of contaminant transferred [kg/s] from process streams to water stream in each water-using unit u_i, i={1,2,…,9}

C_j^S contaminant concentration [ppm] for supply water sources S_j, j={1,2}

F_i^S supply water source stream for water-using unit u_i, i={1,2,…,9}

W_i wastewater stream sent by unit u_i, i={1,2,…,9} to treatment unit

X_{ij} internal water stream between unit u_i and unit u_j

L_i loss water stream of unit u_i, i={1,2,…,9}.

As typically for water streams just flowrate is of interest, in model development stream notation is also used for stream flowrate notation without confusion.

I underline that in my Thesis water minimisation problem is developed. Consequently my research is not based on mass transfer networks approach which is more restrictive for particular case of water networks (Alva-Argaez et al., 1999). In general terms for a complex water network the water minimisation problem is formulated below as an allocation problem.

I consider a general water network with N water-using units, NS supply water sources, K contaminants to be removed and one wastewater treatment unit. It is requested to design network topology and to determine supply water sources allocation, reusing water distribution between units and wastewater streams observing specific restrictions and minimising a certain performance index.

Water network elements are:

$U = \{u_i \mid i = 1,2,...,N\}$ set of water-using units

$S = \{s_j \mid j = 1,2,...,NS\}$ set of supply water sources

$F = \{F_i^s \mid s = 1,2,...,NS, i = 1,2,...,N\}$ set of supply water flowrates for each unit

$C = \{c_k \mid k = 1,2,...,K\}$ set of contaminants

$M = \{m_{i,k} \mid i = 1,2,...,N,\ \ k = 1,2,...,K\}$ mass load [kg/s] matrix for contaminant k transferred in water-using unit u_i

$X = \{X_{ij} \mid i = 1,2,...,N-1, j = 2,3,...,N\}$ matrix of internal water streams

$W = \{W_i \mid i = 1,2,...,N\}$ set of wastewater streams

$L = \{L_i \mid i = 1,2,...,N\}$ set of streams representing water losses in each unit (by evaporation, by penetration, by leakage, etc).

The analysis is made in steady state. Water-using units are considered perfectly mixed vessels such as contaminant concentration C_{ki} in unit u_i is equal to concentration at unit exit. Internal water sources are not considered.

The goal is to design the optimal water network topology minimising certain well defined performance index as total supply water flowrate, total annualised cost, etc.

In my Thesis, I propose an original approach to water minimisation problem according to the principle of driving force equipartition across the unit based on graph theory. A graph is a set of pairs of vertices (or nodes) and of edges (or arcs) which join the vertices. An undirected edge is said to be incident on the two nodes it connects. If the edges have directionality the graph is called digraph (directed graph or oriented graph). The direction of an edge indicates the direction of the flow of property (mass, energy, momentum, information, etc) or a cause-effect relationship (Himmelblau & Bischoff, 1968). A path is a sequence of distinct lines that are connected to each other. A graph forms a single component (also named separated system) if any two points are joined by a path. A loop (recycle) is a path that begins and ends at the same point. If two loops have a line in common they can be linked to form a third loop by deleting the common line. Graph theory is used in different forms in process synthesis. For heat exchanger networks synthesis the lines represent units and the vertices represent streams (Smith, 2005). In process synthesis, Friedler et al., 1992, introduces structural representation of processes using special directed bipartite graphs or process graphs or P-graphs.

In my approach, the water network is an oriented graph starting from water-using units with inlet contaminant-free constraints, which are supplied with fresh water only.

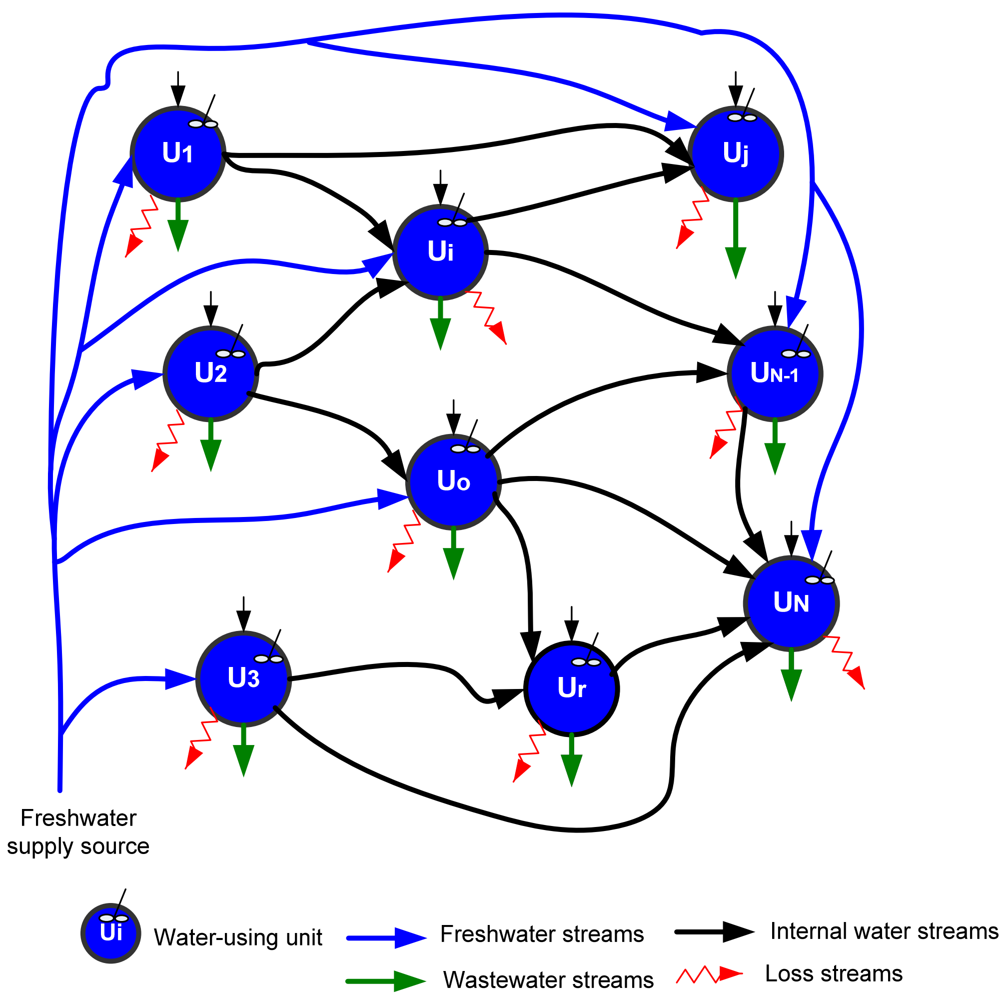


Figure 3. 3 Water network oriented graph for one freshwater source

Any other unit u_i, following the aforementioned ones, receives streams from possibly (but not necessarily) all previous units u_h (h=1,2,...,i-1) and sends streams to probably (but certainly not all) subsequent units u_j (j=i+1,i+2,…,N), as presented in the Fig. 3.3 and published in my papers Lavric et al., 2003; Lavric et al., 2004a. This graph has no recycles (as water recycling is not considered) but has more partitions. This allows me to rank the water-using units inside the water network according to some ranking criteria. As there are no recycles, the mathematical model keeps complexity, but the solution is easier because recurrence is used. As water supply sources can have different degree of contamination, the unit can e grouped to be fed from certain sources forming clusters. Usually the clusters form multicomponent system from graph theory point of view. This approach allows using rationally the water supply sources according to units limiting conditions for contaminants concentrations.

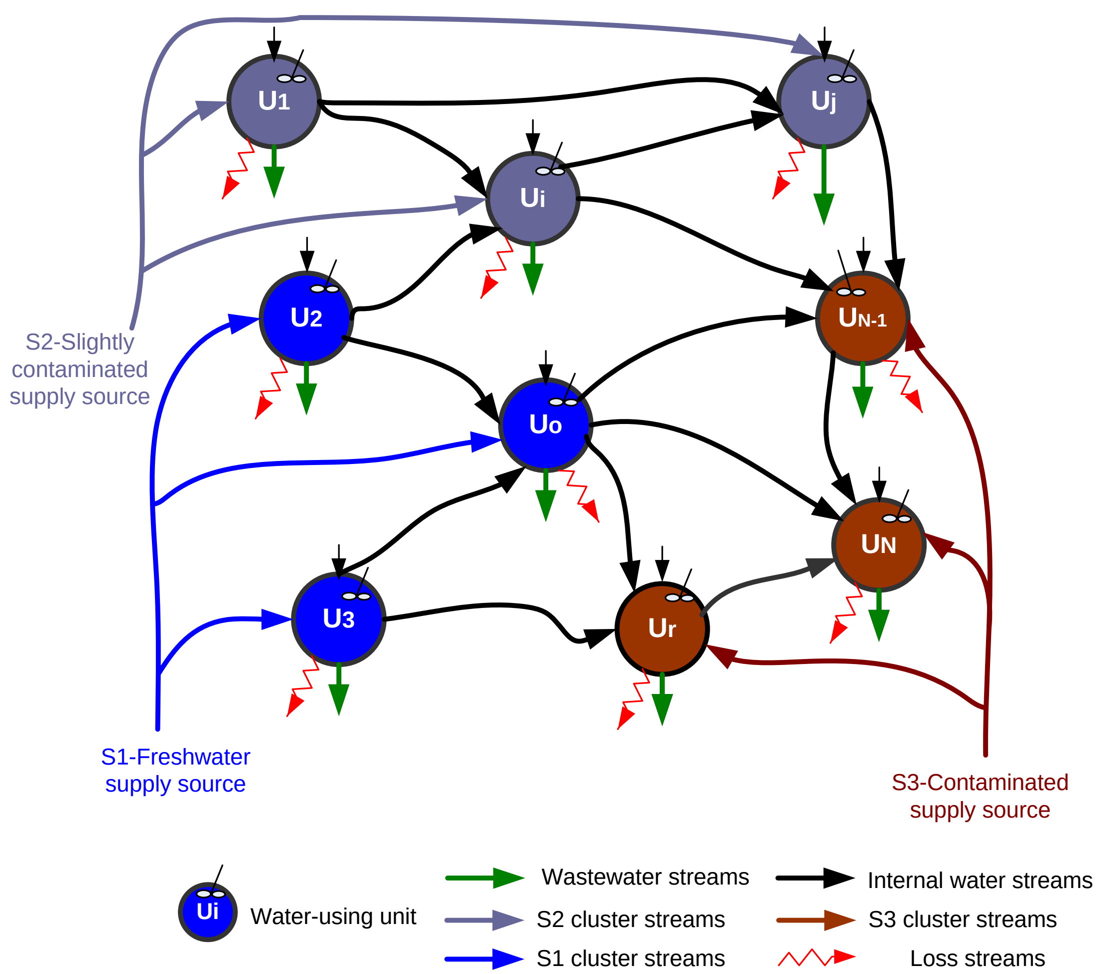


Figure 3. 4 Water network oriented graph with several water contaminated sources

If there are several water supply sources with different contamination level the oriented character of the graph encoding the topology is preserved using each contaminated source to supply its own cluster of water-using units, according to their contaminant level constraints at the entrance as I illustrate in Fig. 3.4. In this figure, since the freshwater source is the most expensive it feeds only the inlet contaminant-free units, grouped into the first cluster. The second cluster consists of the units having moderate restrictions concerning input concentration of contaminants, fed by slightly contaminated water source. The contaminated water source can be, eventually, used to feed the last cluster of units with relaxed restrictions at input, in terms of contaminants concentration. Consequently, the units can be grouped in clusters attached to a given source. This distribution of contaminated sources across the water network topology is also in accordance with the principle of driving force equipartition (Lavric et al., 2004c).

Water network topology encoded as oriented graph (illustrated in Fig. 3.3 and Fig. 3.4) can be adequately represented by an upper triangular matrix of internal flowrates $X = \{X_{ij} \mid i = 1,2,...,N-1, j = 2,3,...,N\}$ and by additional two vectors:

- supply water source flowrates $F = \{F_i^s \mid i = 1,2,...,N\}$
- wastewater flowrates $W = \{W_i \mid i = 1,2,...,N\}$.

This representation is given in Fig. 3.5 as described in my paper Lavric et al., 2005.

Based on this assumption, any water recycling is conceptually avoided. The internal streams become more and more contaminated from the entrance to the exit.

$$\begin{bmatrix} F_1 \\ F_2 \\ F_3 \\ \cdots \\ F_{N-1} \\ F_N \end{bmatrix} \begin{bmatrix} 0 & X_{1,2} & X_{1,3} & \cdots & X_{1,N-1} & X_{1,N} \\ 0 & 0 & X_{2,3} & \cdots & X_{2,N-1} & X_{2,N} \\ 0 & 0 & 0 & \cdots & X_{3,N-1} & X_{3,N} \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & 0 & X_{N-1,N} \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{bmatrix} \begin{bmatrix} W_1 \\ W_2 \\ W_3 \\ \cdots \\ W_{N-1} \\ W_N \end{bmatrix}$$

Figure 3. 5 Formal representation of upper-triangular matrix encoding water network internal flowrates with associated vectors for water source flowrates and wastewater flowrates

Each line of the matrix is associated with streams flowrate emerging of a water-using unit. The uppermost positions are reserved for the units of the inlet contaminant free cluster. In agreement with approaches of Wang & Smith, 1994a, who introduced the concept of *Limiting Water Profile*, I consider each water-using unit to be defined by maximum inlet/outlet concentration and the mass load of the contaminants to be transferred. The flowrate from supply water sources is determined from consistency and feasibility conditions for multiple contaminants.

In literature, different approaches are presented. Wang & Smith, 1994a,b proposed a "shifting" strategy to achieve feasible target within water pinch analysis approach. It was based on modifying inlet and outlet concentrations and mass loads for each water-using unit until all streams were consistently placed for all contaminants. A reference contaminant was chosen to perform shifting of streams and the solution was independent of the selected contaminant. Modifications to the maximum inlet concentrations to achieve the feasibility are considered by Alva-Argaez et al., 1999. The procedure to shift the inlet concentrations is dependent on assumptions regarding the nature of mass transfer. The functional relation, based on Kremser equation, considering fixed mass load distribution, is not a restriction on the basic approach. It is found that the contaminant requiring the highest relative recovery will fix the recovery of all the other contaminants. Savelsky & Bagajewicz, 2003 introduced a formal frame to ensure feasibility and optimality of supply water sources, based on contaminant limiting concentration. For feasibility conditions, the authors defined a key component as the contaminant which reaches maximum outlet concentration to determine freshwater consumption. The necessary conditions of optimality are formulated in a set of theorems with reference to key component outlet maximum concentration and monotonicity of concentration.

In my work, original and high degree of generality conditions are formulated, based on oriented graph topology of water network, considering multiple supply water sources. As Savelsky & Bagajewicz, 2003, water flowrate from supply sources is calculated as maximum of all minimum flowrates requested by each contaminant to keep limiting conditions. The evaluation is made for each water-using unit both for inlet and outlet limiting contaminant concentration as I described in (Lavric et al., 2004a,b,c, Lavric et. al, 2005). In this respect, my original approach is to consider the first necessary condition of optimality slightly modified, taking into account limiting inlet and outlet concentration of the particular unit. So, if a solution for the water network is optimal, then either one of the two restrictions for the inlet and outlet concentrations are fulfilled, or both, for at least one of the contaminants. It can be easily demonstrated that the necessary conditions of optimality are special cases of the principle of the driving force equipartition along a process, which ensures minimum entropy generation for given operating conditions, which is a measure of the process irreversibility.

As a consequence of oriented nature of the graph in ascending order, ranking of water-using units can be performed based on one of following criteria introduced in my papers Lavric et al., 2004a,b,c and Lavric et al., 2005:

- "Load based" criterion (Lcrt) addresses the relationship between the performance of water-using unit (mass load) to rank the units within the graph. Maximum mass load of contaminants for ranked units progressively increases along water network.

-"Maximum Freshwater based" criterion (Fcrt) addresses the maximum flowrate of water from supply sources needed to remove contaminants to rank the units within the graph. Ranking is according their needs for freshwater when reusing is not considered. It should be mentioned that the units with zero limiting inlet contaminant concentration (free contaminant) are always placed first.

Both criteria give same results if the number of water-using units and contaminants are small (Lavric et al., 2003). When the water network is very large (high number of units and contaminants), different topologies and supply water consumption are obtained (Lavric et al., 2005).

3.3. Mathematical model

The mathematical model for the water network is developed for the most general case, covering all the essential aspects of the problem. In this work, mathematical model is not formulated based on a superstructure (which incorporate all relevant water streams within the network under investigation together with all units that introduce or remove waterborne contaminants) (Takama et al., 1990; Rossiter & Ravi, 1995; Alva-Argaez et al., 1999; Yang et al., 2000; Suh & Lee, 2002; Koppol et al., 2003; Feng &Chu, 2004; Karuppiah & Grossmann, 2006).

The mathematical model developed in this chapter do not consider the internal water sources (Feng & Seider, 2001; Cao et al., 2004) and water upgrading through regeneration (to be developed in Chapter 5)(Takama et al., 1990; Feng & Chu, 2004). Treatment unit is not included in the water network (Bagajewicz, 2000; Karuppiah & Grossmann, 2006).

The mathematical model for the water network presented below is based upon the overall and species mass balances around each water using unit together with the associated constraints, based on Limiting Water Profile, in terms of input and output maximum allowable concentrations. This approach is original compared to the above citations. The originality is given by the concept on water network as oriented graph and is supported by the nature of industrial water networks and by physical considerations as equipartition of driving force principle.

3.3.1. Mass balances for the generic water-using unit u_i

A generic water-using unit u_i, is given as in Fig. 3.6. This unit receives water from NS external supply sources (freshwater or slightly contaminated or contaminated) and/or from at most h units effluents (h=1,2,…,i-1), placed before unit u_i (corresponding to Lcrt or Fcrt criteria). Contaminant mass load of pollutant k, m_{ki}, is removed from process streams into water streams.

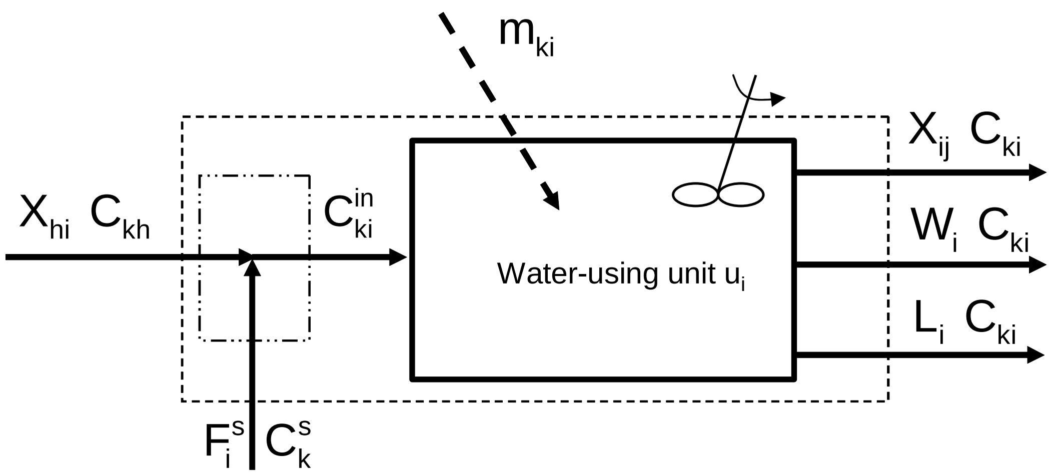


Figure 3. 6 Schematic model of water-using unit, u_i

According to their destination, three kinds of water streams leave the unit: reused streams which can be reused only in next j units (j=i+1,…,N), discharged streams to the treatment unit and losses streams. Each contaminant k is defined by inlet and outlet concentration (C_{ki}^{in} and C_{ki}) at the entrance and exit of unit u_i, respectively.

3.3.2. Total mass balance around water-using unit u_i

$$F_i^s + \sum_{h=1}^{i-1} X_{hi} + \sum_{k=1}^{K} m_{ki} - W_i - \sum_{j=i+1}^{N} X_{ij} - L_i = 0 \qquad \text{i=2,...,N-1}$$

$$F_1^s + \sum_{k=1}^{K} m_{k1} - W_1 - \sum_{j=2}^{N} X_{1j} - L_1 = 0 \qquad \text{in particular for first unit} \qquad (3.\ 1)$$

$$F_N^s + \sum_{h=1}^{N-1} X_{hN} + \sum_{k=1}^{K} m_{kN} - W_N - L_N = 0 \qquad \text{for unit N}$$

In Eqs.3.1, the total flowrate entering in water-using unit u_i (i=2,…,N) is given by the flowrates of supply water F_i^s and all collected flowrates from the preceding units $\sum_{h=1}^{i-1} X_{hi}$, while $\sum_{j=i+1}^{N} X_{ij}$ represents the flowrates sent from unit u_i to the rest of the network.

3.3.3. Partial mass balance for contaminant k around water-using unit u_i

$$F_i^s C_k^s + \sum_{h=1}^{i-1} X_{hi} C_{kh} + m_{ki} - \left(W_i + L_i + \sum_{j=i+1}^{N} X_{ij} \right) C_{ki} = 0, \quad k = 1, 2, ..., K \qquad i=2,...,N-1$$

$$F_1^s C_k^s + m_{k1} - (W_1 + \sum_{j=2}^{N} X_{1j} + L_1) C_{k1} = 0, \quad k = 1, 2, ..., K \text{ in particular for first unit} \qquad (3.\ 2)$$

$$F_N^s C_k^s + \sum_{h=1}^{N-1} X_{hN} C_{kh} + m_{kN} - (W_N + L_N) C_{kN} = 0, \quad k = 1, 2, ..., K \quad \text{in particular for unit N}$$

Eqs.3.2 are written for the most general case, corresponding to contaminated water sources (C_k^s concentration for pollutant k). When dealing with fresh water only, the first term of the left hand side of Eqs. 3.2 vanish.

3.3.4. Partial mass balance for contaminant k at water-using unit u_i input

$$F_i^s C_k^s + \sum_{h=1}^{i-1} X_{hi} C_{kh} - \left(\sum_{h=1}^{i-1} X_{hi} + F_i^s \right) C_{ki}^{in} = 0, \quad k = 1, 2, ..., K \qquad i=2,...,N \qquad (3.\ 3)$$

For the first unit, as there is no internal flow from other units, Eqs.3.3 becomes $C_{k1}^{in} = C_{k1}^{s}$ k=1,2,...,K.

3.3.5. Set of constraints for outlet concentration

The set of constraints for outlet concentration of water-using unit u_i observes the maximum admissible level of concentration for the contaminants in the output water streams, as resulted from technological, corrosion, erosion or any other imperatives. If the water supply could have a certain level of contamination, the constraint can be written for each contaminant k and unit u_i:

$$C_{ki} = \frac{F_i^s C_k^s + \sum_{h=1}^{i-1} (X_{hi} C_{kh}) + m_{ki}}{W_i + L_i + \sum_{j=i+1}^{N} X_{ij}} = \frac{F_i^s C_k^s + \sum_{h=1}^{i-1} (X_{hi} C_{kh}) + m_{ki}}{F_i^s + \sum_{h=1}^{i-1} X_{hi}} \le C_{ki}^{out,max} \qquad \begin{matrix} i=2,...,N-1 \\ k=1,...,K \end{matrix}$$

$$C_{k1} = \frac{F_1^s C_k^s + m_{k1}}{W_1 + L_1 + \sum_{j=2}^{N} X_{1j}} \le C_{k1}^{out,max} \qquad \text{in particular for first unit} \qquad (3.\ 4)$$

$$C_{kN} = \frac{F_N^s C_k^s + \sum_{h=1}^{N-1} (X_{hN} C_{kh}) + m_{kN}}{W_N + L_N} \le C_{kN}^{out,max} \quad \text{in particular for unit N}$$

In the case of equality, in Eqs 3.4. minimum water source flowrate specific to each contaminant k and each unit u_i, corresponding to outlet concentration imposed constraints can be calculated.

$$F_{ik}^{s,min}\Big|_{out} = \frac{\sum_{h=1}^{i-1} X_{hi}(C_{kh} - C_{ki}^{out,max}) + m_{ki}}{C_{ki}^{out,max} - C_k^s} \qquad \text{(i=2,...,N, k=1,2,...,K)}$$

$$F_{1k}^{s,min}\Big|_{out} = \frac{m_{k1}}{C_{k1}^{out,max} - C_k^s} \qquad \text{in particular for first unit} \tag{3. 5}$$

For freshwater supply, the set of constraints for outlet concentration, for each contaminant k, becomes:

$$C_{ki} = \frac{\sum_{h=1}^{i-1}(X_{hi}C_{kh}) + m_{ki}}{W_i + L_i + \sum_{j=i+1}^{N} X_{ij}} = \frac{\sum_{h=1}^{i-1}(X_{hi}C_{kh}) + m_{ki}}{F_i^s + \sum_{h=1}^{i-1} X_{hi}} \le C_{ki}^{out,max} \qquad \text{i=2,...,N-1}$$

$$C_{k1} = \frac{m_{k1}}{W_1 + L_1 + \sum_{j=2}^{N} X_{1j}} \le C_{k1}^{out,max} \qquad \text{in particular for first unit} \tag{3. 6}$$

$$C_{kN} = \frac{\sum_{h=1}^{N-1}(X_{hN}C_{kh}) + m_{kN}}{W_N + L_N} \le C_{kN}^{out,max} \qquad \text{in particular for unit N}$$

In Eqs. 3.4 and 3.6, the total mass balance (Eqs. 3.1) is used to express the contaminant k concentration for unit u_i, as function of supply water stream and streams from preceding units parameters.

3.3.6. Set of constraints for inlet concentration

The set of constraints inlet for concentration concerns to observe the maximum admissible input concentration for the contaminants, related to the technological, corrosion, erosion or any other imperatives. Considering the general case, when the supply water contains an acceptable level of contamination, the mass balance for the contaminant k at the entrance of the water-using unit u_i is given by Eqs. 3.7:

$$F_i^s C_k^s + \sum_{h=1}^{i-1} X_{hi} C_{kh} = \left(F_i^s + \sum_{h=1}^{i-1} X_{hi} \right) \cdot C_{ki}^{in} \qquad \text{i=2,...,N-1}$$

$$F_N^s C_k^s + \sum_{h=1}^{N-1} X_{hN} C_{kh} = \left(F_N^s + \sum_{h=1}^{N-1} X_{hN} \right) \cdot C_{Ni}^{in} \qquad \text{in particular for unit N} \tag{3. 7}$$

Eqs. 3.7 allow writing explicitly the set of restrictions related to maximum inlet concentration for each contaminant and for each water-using unit:

$$C_{ki}^{in} = \frac{F_i^s C_k^s + \sum_{h=1}^{i-1} X_{hi} C_{kh}}{F_i^s + \sum_{h=1}^{i-1} X_{hi}} \le C_{ki}^{in,max} \qquad i=2,...,N \;\; k=1,2,...,K \tag{3. 8}$$

For equality in Eqs. 3.8, minimum water source flowrate for each contaminant k and each unit u_i corresponding to inlet concentration imposed constraints can be calculated.

$$F_{ik}^{s,min}\Big|_{in} = \frac{\sum_{h=1}^{i-1} X_{hi}(C_{kh} - C_{ki}^{in,max})}{C_{ki}^{in,max} - C_k^s} \qquad (i=2,...,N,\ k=1,2,...,K) \tag{3. 9}$$

When only freshwater is available, the set of restrictions simplifies for each contaminant:

$$C_{ki}^{in} = \frac{\sum_{h=1}^{i-1} X_{hi} C_{kh}}{F_i^s + \sum_{h=1}^{i-1} X_{hi}} \le C_{ki}^{in,max} \tag{3. 10}$$

This concludes mathematical model development for the generic water-using unit, u_i. A water network is abstracted as an oriented graph of water-using units, interlinked such that there is no flow allowed backwards, from unit u_i to unit u_h, when i>h

Mathematical model is original, due to elements of originality of physical model and to complexity of approach. Practically, any number of contaminants, supply water sources and water-using units is possible to be considered. As demonstrated by the case studies, this model allows solving easily large industrial problems. Generally, the models presented in the literature can solve only problems not too complex (i.e. seven water-using units and three contaminants (Bagajewicz, 2000), or ten water-using units and three contaminants (Alva-Argaez et al., 2006).

3.4. Design criteria

Optimisation problem regards the water-using system in a plant as a whole by considering how to allocate the **quantity** and **quality of water** in each water-using unit so as to maximise water reusing and minimise wastewater discharge requirement of the entire unit in a direct way (Bagajewicz et al., 2000). For a new water-using system this procedure is called “design”, and for an existing network the procedure is called “retrofit”.

The optimisation of the wastewater network is fully dependent upon the objective envisaged. Generally speaking, this can be reduced to either a complex allocation problem, when there are several contaminated sources available, with different degrees of contamination (minimum supply water consumption), or an investment and/or operating costs problem, when piping and pumping costs are of primary importance (minimum topological index and minimum total cost). Although it may be seem that the best approach would be to jointly use these criteria, optimising the wastewater network in terms of allocation of available resources may damage the topology, when there is more than one water supply (Lavric et al., 2005).

3.4.1. Minimum supply water design criteria

The best topology of water-using network is obtained formulating an optimisation problem to ensure the minimum supply water consumption:

$$\min \sum_{s=1}^{NS} \sum_{i=1}^{N} F_i^s \tag{3. 11}$$

subjected to constraints, Eqs.3.1 - 3.10. This represents a NLP problem with non-convex objective function, suitable to be solved with genetic algorithm (GA).

3.4.2. Deriving the design criteria

The optimisation problem at hand, finding the optimum water resource allocation and network topology, with minimum supply water consumption has no trivial solution, since the number of variables outcome the number of equations and a proper objective function is derived.

The independent variables for solving the water network problem are the internal mass flowrates between water-using units: $X = \{X_{ij} \mid i = 1,2,...N-1,\ j = 2,...,N\}$. As presented in paragraph 3.2, the water network is an oriented graph so, the total number of independent variables is N(N-1)/2.

The parameters of the problem are:

N number of water using units

K number of contaminants

NS number of water sources

$M = \{m_{ki} \mid i = 1,2,...,N,\ k{=}1,2,...,K\}$ set of mass load per unit and contaminant

$L = \{L_i \mid i = 1,2,...,N\}$ set of water losses for each unit

$C^s = \{C_k^s \mid k = 1,2,...,K,\ s = 1,2,...,NS\}$ set of contaminants concentration for each water supply source

$C^{in,max} = \{C_{ki}^{in,max} \mid k = 1,2,...,K,\ i = 1,2,...,N\}$ set of inlet limiting concentration per contaminant and unit

$C^{out,max} = \{C_{ki}^{out,max} \mid k = 1,2,...,K,\ i = 1,2,...,N\}$ set of outlet limiting concentration per contaminant and unit.

The dependent variables of the problem are calculated from model equations:

$F^s = \{F_i^s \mid i = 1,2,...,N\}$ set of water supply source flowrates for each u_i

$W = \{W_i \mid i = 1,2,...,N\}$ set of wastewater flowrates from each u_i

$C^{in} = \{C_{ki}^{in} \mid i = 1,2,...,N\ ;\ k = 1,2,...,K\}$ set of concentration of contaminant k at the entrance of u_i

$C^{out} = \{C_{ki} \mid i = 1,2,...,N\ ;\ k = 1,2,...,K\}$ set of concentration of contaminant k at the exit of u_i

The total number of dependent variables is:

dim(W) + dim(F^s) + dim(C^{in}) + dim(C^{out}) = N + N + NK + NK = 2N + 2NK variables.

Due to the cascaded nature of the topology, all the information associated with the preceding water-using units are already computed, i.e. X_{hi} and C_{kh}, while C_k^s and $C_{ki}^{in,max}$ are problem parameters. So, there are K possible flowrates for the water supply, as resulted from Eqs. 3.9. To observe the constraints Eqs. 3.8, the maximum value of minimum water supply should be kept, this should correspond to the limiting concentration of a contaminant denoted *p*.

$$F_{i,in}^{s,min} = \max_{k=1}^{K} F_{ik}^{s,min}\Big|_{in} \tag{3. 12}$$

Similarly, for flowrates calculated with Eqs. 3.5, the maximum value should be found, this should correspond to the limiting concentration of a contaminant denoted *q*.

$$F_{i,out}^{s,min} = \max_{k=1}^{K} F_{ik}^{s,min}\Big|_{out} \tag{3. 13}$$

As final notice, both constraints Eqs. 3.4 and 3.8 hold for the largest value of the two previously calculated water supply flowrates from Eqs.3.12 and 3.13. Consequently, the value of minimum flowrate from supply source to unit u_i, is calculated with:

$$F_i^s = \max(F_{i,in}^{s,min}, F_{i,out}^{s,min}) \tag{3. 14}$$

$F^s = \{F_i^s \mid i = 1,2,...,N, s = 1,2,...,NS\}$ are the components of the objective function to be minimised. The corresponding contaminant (*p* or *q*) is the critical component.

The total number of equations involved in these calculations can be evaluated from above presentation : *N* equations for F_i^s, *N* equations for W_i, $N \cdot K$ equations for C^{in}

and $N \cdot K$ equations for C^{out}, i.e. a total number of $2N + 2\mathrm{N} \cdot \mathrm{K}$ equations, equal with the number of dependent variables.

The sequence of several calculations is presented in Annex 1.

3.5. The optimisation algorithm

Optimisation algorithm, based on superstructure, used to solve NLP problem, in most cases is simplified through assumptions or heuristic rules. Such simplification makes it easier for specific optimization methods to determine the optimal solution which turns to be sub-optimal. The main disadvantages for these methods are (Garrard & Fraga, 1998): the need to simplify the nonlinear equations to guarantee global optimality, the need to find a good, feasible, starting guess and, in some cases, a dramatic increase in size of the solution space as the problem expand.

Genetic Algorithm (GA) methods do not require such simplifications, giving them a significant advantage in finding a global optimal solution. GA optimisation is an evolutionary, directed search technique, based on the theory of natural selection and the mechanisms of population genetics, that evaluates hundreds of thousands of possible solutions as it converges to the best solution. GA kept track of a population of potential solutions being less sensitive to arbitrary initial guess. The evolutionary nature of the GA optimisation approach is defined by: the initial population, randomly generated, but containing its characteristic variability; the fitness associated with each individual in the population, assessed according to a fitness function; the survival probability of each individual, proportional to its fitness; the selection of individuals, based on probability and breeding through a genetic transformation process of cross-over and mutation, ensuring that the solution is not trapped into a local optimum environment. The main benefits of GA are: provision of substantially lower cost solutions; identification of different solutions with similar objective functions, so the user can choose from the preferred one; relatively easy to analyse, complex problems; creation of an optimal design benchmark and the continuous drop of objective function and raise of benefits/performance.

For solving the NLP problem for optimal allocation of water resources and finding the best network topology, there was implemented a hybrid variant of a classical GA (Lavric et al., 2004b; Raducan et al., 2004). The main idea is to introduce the independent variables in a chromosome (or individual) which is formed by genes.

In our case, the chromosome is the set of internal flowrates between different water-using units (X). A gene contains the flowrate X_{ij}. These flowrates have upper bound as maxim admissible water flowrate:

$$F_i^{max} = \max_{k=1}^{K} \frac{m_{ki}}{C_{ki}^{out,max} - C_{ki}^{in,max}} \tag{3. 15}$$

The restrictions are coped with during the population generation, eliminating those individuals outside the feasible domain.

The fitness function is based on objective function, Eq. (3.11), in a normalised form, to keep the values in [0,1] domain, to reduce or enlarge the difference between good and bad individuals. The fitness measures how good or useful is a chromosome (a particular solution encoded by the chromosome). A good fitness function increases the probability of selecting the individuals. In this implementation, a threshold of 65% is considered for fitness to be selected for crossover (crossover probability).

The individuals interbreed according to their frequency of selection, using one-point crossover method and then mutation is applied to randomly selected individuals of the new generation.

One of the main problems, when using GA, is how to choose the most appropriate parameters values (i.e., the population size, maximum number of generations, mutation and crossover rate). This is normally a trial and error process which takes a considerable amount of time.

Being involved in this statement (Lavric et al., 2004a; Lavric et al., 2004b; Lavric et al., 2005), I can say that it turns out to be harder to fine tune the parameters of the GA (population size: 10000; maximum number of generations: 2500; crossover rate: 65%, mutation probability 0,5%, shrinking standard deviation of individuals upper bound (maximum flowrate): 99,9%; global admissible error: 0,1%).

To solve mathematical model for optimisation of water network, it is developed an optimisation procedure (Lavric et al., 2005).

The computation of the objective function, Eq.(3.11) is performed in following steps, *keeping in mind that the upper triangular matrix X, whose elements are encoded in a chromosome, is an individual from a population bounded by conditions (3.15), as generated in any standard GA*.

1. *Reorder the units*, by load (Lcrt criterion) or maximum supply water needs (Fcrt criterion), such as the first in series are the ones having the lowest limits on input

contaminant concentration, but not lower than the contaminated supply water; if the water source is too contaminated, another source is picked-up.

2. *Compute the minimum supply water flowrate* for water-using unit u_i, based on Eqs. (3.5) and (3.9), with the individual delivered by GA, observing that, due to the oriented nature of the graph, the computations involve only the up-stream arches; for the first unit, at least, this is equivalent with having only supply water as input.
3. *Compute the wastewater flowrate* for water-using unit u_i, according to Eqs.3.1;
   a. For negative values of wastewater flowrate and no losses, this means there is too much water down-stream, so diminish-it subtracting the wastewater flowrate proportionally from every down-stream arch. When losses are present, subtract the wastewater flowrate from the minimum supply water flowrate. Replace, then, the negative value with zero.
   b. For positive but less than a threshold value (a custom value is 1 t/h), the wastewater flowrate should be neglected, from economic considerations. In order for the mass balance to hold, this flow should be proportionally distributed down-stream, only to non-zero arches.
4. *Compute the unit concentrations* around each unit.
5. *Return the objective function*, summing up the minimum supply water flowrate for all the water-using units.

Following these steps, the optimal solution is obtained in terms of the minimum supply water.

This algorithm is coded into original software, whose main window is presented in Annex 2 and also in some publications (Lavric et al., 2004a; Lavric et al., 2004b; Lavric et al., 2005).

3.6. Graphical representation of water network

Visualisation of water network topology is of practical interest. Users need to get graphical representations of water-using units and the whole network links that are selected by optimisation tool. This representation can be made traditionally (El-Halwagi, 1990; Bagajewicz, et al., 1999; Alva-Argaez et al., 1998; Cao et al., 2004; Lavric et al., 2004b).

These types of representation are acceptable for water networks of reduced complexity underlying the links and the flowrates between different units. When more streams go to same unit these representations become difficult to understand (Fig.3.7).

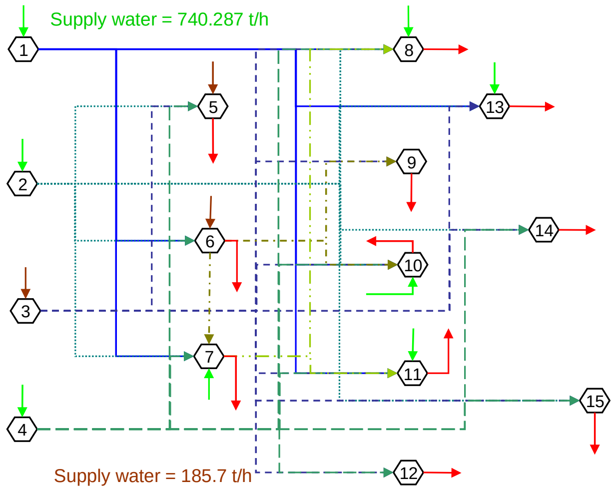


Figure 3. 7 Representation of simple water network (Lavric et al., 2004 b)

If modifications are done, it is very complicated to trace them. From my expertise gained in last years, to harvest more information in a more relevant way the graphical representation of water networks, in my last paper (Iancu et al., 2007) I proposed a new and original type of representation, to offer user easier access to information. Main elements are the water stream (represented as an arrow), water-using unit, water source and water sink, as Fig. (3.8). If the stream does not exist, there is no arrow pointing towards the sink.

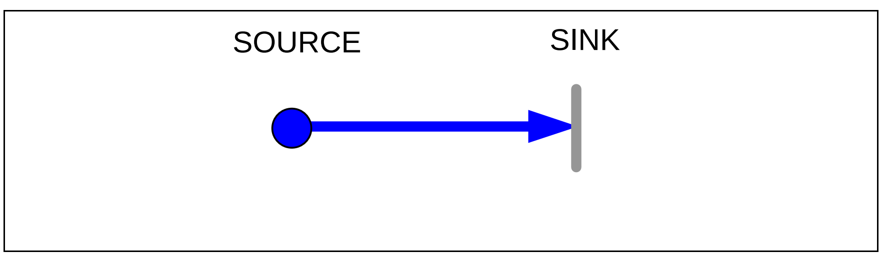


Figure 3. 8 Representation of water stream from source to sink

Inlet external water streams are represented as an arrow between a supply water source (blue circle) and a sink (grey line). Outlet external water streams are represented as an arrow between a sink and a treatment unit. If a source (freshwater) feeds more sinks (water units), the representation is like in Fig. 3.9. A supply water stream (blue line) feed Sink 1. The effluent from Sink 1 is reused in Sink 2, Sink 4,…, Sink N, and also a part of these streams are sent to treatment unit to be regenerated (green line). If Sink 3 doesn't receive water from Sink1 is represented as a line without arrow, as in Fig.3.9.

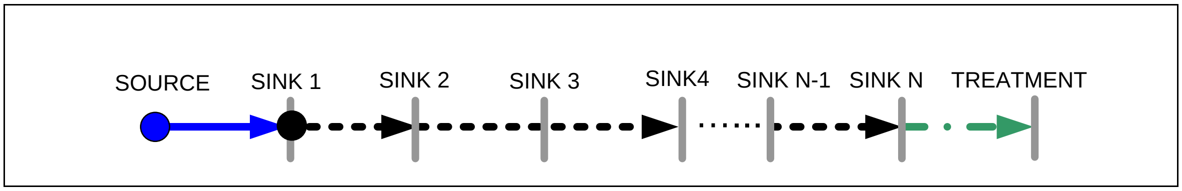


Figure 3. 9 Representation of water streams from one source to many sinks

Using this original concept of coding, the entire water-using network can be represented as in Fig. 3.10.

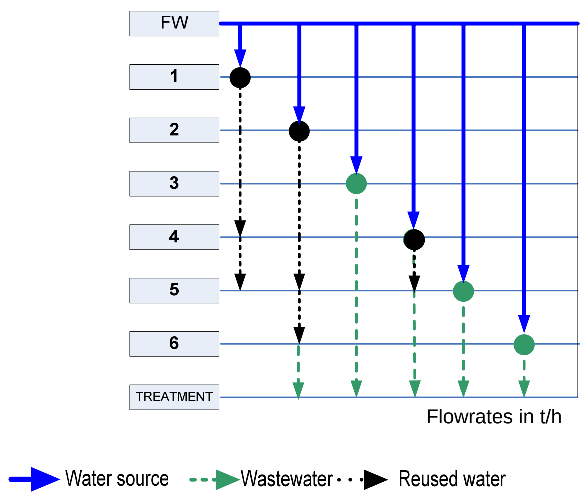


Figure 3. 10 Representation of topology for water-using network

Each water unit is placed on an interval, where water and wastewater streams enter or exit. Around each interval, the mass balance can be made, as mass flowrate of water streams coming from sources and from other water-using units enter in the interval is the same with a mass flowrate of water streams which leave the interval.

3.7. Water network optimisation case studies

A water network is characterized by the following data:

- limiting flowrate of supply water (the water flowrate that actually passes through the unit and comes into contact with process streams), specified for each water-using unit or mass load of contaminants picked up from process streams by water streams,

- inlet maximum concentrations of contaminant for each unit

- outlet maximum concentrations of contaminant for each unit

- total flowrate of water supply sources available on the site.

The following steps are required for optimisation of water network:

1. Formulation of optimisation criteria

2. Optimise the water network based on process constraints (flowrate, contaminant concentrations), using GA algorithm

3. Design the network which satisfies the optimal solution

3.7.1. Literature test case study

In order to test the optimisation procedure for water network topology, it is proposed to get data from literature. There are many examples of water networks from industrial sector (as oil refinery, chemical complex, pharmaceutical plant, paper mill) from literature which are optimised using different methods (graphical or mathematical programming).

A case study proposed by Savelski *et al.*, 1999 related to a petrochemical site is analysed to test the optimisation procedure described above, using GA.

Table 3. 1 Water-using units data, from Savelski et al., 1999

Unit Nr	Contaminants	Load (kg/h)	$C^{in,max}$ (ppm)	$C^{out,max}$ (ppm)
1	A	3.40	20	120
	B	414.80	300	12500
	C	4.59	45	180
2	A	5.60	120	220
	B	1.40	20	1000
	C	520.80	200	9500
3	A	0.16	0	20
	B	0.48	0	60
	C	0.16	0	20
4	A	0.80	50	150
	B	60.80	400	8000
	C	0.48	60	120
5	A	0.75	0	15
	B	20.00	0	400
	C	1.75	0	35
6	A	2.00	10	70
	B	100.70	200	600
	C	2.50	20	90
7	A	1.80	25	150
	B	6.80	230	1000
	C	0.60	20	220
8	A	3.00	5	100
	B	102.30	45	4000
	C	8.14	50	300
9	A	70.00	13	1000
	B	1.90	200	3000
	C	4.00	5	200
10	A	4.00	10	100
	B	10.30	90	500
	C	9.00	70	800

The initial network considered by those authors has 10 water-using units which use water directly from only one water supply source, no reusing streams exist. In each water-using unit, 3 contaminants (A, B, C) can be transferred. The data for this analysis is presented in Table 3.1. No water loses from neither unit are taken into account. For water network optimisation Savelski associated to the network a superstructure, where the nodes represented water units and the lines represented streams linking two units. To solve this superstructure the authors proposed a mathematical programming tool based on *branch and bound* procedure. They introduced necessary conditions of optimality which reduce the initial MINLP problem to a sequence of linear problems. They define the conditions of optimality for a process key component as:

1. *Maximum outlet concentration*: all fresh water-using units reach their maximum possible outlet concentration.
2. *Concentration monotony*: at every process, the outlet concentration is not lower than the concentration of the combined water stream coming from all the precursors.

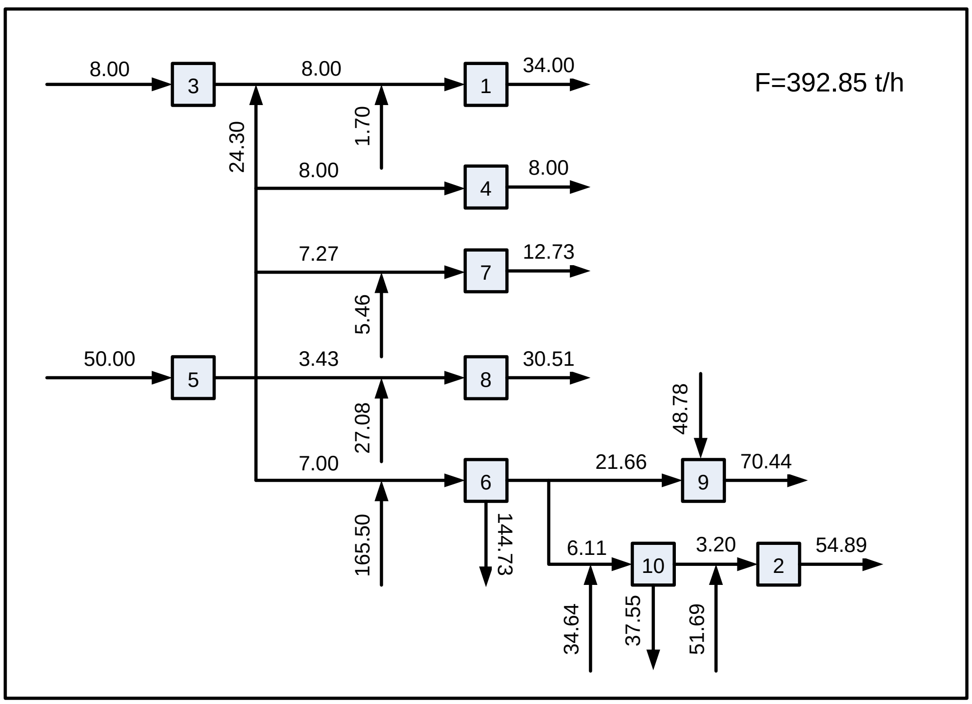


Figure 3. 11 Optimal solution for the water system test case, Savelski et al., 1999

A methodology based on combinatorial optimisation in which a tree searching technique with branch and bound procedure is used by author to solve a tree processes system which cover all possibilities. The optimal solution identified by Savelsky for this case study and guaranteeing as a global optimal solution is 392.85 t/h fresh water consumption. The topology of this network satisfying this optimal solution is presented in Fig. 3.11. This procedure guarantees optimal solution for all water-using units which are terminal units.

GA optimisation procedure, presented in paragraph 3.5, is used to recalculate the optimal network for this case study.

First of all, all the water units are ordered by "*mass load*" of contaminants (Lcrt criterion) which are transferred between process streams and water streams or by "*freshwater flowrates*" (Fcrt criterion) needed in the network. To order the network by Lcrt criterion, mass loads for all contaminants and all water-using units are compared to find the contaminant which has the biggest influence, Fig.3.12 .

Then, the contaminant with highest load at the network level is picked-up, then the graph is ordered putting first the unit with the lowest outlet concentration and last, the unit with the highest outlet concentration. As an exception, first water-using units of the graph should be those with the lowest contaminant limits.

In this case study (as in Fig.3.12), the contaminant C has the maximum mass load, so this contaminant determines the range, as in Table 3.3:

Table 3. 2 Units ranking after mass load criterion (Lcrt)

Water Unit Nr.	U3	U5	U6	U4	U1	U9	U7	U8	U10	U2
Mass load (kg/h)	0.16	1.75	2.50	0.48	4.59	4.00	0.60	8.14	9.00	520.80
$C^{out,max}$ (ppm)	20	35	90	120	180	200	220	300	800	9500

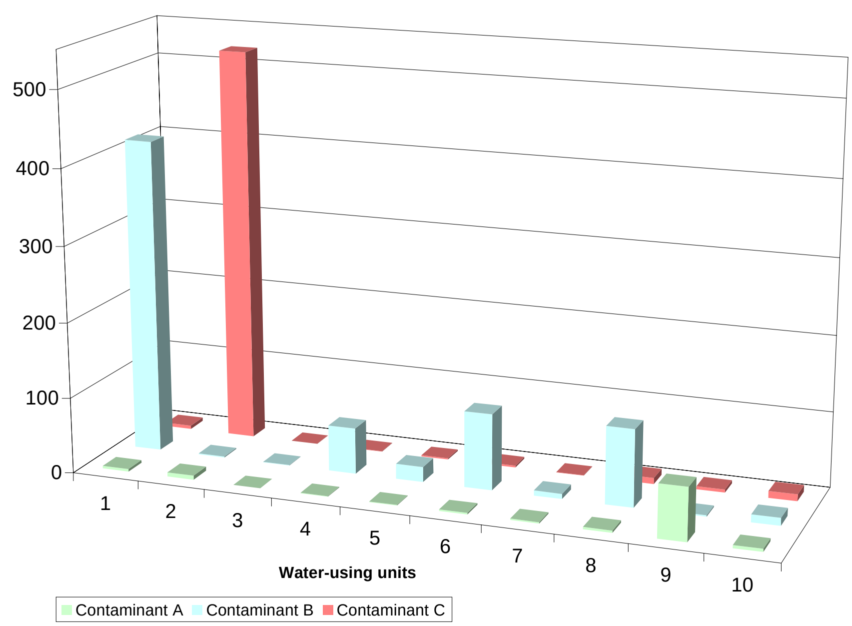


Figure 3. 12 Mass load of contaminants for each water-using unit

If the units are ordered by "*freshwater flowrate*" criterion, first calculate the sum of water flowrates which is needed to transfer each contaminant and then is made an ascending order of flowrates as in the following table:

Table 3. 3 Units ranking after freshwater flowrate criterion (Fcrt)

Water unit Nr.	U3	U4	U7	U10	U8	U9	U1	U2	U5	U6
C1 Flowrate (t/h)	8.00	8.00	14.40	44.44	31.57	70.92	34.00	56.00	50.00	33.33
C2 Flowrate (t/h)	8.00	8.00	8.83	25.12	25.87	0.68	34.00	1.43	50.00	251.75
C3 Flowrate (t/h)	8.00	8.00	3.00	12.33	32.56	20.51	34.00	56.00	50.00	35.71
$\sum$ Flowrate (t/h)	24	24	26.23	81.89	90.00	92.11	102.00	113.43	150.00	320.79

When applying the GA proposed optimisation procedure, the optimal topology presented in Fig. 3.13 is determined, for which the global minimum fresh water flowrate is 389.87 t/h, thus declassifying the previous optimal solution into a local optimum.

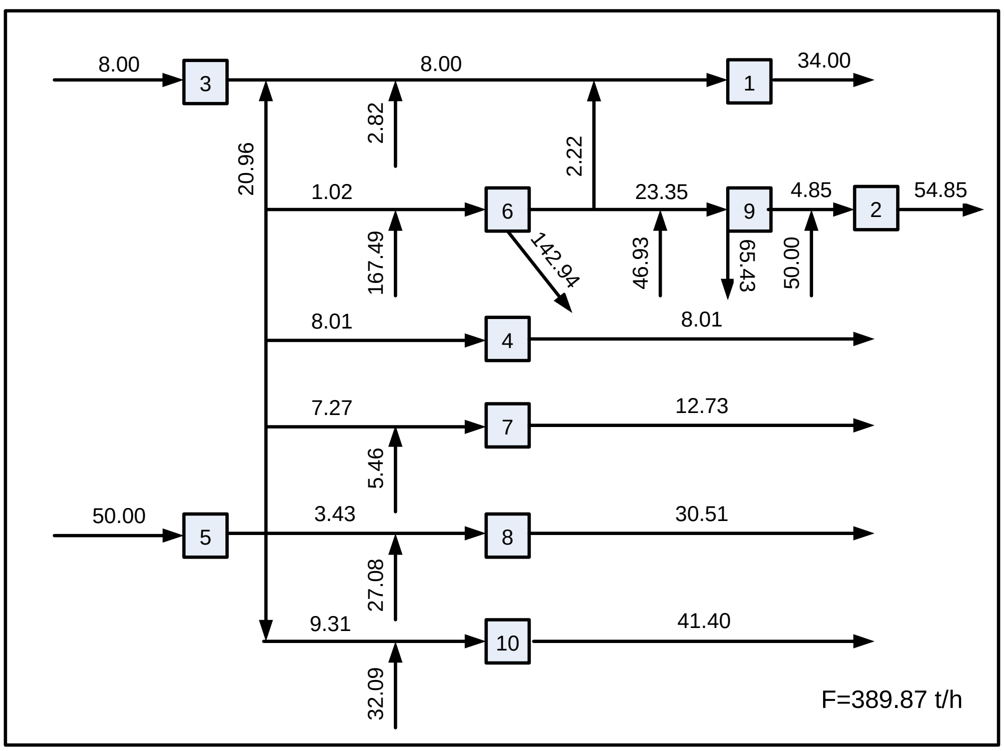


Figure 3. 13 GA optimal solution for the water system test case

Taking into account the stochastic nature of the GA, several replicates are made for this case, starting from different points, in order to be sure that the global optimum is achieved. These results are the same. Basically, the topology given by Savelski *et al.*,1999 is preserved, except the new connections between units 6 and 1, 9 and 2 and 5 and 10; also, the former connection between units 10 and 2 is broken. The solution found for this rather difficult test case proved the capacity to give good solutions of above presented optimisation procedure based on GA, observing, always, all the constraints associated to the network. The procedure is original being different on other approaches. The procedure is more effective because, as is presented in next paragraphs, more complicated case studies as tackled in literature can be solved easily.

3.7.2. Optimal design with minimum supply water flowrate

In this paragraph a case study illustrates the new solution methodology for design of water networks for oil refining and petrochemical sites. The results are published in Lavric et al., 2005. Optimisation criterion is minimisation of water supply flowrate.

Abbreviations used are given in Table 3.4.

Table 3. 4 Abbreviations of water-using units and contaminants oil refinery case study

Water using Units		Contaminants	
U1	Cooling Tower HAMON	C_1	Salts
U2	Cooling Tower MPX	C_2	Chlorine
U3	Cooling Tower RC2	C_3	Alkalinity
U4	Cooling Tower RC1	C_4	Suspended solids
U5	Cooling Tower CC	C_5	Organics
U6	Blowdown	C_6	Extractible
U7	Visbraking		
U8	Pumping		
U9	Washing		
U10	CDU+VDU		

Cooling towers are used within water cooling systems to reduce by evaporation the temperature of water used as cold utility. Evaporation of a fraction of water in air stream (in natural or forced circulation) provides cooling effect. Oil refineries use large number of cooling water streams which normally do not come into contact with oil product streams and contain less contaminants than units water streams. Almost all cooling water streams are recycled with a bleed (or blowdown stream) to keep specific contaminants in acceptable limits. Cooling water may contain chemical additives used to prevent scaling and biological growth in heat exchanger networks. Process water that is contaminated by direct contact with oil type products (in different mass transfer operations or in washing operations) accounts for a significant quantity of total oil refinery wastewater. Data for each water-using unit is given in Table 3.5.

Table 3. 5 Limiting data for industrial case study

	Contaminant	U1	U2	U3	U4	U5	U6	U7	U8	U9	U10
Mass load of contaminant, kg/h	C1	31.2	16.40	1.20	4.80	2.64	132.60	8.20	12.10	10.35	8.62
	C2	7.80	4.10	1.325	5.30	2.79	124.80	42.00	14.55	12.00	1.95
	C3	7.8	4.10	4.25	4.10	3.25	50.70	3.56	7.73	2.12	3.4
	C4	5.46	2.87	3.35	1.40	2.12	1.95	11.20	5.50	3.20	2.50
	C5	5.46	2.87	5.35	2.40	5.12	6.78	10.64	6.17	3.04	7.70
	C6	109.59	57.61	8.98	35.90	10.77	62.40	103.60	1.35	29.60	9.90
Limiting inlet concentration, ppm	C1	400	400	160	160	160	160	400	400	400	400
	C2	200	200	35	35	35	35	150	150	150	150
	C3	400	400	200	20	20	15	150	150	150	150
	C4	30	30	30	30	30	10	10	10	10	10
	C5	30	30	30	30	30	10	12	12	12	12
	C6	630	630	240	240	240	240	630	630	630	630
Limiting outlet concentration, ppm	C1	800	800	400	400	600	500	450	450	450	450
	C2	300	300	300	300	500	350	300	300	300	300
	C3	500	500	250	250	200	280	350	250	350	50
	C4	100	100	100	100	500	150	50	100	50	100
	C5	100	100	100	100	500	120	50	120	50	120
	C6	2235	2335	2135	2535	2735	400	1000	830	1000	730

Typical plants producing such effluents are: crude oil desalting, steam stripping, fractionator reflux drum drains and cleaning operations. Treatment of oil-contaminated wastewater usually involves separation of oil, water and solids by various physical and/or chemical processes. Many of these are sour water streams and are also subjected to treatment to remove hydrogen sulphide, carbon dioxide and ammonia. The influence of water supply contamination is analysed in this case study.

For each scenario, the units are ranked after two criteria: Fcrt and Lcrt, as presented above. In Table 3.6, limiting data for the available water supply sources are given.

Table 3. 6 Limiting data for contaminated water sources case study

	Contaminant	Source S1	Source S2	Source S3	Source S4
Limiting concentration for water sources, ppm	C1	0	160	20	400
	C2	0	30	20	150
	C3	0	15	15	150
	C4	0	10	8	30
	C5	0	10	6.5	30
	C6	0	240	140	630

3.7.2.1. Scenario A – freshwater source

In the first scenario, I consider that water supply is fresh, non-contaminated. No losses are taken into account. Freshwater supply flowrate, without water reuse, is 955.8 t/h. The presence of 6 contaminants generates a highly NLP problem. The results of optimisation are presented in two formats to underline the advantage of new (original) graphical format described in paragraph 3.6. Data file is prepared with a such structure accepted by the dedicated software to implement GA: number of units, number of contaminants, mass loads matrix (units x contaminants), inlet maximum concentration matrix (units x contaminants) and outlet maximum concentration matrix (units x contaminants), as presented in Annex 3. The importance of ordering criterion Lcrt or Fcrt is discussed.

Mass load criterion (Lcrt) - if water-using units are ordered by *mass load of contaminant* the optimum flowrate from water source is 832.2 t/h instead of 955.8 t/h (for base case - no water reuse). The water network, reuses 191.4 t/h from different units, which are not restricted by contaminant inlet concentrations. In Fig.3.14, water reuse streams are presented:

From unit 3 $\rightarrow$ 4, 6, 7

From unit 7 $\rightarrow$ 8, 10, 6, 1, 2

From unit 9 $\rightarrow$ 10, 6, 5

From unit 6 $\rightarrow$ 1, 2

As direct consequence freshwater saving is about 13%.

Freshwater consumption criterion (Fcrt) - if water-using units are ordered by *freshwater consumption*, the optimum flowrate from the source is 899.8 t/h, instead of 955.8 t/h (for base case - no water reuse), obtaining about 6% fresh water saving, reported to base case.

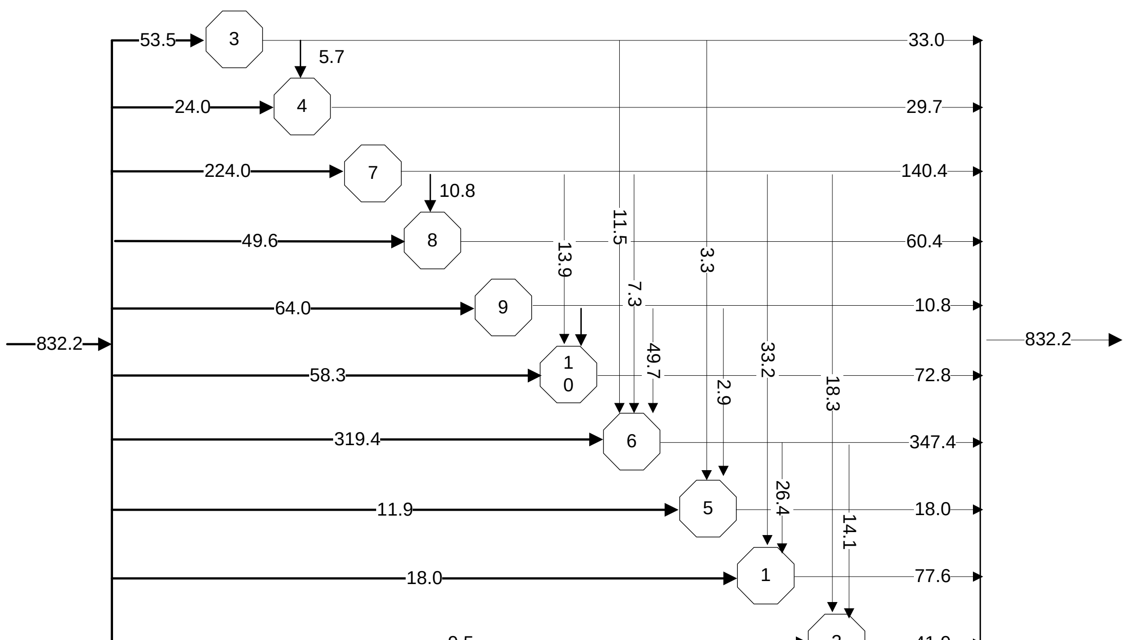


Figure 3. 14 GA optimal solution for the water system, Scenario A- Lcrt criterion

Network topology is presented in Fig.3.15. Reuse is produced by following streams :

From unit 4 $\rightarrow$ 2, 1

From unit 3 $\rightarrow$ 6

From unit 10 $\rightarrow$ 8, 7

It is important to notice that water-using units ranking criterion (to generate oriented graphs) is quite significant to get optimal topology and water consumption as presented in Fig.3.14 and Fig.3.15 due to the complexity of the problem. For the ranking criteria, fresh water saving difference is not very big (about 7% from the total flowrate 67.6 t/h), but topology is different.

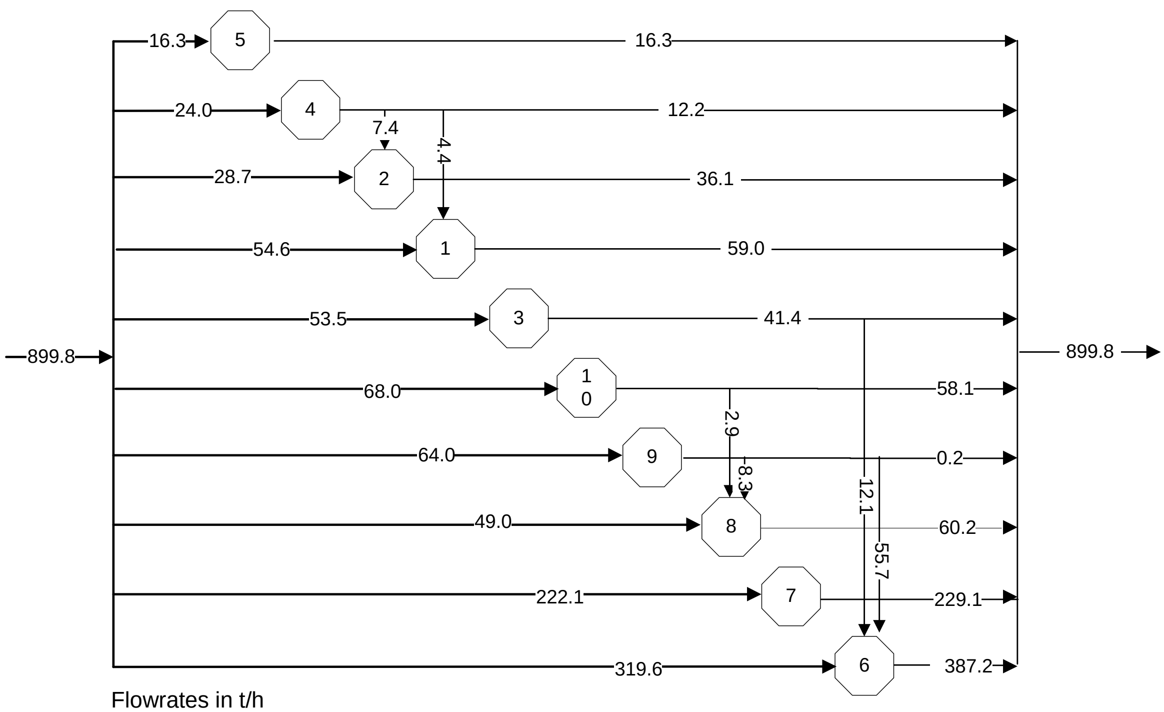


Figure 3. 15 GA optimal solution for the water system, Scenario A- Fcrt criterion

This suggests that for taking decisions in practical cases other optimisation criteria should be addressed (economic, topological) and results compared. It should be noted as well that the change in network topology - the gain in fresh water is compensated through a higher degree of internal water reuse.

When network topology is very complicated, there are a lot of connections between units. Water re-use involves introducing additional pipes, the connection system being quite difficult to visualise in traditional representations. Regarding the visualisation of analysis results for this case study it is to notice that different topologies are not easily to read (Fig.3.7). For this reason, these topologies are illustrated with my original representation of water-using network proposed in this work (Iancu et al., 2007). Using concepts introduced in Figs.3.8 and 3.9, the water network can be drawn like in Fig.3.16 (for “mass load” criterion - Lcrt) and Fig.3.17 (“freshwater consumption” criterion - Fcrt).

In this representation it is very easy to identify the water sources, the types of streams (from source, reused water or wastewater to treatment), to check the mass balance around each water using unit and around the whole network. Different scenarios for re-using water are easier to analyse. In this case study, each water unit is fed by freshwater, some of them produce wastewater streams which are sent to

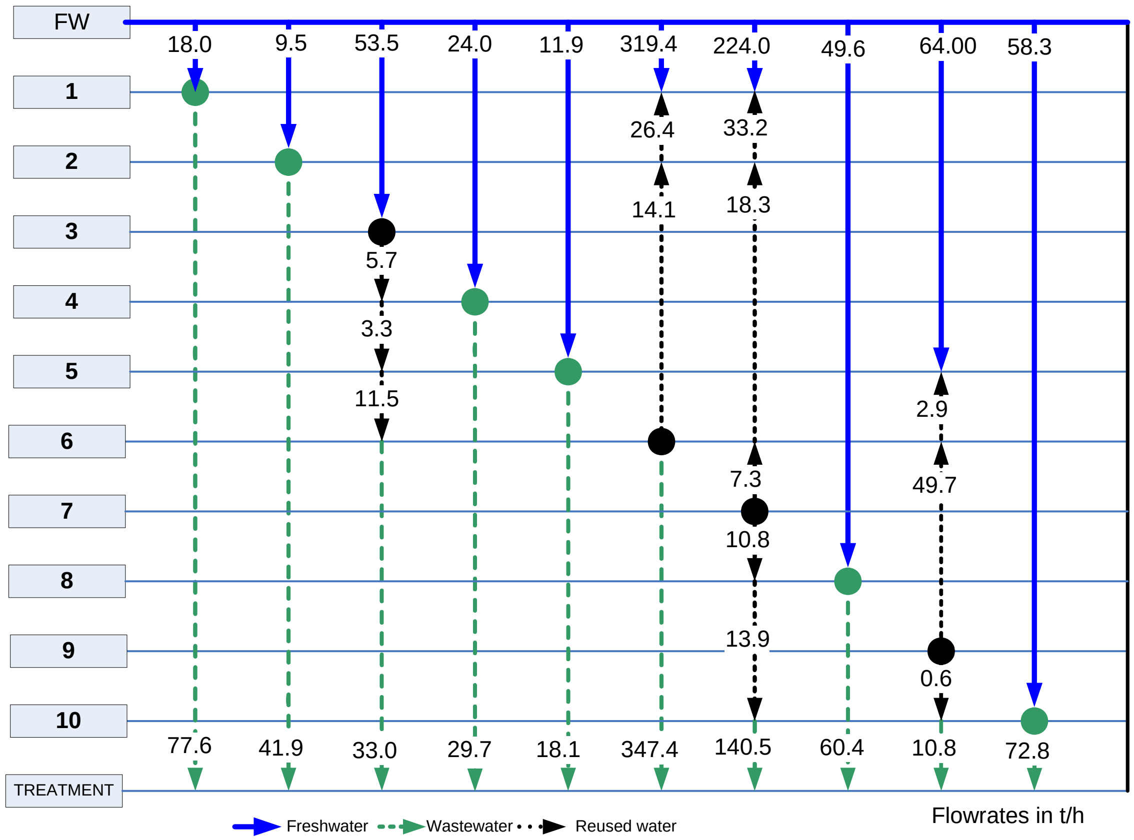


Figure 3. 16 New representation of GA optimal solution for Scenario A- Fcrt criterion – S1

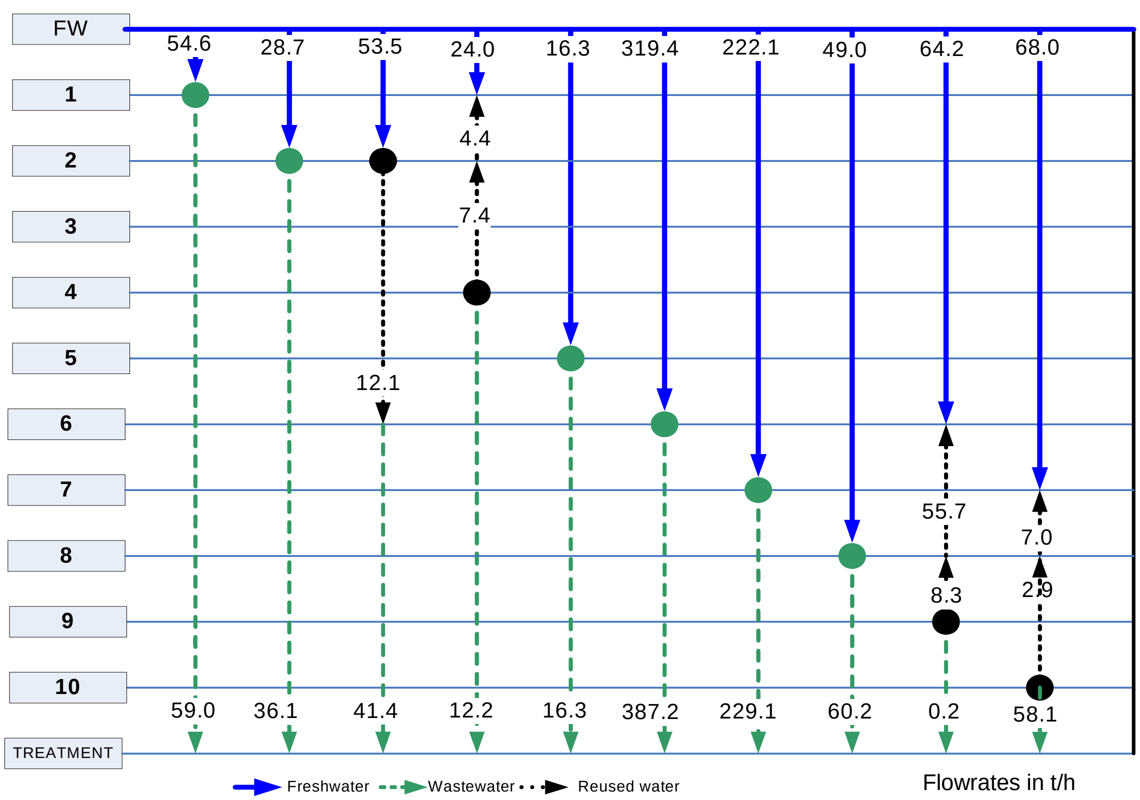


Figure 3. 17 New representation of GA optimal solution for Scenario A- Lcrt criterion – S1

treatment unit (U1, U2, U4, U5, U8, U10). Effluents from some units (U3, U6, U7, U9) are reused or sent to treatment. The reusing effluents policy can be seen very well from this representation, so each solution can be easily ranked. Some economical or technological constraints can be taken into account for this choice.

3.7.2.2. Scenario B – Influence of water supply source contamination

Sometimes, the complexity of the nonlinear mathematical model, combined with difficulty to solve it, especially when there are multiple contaminants and many restrictions, impose linearisation as an alternative technique (Bagajewicz, 2000; Wang *et al.*, 2003). Availability of multiple water resources, with different degree of contamination, creates some difficulties to choose which water supply to be used. Same case study can be solved, with GA as optimisation approach, when several water resources are available. As in the case of contaminant-free water supply, an optimal water network for minimum water flowrate will be determined, keeping same data (10 unit operations, six contaminants and same limiting compositions, as in Table 3.5. Four water sources are available with contamination level shown in Table 3.6. Analysing the input restrictions, it is easy to notice that Source 4 cannot be used alone to feed all water using units, since its contamination level is higher than the inlet maximum accepted contamination for some units. So, it has to be used jointly with one of the other three water sources. As the level of contamination of the supply water increases, the mass transfer driving force for each water using unit decreases together with its degrees of freedom at inlet. Uncontaminated supply water can be used to diminish the pollution level of the water stream from water using unit u_i, allowing the reuse of some streams coming from previous water using units, even if their exit concentrations are higher. As the contamination level of the supply water increases, up to the inlet restrictions, less and less reused water can be used to make-up the inlet stream of the water unit operation u_i. So, the topology tends to stiffen up to the point where there is no internal reuse, when the contamination level of the supply water equals the inlet restrictions for each and every unit.

When contaminated supply water is used, finding optimal solution hardens, several approaches being possible:

- To use one contaminated water supply at the time and to keep the optimum-so-far solution,
- To use all the available sources, supplying, first, the units with the input limits equal to the existing contaminant level, or

- To decouple the original problem into sub-problems, based upon the available water resources and accepted level of input contaminants for several units, then to reunite the local solutions.

In this scenario, I apply the methodology to determine the optimum network for minimum water flowrate, separately, with supply water from sources S2, S3 and S4 to underline the contamination influence on water network topology.

When Source S2 is used, the optimal solution for water network is degenerated (as presented in Fig 3.18), since no internal reuse is possible, due to the match between the inlet restrictions and the contamination level of this supply water. Water flowrate increases, with 231.1 t/h (when Fcrt ranking criterion is used), due to water source contamination level.

When Source S3 is considered as supply source (this is less contaminated as Source S2), the topology is a little bit modified, as presented in Fig. 3.19. 46.5% from effluent water of unit 6 is reused in other units: U1, U2, U3, U4, U7, U8, U9. It is possible to conclude that Source S3 can be used alone as water supply. Reuse strategies can be noticed.

Water Source S4 cannot be used alone as supply water source for this network, as mentioned above (water using units U3, U4, U5 and U6 have concentration limit for 1st contaminant at 160 ppm). So this source cannot provide alone feasible solution. In this respect a combination between Source S2 and Source S4 is presented in next paragraph.

In conclusion, for one water source, internal water reuse increases from no-reuse when Source S1 is connected (Fig. 3.16 and Fig. 3.17) to intensive water reuse when Source S3 is connected, Fig. 3.19. No water re-use when connecting Source S2. The network is stiffened, as presented in Fig.3.18. When the contamination level of water supply increases, water flowrate increases too, to compensate mass transfer driving force decrease for each water-using unit.

In the case of Source S3, whose contamination level is intermediate, between Source S1 and Source S2, the decrease in the driving force is balanced by an increase of network internal complexity (for water reuse and flow).

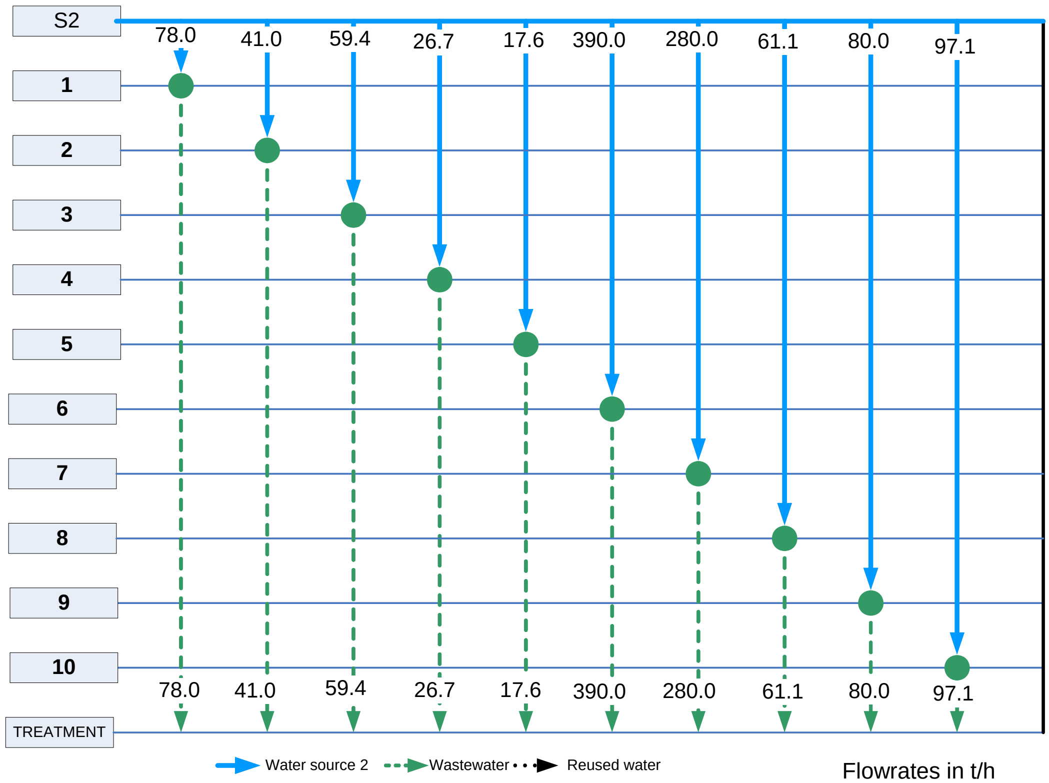


Figure 3. 18 GA optimal solution for Scenario B – Fcrt criterion – S2

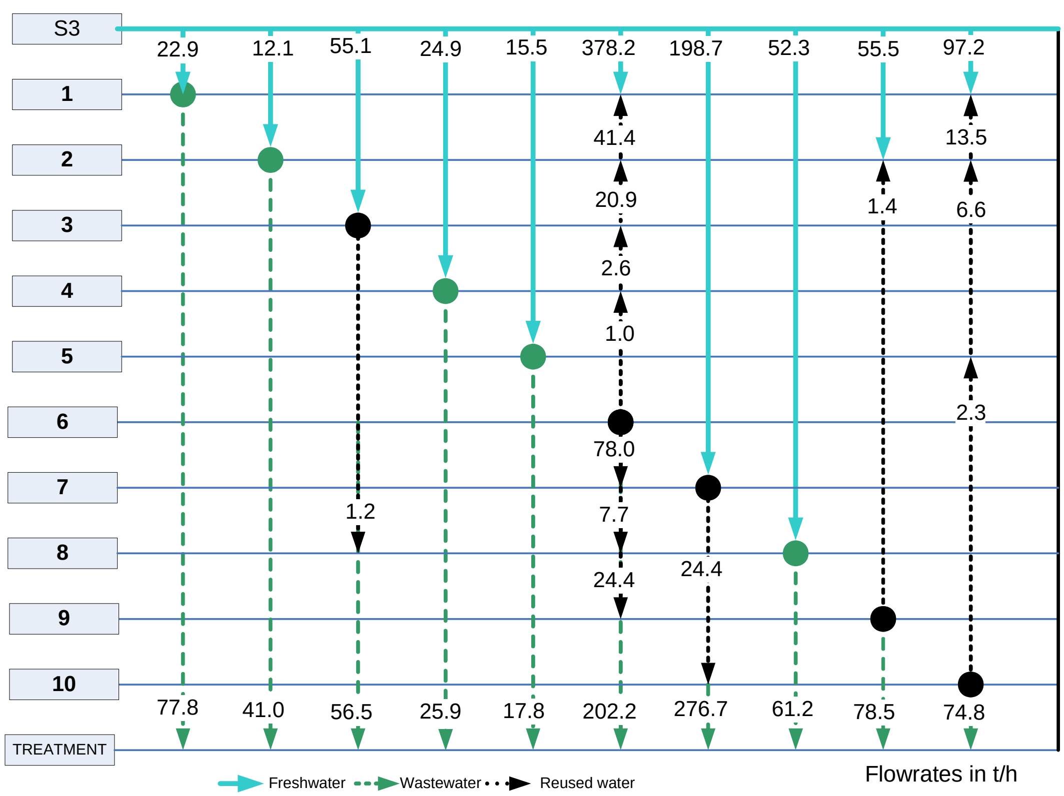


Figure 3. 19 GA optimal solution for Scenario B - Fcrt criterion - S3

3.7.2.3. Scenario C – multiple supply water sources

Under the imperative of reducing the operating costs, while reducing fresh water consumption, the best strategy is to jointly use two or more water supply sources, allocated corresponding to their contamination level. When using multiple supply sources, the software computes the difference between inlet imposed concentration level for each water using unit and the contaminant supply source level. The source with the minimum positive difference is allocated for the given unit operation. Thus, the most contaminated sources are used first and the less contaminated sources are used only when really needed, thereby decreasing the supply water costs.

Based upon this strategy, I present the optimal topology of water network when two or more sources can be combined. Considering possibility to combine any of the four sources, as expected, the preferred sources (since they are the closest to inlet restrictions for water using units and cheapest), Source S2 and Source S4, are selected. The optimal result is represented in Fig. 3.20.

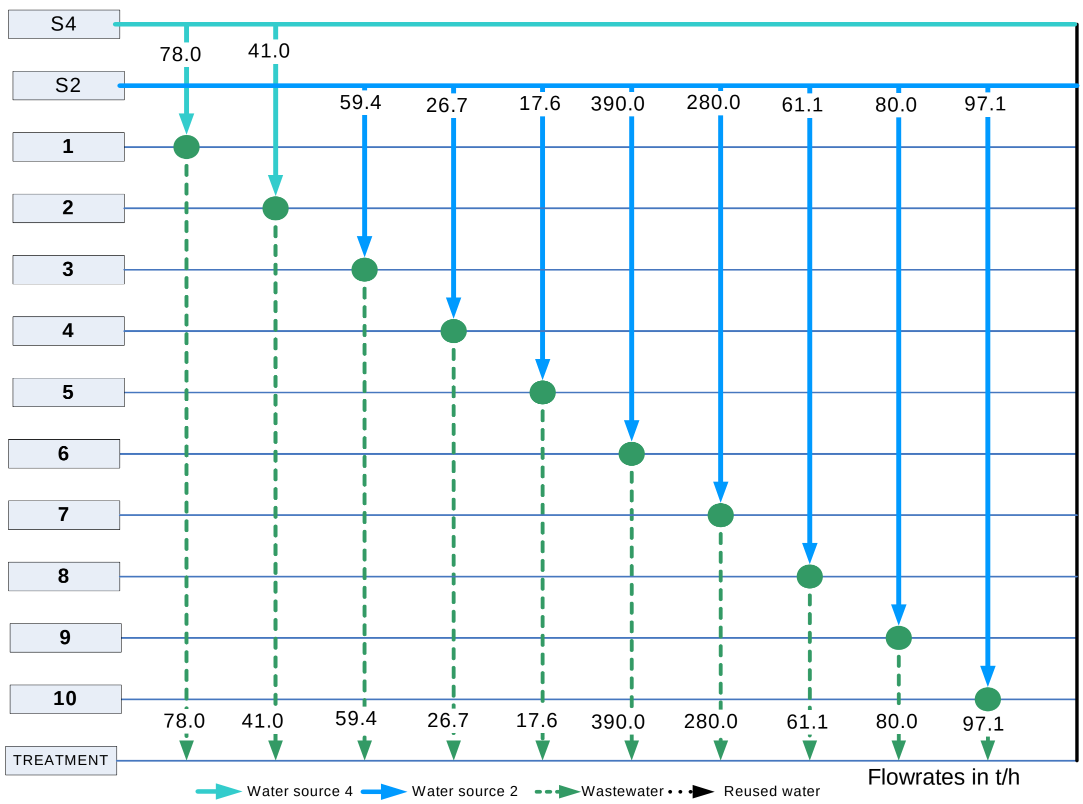


Figure 3. 20 GA optimal solution for Scenario C - Fcrt criterion S2 & S4

Optimal water network topology is again degenerated, no water re-use is acceptable due to global high level of contamination of water sources. The drawback is that, again, the network is made less flexible; no water reuse is possible, since the supply water matches the inlet restrictions. For the cases when the match is not complete, the difference, in terms of concentrations, is sufficiently small to avoid the possibility of any water reuse, due to the large contaminant concentrations coming from previous units. The water networks depicted in Figs.3.17 and 3.18 have the same topology, because the water from the most polluted source is used only for units U1 and U2. These water streams have enough mass transfer potential to completely remove the contaminants as water streams from Source S2.

3.7.3. Large scale water network with multiple supply sources

Integrated oil refining site is composed of very complex processes, exchanging materials, energy and water. The aim of oil refining processes is to separate different organic compounds from the crude oil and to convert lower value compounds into high value ones. The general order of processing is desalting, primary distillation, and secondary processing (i.e., cracking, treating, reforming, sulphur removal, hydrogenation, isomerisation, etc.). Desalting is a washing process where water is added to the crude, mixed and then separated to remove salts, clay and other suspended particles. Distillation involves heating the crude so that different fractions (compounds that boil at different temperatures) can be separated. Special equipment and technologies allow to separate well defined fractions (gasoline, fuel jet, diesel, etc). Many different products result from oil refining: petroleum products with different quality; products with enhanced value because of the addition of other compounds, etc. Secondary processing generally involves thermal treatment and/or the use of catalysts and/or hydrogen to convert in high value products lower quality petroleum fractions. Wastes are generated throughout the refinery processes. Major waste streams include process wastes (e.g., wastewaters from desalting operations, spent catalyst from refining processes), equipment cleaning wastes (e.g., sludge from tank cleaning) and wastewater treatment wastes.

In a typical oil refinery, water is a major element in process integration, being used either as heat utility (steam production and cooling agent in heat exchanger networks) or as mass separation agent (removes contaminants from process streams). At its turn, steam can be used as heating agent, power agent in steam turbines and mass separation agent (for stripping in direct contact with process streams). Water effluents are loaded with different contaminants as: inorganic or organic compounds, salts, suspended solids, biodegradable compounds. Contaminants are removed from wastewater streams in an “end of pipe” manner in special treatment facilities. Effluents of treatment units which observe legal regulations can be discharged into environment (rivers, lakes, etc). In process operations and heat utility systems an important quantity of water is lost in environment by evaporation or by accidental loses and cannot be recovered, these amounts are taken from water sources as make-up.

3.7.3.1. Water streams

On oil refinery site analysed in this paragraph the following types of water streams are identified :

- Water process streams (technological water) to be involved in chemical reaction systems (as reactant or as solvent) or in mass transfer operations (liquid-liquid extraction, distillation, absorbtion/desorbtion)
- Wastewater streams (effluents) after water being in contact with process steams (oil product from desalination or washing tanks, acid water from neutralization, etc)
- Unusable water streams – cannot be reused (from chemical reaction, from evaporation)
- Heat utility agents in heat exchangers: steam condensation or cooling water as well as cooling agent for pumps
- Power agent in turbines and liquid pumps
- Mass separation agent for purification of products or environment (in absorption, liquid-liquid extraction, washing, etc)
- Other water streams (rain water, drinking water, accidental runaways, etc).

In Fig.3.21 I present the ratio for different types of water streams for the site water system taken into account.

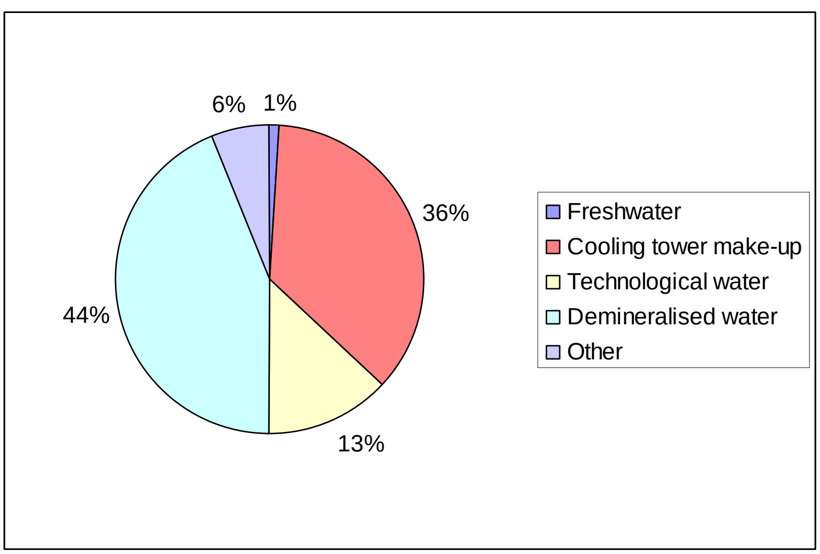


Figure 3. 21 Using ratio of water streams in refinery

3.7.3.2. Contaminants

Environmental protection issues are very important for oil refinery operation. Legislation and safety/health regulations compliance involve important costs which become critical now when oil price and other costs escalate rapidly. Oil refineries produce a wide range of water effluents with high degree of hazard to the environment. Some of these contaminants come with crude oil, while others result in oil refinery processes and secondary operations. Waste water typically contains hydrocarbons, dissolved materials, suspended solids, hazardous organic compounds (as phenols), inorganic compounds (as ammonia, sulphides, acids, alkalis, metal ions) and other contaminants. Carbon dioxide loaded waters are also to be taken into account especially for climate change concerns. There is also the risk of accidental spills and leaks for a wide range of flammable, hazardous and highly toxic chemicals.

For the system analysed, there were identified as highly significant following contaminants, which are presented in the process effluents, as presented in Table 3.7:

Table 3. 7 List of identified contaminants on studied oil refinery site

Abreviation	Contaminant
C1	Salts
C2	Chlorine
C3	Alkalinity
C4	Suspended solids
C5	Organics
C6	Extractibles

3.7.3.3. Water network

On oil refinery site there are a lot of units which use water from different sources and produce important number of wastewater streams. There are identified as highly significant 15 water using units (as abbreviated in Table 3.8). Four different water sources with different contamination level and unit costs are presented in Table 3.9. So, underground water is the most expensive water source and decarbonated water is the cheapest one. For optimisation strategy it is better to identify which supply source can be used from economical and technological point of view.

The topology of water network for the refinery site is presented in Fig. 3.21.

On the site there are three cooling towers (denoted LOB, FCC and CD) which use water as cooling agent to remove heat from heat exchanger network allocated to each tower.

Table 3. 8 Abbreviations of water units on an oil refinery site

U1	FCC cooling tower	U11	Propane Deasphalting
U2	CD cooling tower	U12	Hydrobon
U3	LOB cooling tower	U13	Bitumen unit
U4	Demineralisation	U14	Sodium sulphite
U5	Storage facilities	U15	Demercaptanisation
U6	Crude distillation unit	S1	Underground water
U7	Gas fractionation	S2	River water
U8	Gasoline hydrotreating	S3	Decarbonated water
U9	Gasoil hydrotreating	S4	Lake water
U10	Visbreaking		

Table 3. 9 The contamination level and unit costs for the available supply water sources: S1-underground water, S2-river water, S3-decarbonised water, S4- lake water

Contaminant \ Water supply source		S1	S2	S3	S4
Contaminant level (ppm)	C1	0	2	31	9
	C2	0	3	16	8
	C3	0	5	24	3
	C4	0	2	30	6
	C5	0	3	28	5
	C6	0	5	27	9
Price ($/t)*		0.56	0.20	0.05	0.25

* Romanian Agency for Foreign Investment, 2005

Significant amount of effluents is purged to avoid the accumulation of contaminants. These water streams are possible new sources of water to be reused in site water network. To cover water purges and evaporation flowrates, each cooling tower receives a certain flowrate of supply water which is mixed with recycled water (make-up). The other water using units use huge amounts of water and there are no reuse options, so the effluents from these units can be also sources in reuse strategy. The water streams from Drinking Water, Fire Brigade System and Tank Washing are not considered in analysis because there are small possibilities to recover these streams. The effluents from cooling tower are mixed together and sent to treatment unit and then discharged into environment. The other effluents are sent directly to environment.

Process integration methodology presented in this thesis aims to find the optimal water network from economical or technological point of view using limiting data for contaminants imposed at the entrance and at the exit of water-using units (Table 3.10).

Table 3. 10 Limiting data for oil refinery water network case study

	Contaminant	U1	U2	U3	U4	U5	U6	U7	U8	U9	U10	U11	U12	U13	U14	U15
Mass load of contaminant, g/h	C1	2,303	160	9,100	2,640	7,020	2800	400	390	300	600	150	150	40	10	30
	C2	7,350	320	11,900	1,200	4,680	700	100	260	540	400	150	50	40	10	20
	C3	490	40	2,100	5,760	11310	2450	350	572	3400	400	150	50	40	10	20
	C4	6,085	15,200	15,750	2,160	7410	3150	450	520	1800	1800	600	200	160	40	40
	C5	1,470	160	1,400	288	390	350	50	0	200	200	0	50	40	10	10
	C6	0	0	7	0	7800	25	2	3	2	2	6000	750	800	100	200
Limiting inlet concentration, ppm	C1	300	130	150	150	150	140	130	130	130	130	120	130	120	120	130
	C2	120	110	120	120	120	85	85	85	110	85	80	80	80	80	85
	C3	32	30	35	40	100	40	40	35	60	30	30	30	30	30	30
	C4	300	270	300	300	240	220	220	210	220	220	215	215	215	215	215
	C5	20	15	25	15	22	22	23	20	22	22	22	22	22	22	22
	C6	0	0	0	0	100	2	5	1	1	1	100	20	20	20	25
Limiting outlet concentration, ppm	C1	600	150	250	350	300	200	200	150	150	150	130	150	130	130	150
	C2	250	140	250	200	200	100	100	100	150	100	90	90	90	90	100
	C3	40	35	60	200	320	100	100	74	200	50	40	40	40	40	50
	C4	435	310	435	450	400	300	300	250	300	300	250	250	250	250	250
	C5	40	30	40	34	30	30	30	20	30	30	30	30	30	30	30
	C6	10	10	10	10	2,000	5	10	10	10	10	400	150	200	100	200

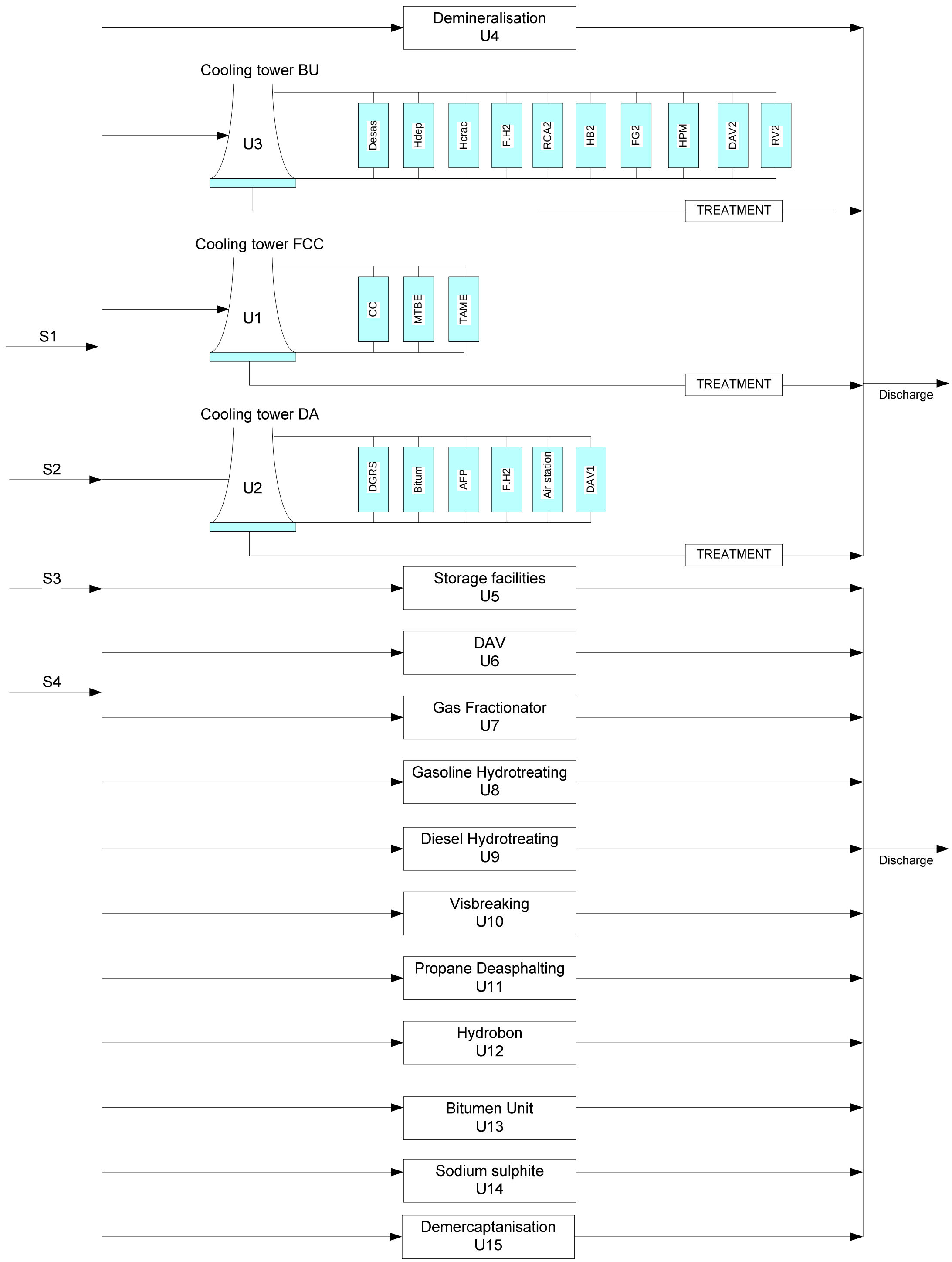


Figure 3. 22 Water network in oil refinery

Desas – Desasphalting
CC – Catalytic Cracking
DGRS – Sulphur Removing Unit
Hcrac – Hydrocracking
F.H2 – Hydrogen Unit
RCA2 – Catalytic Reforming
HB2 – Naphta Hydrotreating
HPM – Diesel Hydrotreating
FG2 – Gas fractionation plant

DAV1, DAV2 – Crude distillation unit
RV2 – Visbracking unit
MTBE – MTBE unit
AFP – Storage facilities

3.7.3.4. Existing situation - each unit is fed by freshwater only, no water reuse

Analysed industrial water network uses only freshwater as water source and there is no reuse strategy. Consequently, the network topology is very simple as drawn in Fig.3.23. The maximum amount of freshwater needed to satisfy this network is 1198.8 t/h, as presented in Table 3.11. From this amount, 326 t/h is lost, due to evaporation in the cooling towers and 872.8 t/h is send to treatment unit. This is the maximum amount of freshwater needed, so, some solutions are requested by site management team to reduce water consumption considering reuse strategy. For this reason, in following paragraphs, I propose some optimisation scenarios as illustration of the methodology developed in paragraph 3.3, based on GA. Minimum supply water consumption is calculated and associated topology is drawn for the two ranking criteria (Lcrt and Fcrt).

Table 3. 11 The maximum fresh water for each unit – existing situation

Original water unit	Maximum freshwater flowrate (t/h)	Losses (t/h)
U1	199.5	126.0
U2	400.0	20.0
U3	296.7	180.0
U4	36.0	-
U5	58.5	-
U6	58.3	-
U7	40.0	-
U8	19.5	-
U9	25.0	-
U10	30.0	-
U11	20.0	-
U12	7.5	-
U13	5.0	-
U14	1.3	-
U15	1.5	-
Total flowrate (t/h)	**1198.8**	**326.0**

3.7.4. Optimisation of water network

Based on different strategies of ranking water-using units and supply water sources, the following optimisation scenarios are studied to determine minimum flowrate of supply water sources for the large industrial site presented in paragraph 3.7.3.

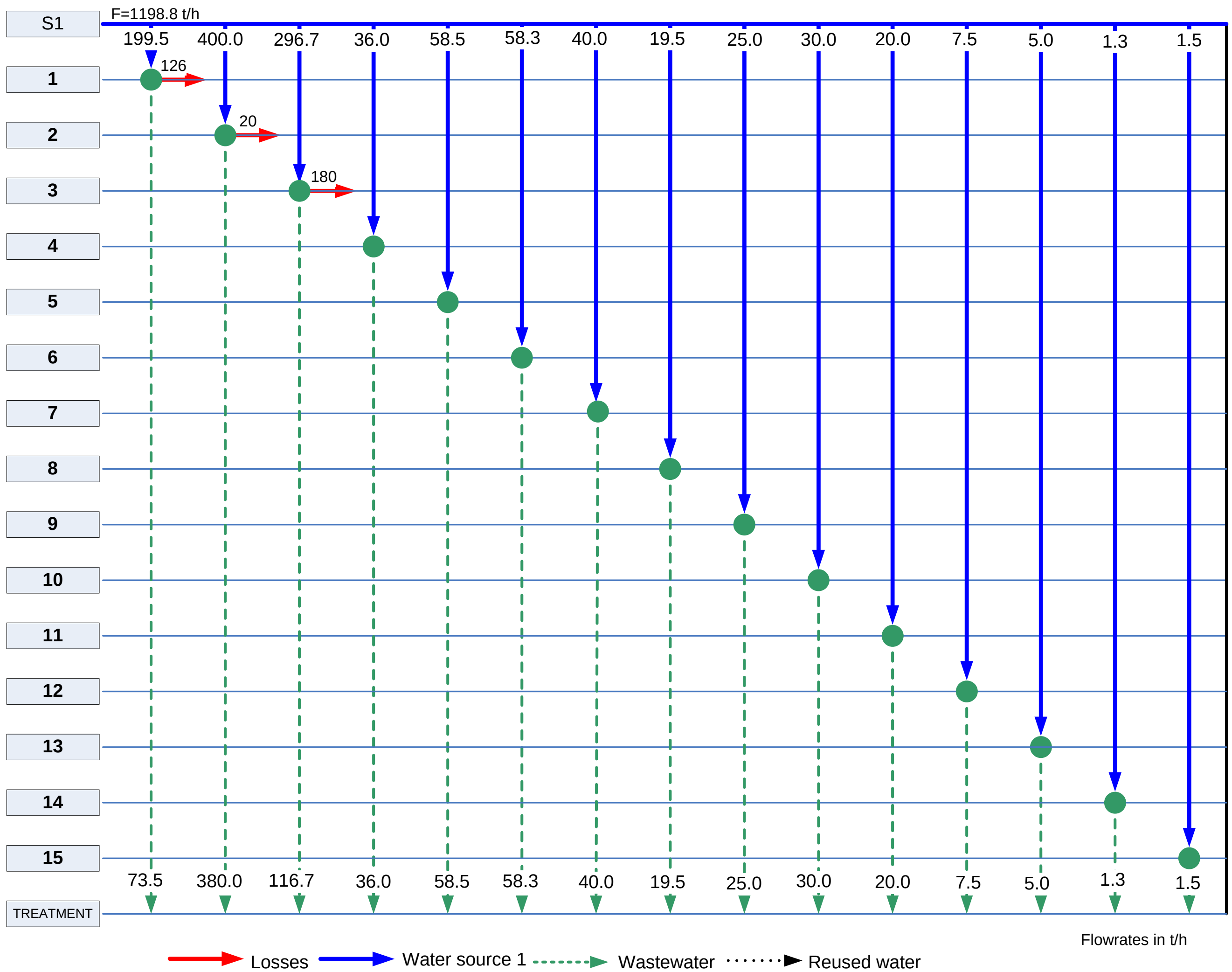


Figure 3. 23 Existing network topology: Freshwater source only

As I present in Table 3.9 four water supply sources are available on the industrial site. The existing water network uses just the freshwater source which has however a limited capacity. To allow new extension on the site the other three sources should be considered as well. The scenarios present the possibilities to reduce the freshwater flowrate and the influence of contaminated water sources on water network topology. The scenarios are formulated as optimisation problems with objective function flowrate of supply water (paragraph 3.4.1). In Scenario A only freshwater supply S1 is considered. When more water supplies are chosen water unit operations can be grouped in clusters. In Scenario B two supply sources (S1&S2) are considered, in Scenario C additional supply source is taken into account (S1&S2&S3) and finally in Scenario D all supply sources are considered (S1&S2&S3&S4). For each scenario relevant variables are calculated: minimum freshwater flowrate, minimum wastewater flowrate and reused water flowrate for each water-using unit. Based on these variables, water network topology is drawn and water balance table can be created.

3.7.4.1. Optimisation Scenario A: Freshwater source

a) Ranking water network

First step in optimisation strategy is to rank the water-using units to obtain the oriented graph associated to water network. As presented above, I propose two ordering criteria: by mass load of contaminants (Lcrt) or by freshwater usage to remove entire amount of contaminants from process streams (Fcrt). Despite the fact that sometimes different results can be obtained applying these criteria, both results can have practical importance in well established real situations. In Table 3.12, water-using units ranking (automatically generated by GA application software) and water source allocation for each water-using unit (only freshwater for this scenario) are presented.

Table 3.12 Allocation of water sources for ordered water network: Scenario A (Freshwater source)

Original water unit		Fcrt		Lcrt	
		Ranking water units	Allocated water source	Ranking water units	Allocated water source
U1		U1	S1	U1	S1
U2		U3	S1	U3	S1
U3		U9	S1	U9	S1
U4	corresponds to	U5	S1	U8	S1
U5		U13	S1	U7	S1
U6		U4	S1	U13	S1
U7		U15	S1	U10	S1
U8		U10	S1	U12	S1

U9	U11	S1	U6	S1
U10	U14	S1	U14	S1
U11	U8	S1	U2	S1
U12	U7	S1	U11	S1
U13	U12	S1	U15	S1
U14	U6	S1	U4	S1
U15	U2	S1	U5	S1

I notice that each criterion produced different water-using units ranking. The results of optimisation methodology described in paragraph 3.5 are presented below

b) Total supply water flowrate

Table 3.13 Minimum water source flowrate per water-using units: Scenario A (Freshwater source S1)

Water-using unit	**Minimum flowrate Source S1 (t/h)**	
	Fcrt	**Lcrt**
U1	131.9	131.9
U2	70.5	69.9
U3	204.5	204.5
U4	0.0	0.0
U5	0.0	0.0
U6	0.0	4.7
U7	28.5	30.9
U8	1.7	5.7
U9	2.0	2.0
U10	0.0	0.4
U11	0.7	0.0
U12	0.0	1.3
U13	0.0	0.8
U14	0.4	0.7
U15	1.9	0.0
Total flowrate (t/h)	**442.1**	**452.8**

c) Total wastewater flowrate

Table 3.14 Wastewater flowrate per water-using units: Scenario A (Freshwater source S1)

Water-using unit	**Minimum wastewater flowrate (t/h)**	
	Fcrt	**Lcrt**
U1	0.0	0.0
U2	51.0	20.5

U3	0.0	0.0
U4	0.4	17.0
U5	0.0	8.9
U6	40.1	35.0
U7	0.2	30.4
U8	0.1	0.1
U9	0.0	0.0
U10	1.6	0.2
U11	3.9	2.5
U12	17.2	0.0
U13	0.3	0.2
U14	1.0	2.5
U15	0.3	9.5
Total flowrate (t/h)	**116.1**	**126.8**

d) Total reused water flowrate

Table 3.15 Reused water flowrate for each water-using unit: Scenario A (Freshwater source S1)

Water-using unit	Reused water flowrate (t/h)	
	Fcrt	Lcrt
U1	0.0	0.0
U2	0.5	0.0
U3	0.0	0.0
U4	2.6	17.0
U5	0.3	8.9
U6	40.1	32.5
U7	6.4	2.0
U8	8.9	5.0
U9	0.0	0.0
U10	3.8	3.1
U11	5.6	10.6
U12	19.7	16.2
U13	2.0	1.4
U14	4.9	6.0
U15	3.5	9.5
Total flowrate (t/h)	**97.8**	**112.2**

e) Savings of supply water

If reused water is allowed, when the water network is fed by only one water source (freshwater S1), the minimum supply water flowrate for the network has different values for each criterion (Fcrt - 442.1 t/h vs Lcrt - 452.8 t/h). Consequently, 62-63 %

savings is obtained, compared to existing topology presented in Fig. 3.23. It is important to notice that important amount of water is lost by evaporation in cooling towers (326.0 t/h). The distribution of minimum supply water flowrate for each water-using unit is presented for Fcrt criterion in Fig.3.24.

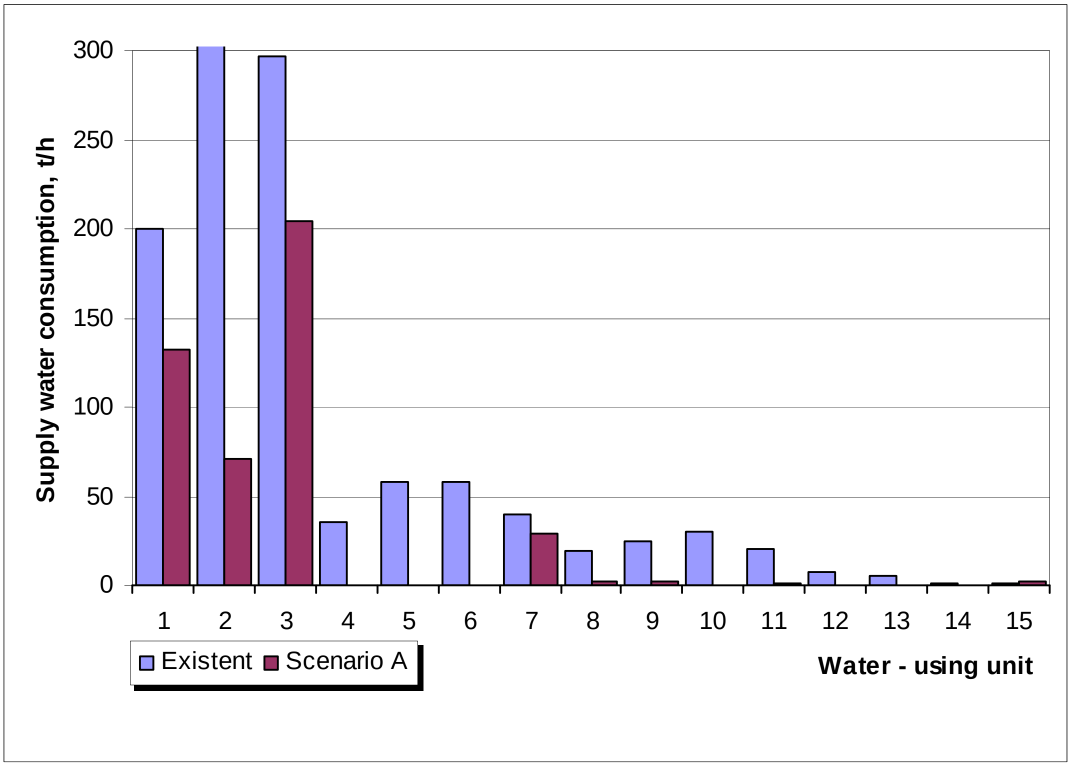
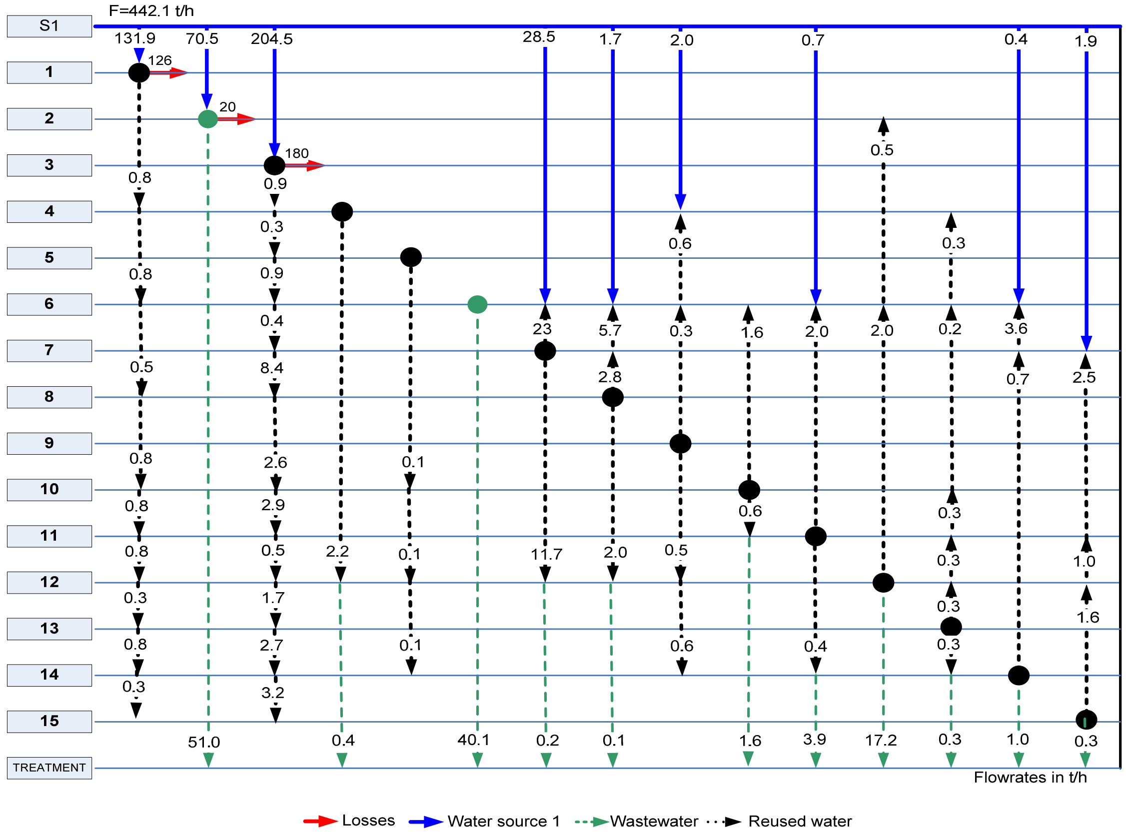
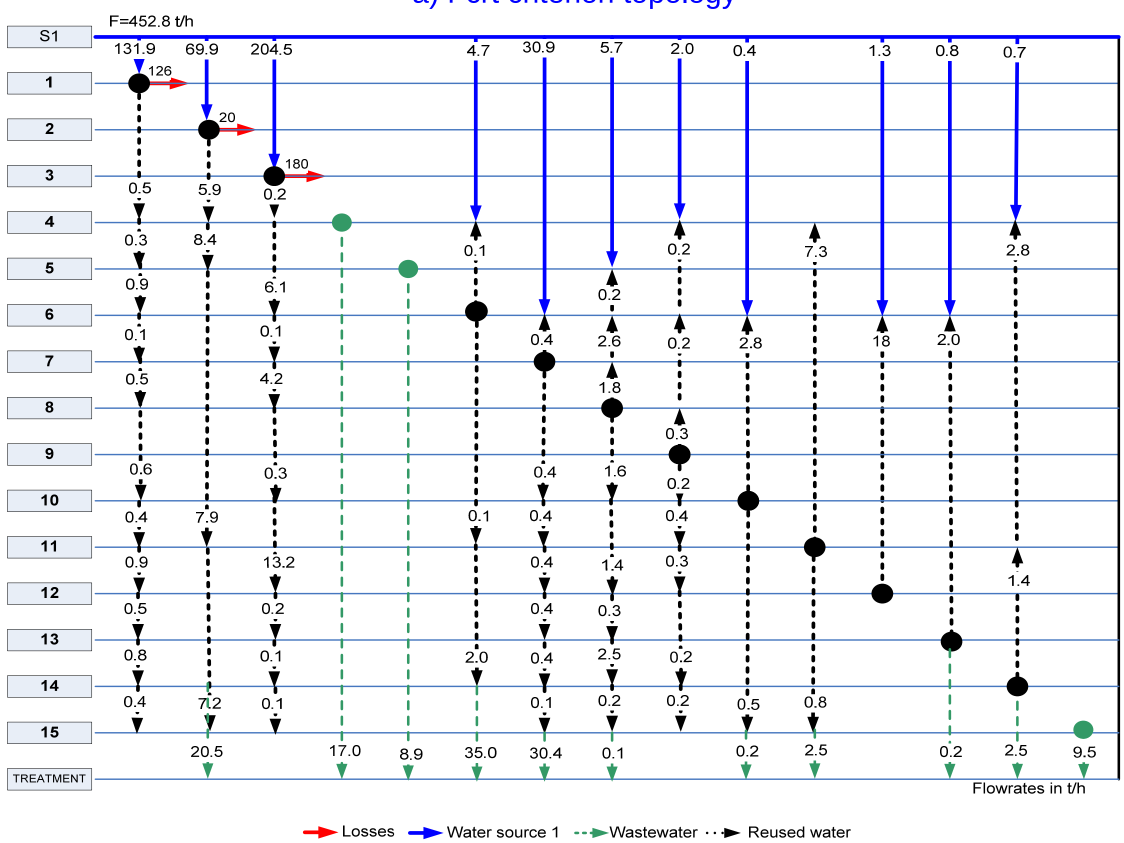


Figure 3. 24 Minimum water flowrate for Existing vs Scenario A – Fcrt criterion

Figure 3. 25 Water usage ratio for: Scenario A (Freshwater source) – Fcrt criterion



a) Fcrt criterion topology



b) Lcrt criterion topology

Figure 3. 26 Water network topology: Scenario A (Freshwater source)

Only four water-using units (U1, U2, U3 and U9) use the higher flowrate (but less than in existing situation). The other units receive reused water from different units, the percentage of distribution of two sources (freshwater and reused water) on each unit is presented in Fig. 3.25. Units U4, U5, U6, U10, U12 and U13 receive only reused water for Fcrt criterion.

f) Water network topology

Though the consumption of freshwater is approximately the same (442.1 t/h vs. 452.8 t/h), water network topology is different for both ordering criteria. New pipes should be installed because the water streams are spitted (i.e. for Fcrt criterion – effluent streams from U1 and U3 are spitted in 9 streams respectively in 11 streams to be reused in other units). Some pipes from supply water source to water using units and from water using units to treatment unit are not used because water flowrate is nil (i.e. Fcrt criterion - supply water pipes to U4, U5, U6, U10, U12, U13 or treatment pipes from U1, U3, U5 and U9).

The GA application software calculates also the total *active length of piping system (ℓ)* as total length of pipes needed for reusing water: ℓ_{Fcrt}= 51,630 m, ℓ_{Lcrt}= 53,555 m. Both topologies can be chosen as a best solution of optimisation: Fcrt ranked topology uses a lower supply water flowrate (442.1 t/h) and has lower total length (51,630 m) compared to Lcrt ordered topology (F=452.8 t/h and ℓ_{Lcrt}= 53,555 m). So, an economic optimisation criterion could give more information for supporting the decision to choose the best topology, for same scenario. I will resume this case in next chapter.

3.7.4.2. Optimisation Scenario B: Water sources S1 & S2

a) Ranking of water network and allocation of water-supply sources

In this scenario two water supply sources are considered available for the water network. The distribution of water-using units per each water source is presented in Table 3.16, according to cluster concept presented in paragraph 3.2 and Lavric et al 2005. This is an original contribution of my work. Ranking is different compared to Scenario A, because the units are ordered as function of water source clusters, depending on accepted inlet concentration of contaminants. The allocation of water supply sources is made as follows :

S1 cluster ={U1, U3, U9, U13}

S2 cluster ={U2, U4, U5, U6, U7, U8, U10, U11, U12, U13, U14, U15}

Table 3.16 Allocation of water sources for ranking water network: Scenario B (Water sources S1 & S2)

Original water unit		Fcrt		Lcrt	
		Ranking water units	Allocated water source	Ranking water units	Allocated water source
U1		U1	S1	U1	S1
U2		U2	S2	U2	S2
U3		U3	S1	U3	S1
U4		U7	S2	U7	S2
U5		U9	S1	U9	S1
U6		U5	S2	U8	S2
U7		U13	S1	U13	S1
U8	**corresponds to**	U4	S2	U10	S2
U9		U15	S2	U12	S2
U10		U10	S2	U6	S2
U11		U11	S2	U14	S2
U12		U14	S2	U11	S2
U13		U8	S2	U15	S2
U14		U12	S2	U4	S2
U15		U6	S2	U5	S2

I notice that each criterion produced different water-using units ranking. The results of optimisation methodology described in paragraph 3.5 are presented below

b) Total supply water flowrate

Table 3.17 Minimum water source flowrate per water-using units: Scenario B (Water sources S1 & S2)

Water-using unit	Minimum flowrate Source 1 (t/h)		Minimum flowrate Source 2 (t/h)	
	Fcrt	Lcrt	Fcrt	Lcrt
U1	131.9	131.9	0.0	0.0
U2	0.0	0.0	355.1	355.1
U3	204.5	204.5	0.0	0.0
U4	0.0	0.0	0.0	0.0
U5	0.0	0.0	0.0	0.0
U6	0.0	0.0	0.0	0.0
U7	0.0	0.0	39.9	39.9
U8	0.0	0.0	0.0	0.0
U9	2.0	2.0	0.0	0.0
U10	0.0	0.0	0.0	0.0
U11	0.0	0.0	0.0	0.0
U12	0.0	0.0	0.0	0.0
U13	0.0	0.0	0.0	0.0
U14	0.0	0.0	0.0	0.0

U15	0.0	0.0	0.0	0.0
Total flowrate (t/h)	**338.4**	**338.4**	**395.0**	**395.0**

I notice that both criteria give same results. Supply water flowrate is bigger compared to Scenario A (733.4 t/h vs 442.1 t/h for Fcrt). Effective usage of Source S1 dropped with important amount, if I consider that losses represent 326 t/h. Source S2 flowrate is bigger than source S1 flowrate, allowing savings from source S1 for this Scenario by ~ 24 %. This could be an important decision factor if source S1 has limited capacity.

c) Total wastewater flowrate

Table 3.18 Wastewater flowrate per water-using units: Scenario B (Water sources S1 & S2)

Water-using unit	**Minimum wastewater flowrate (t/h)**	
	Fcrt	**Lcrt**
U1	0.0	0.0
U2	0.0	20.7
U3	0.0	1.8
U4	0.0	106.1
U5	0.0	75.8
U6	51.4	35.7
U7	0.0	4.8
U8	66.7	4.8
U9	0.0	0.2
U10	40.5	0.1
U11	69.4	0.0
U12	127.9	34.7
U13	0.0	0.0
U14	9.1	26.9
U15	42.4	95.8
Total flowrate (t/h)	**407.4**	**407.4**

More wastewater is produced in this scenario due to global increase in water supply flowrate.

d) Total reused water flowrate

In Table 3.19, reused water flowrate for each unit is presented.

Table 3.19 Reused water flowrate for each water-using unit: Scenario B (Water sources S1 & S2)

Water-using unit	**Reused water flowrate (t/h)**	
	Fcrt	**Lcrt**
U1	0.0	0.0
U2	0.0	0.0
U3	0.0	0.0
U4	26.4	109.3
U5	62.7	75.8
U6	51.4	53.7
U7	0.0	4.8
U8	68.6	4.8
U9	0.0	0.2
U10	61.7	0.1
U11	84.4	0.0
U12	133.3	34.7
U13	7.8	0.0
U14	63.8	26.9
U15	47.6	95.8
Total flowrate (t/h)	**607.7**	**585.5**

e) Savings of supply water

When using two water sources (S1&S2), the minimum supply water flowrate for the network is 733.4 t/h (338.4 t/h from S1 and 395.0 t/h from S2), for both ranking criteria. This is a bigger value compared to Scenario A, because freshwater is mixed with slightly contaminated water from S2. However total supply water saving of 38.8% and freshwater (S1) saving of 71.8% vs existing situation is obtained. Compared to Scenario A, the consumption of freshwater is reduced with 23.5%. Consumption of supply water for each water-using - Scenario B vs existing water flowrate is given in Fig. 3.27. In water-using unit U2, the water demand is increased because contaminated source S2 is used. Reused water flowrate increases several times in this scenario compared to Scenario A : 607.7 t/h (vs 97.8 t/h) for Fcrt and 585.5 t/h (vs 112.2 t/h) for Lcrt. In Fig. 3. 28, distribution of supply water sources and reused water per each water-using unit is presented.

f) Water network topology

For this scenario, the network topology is modified compared to Scenario A. There are streams between water-using units as in scenario A, but only 5 water-using units receive water from supply sources. Units U1, U3 and U9 receive water from S1

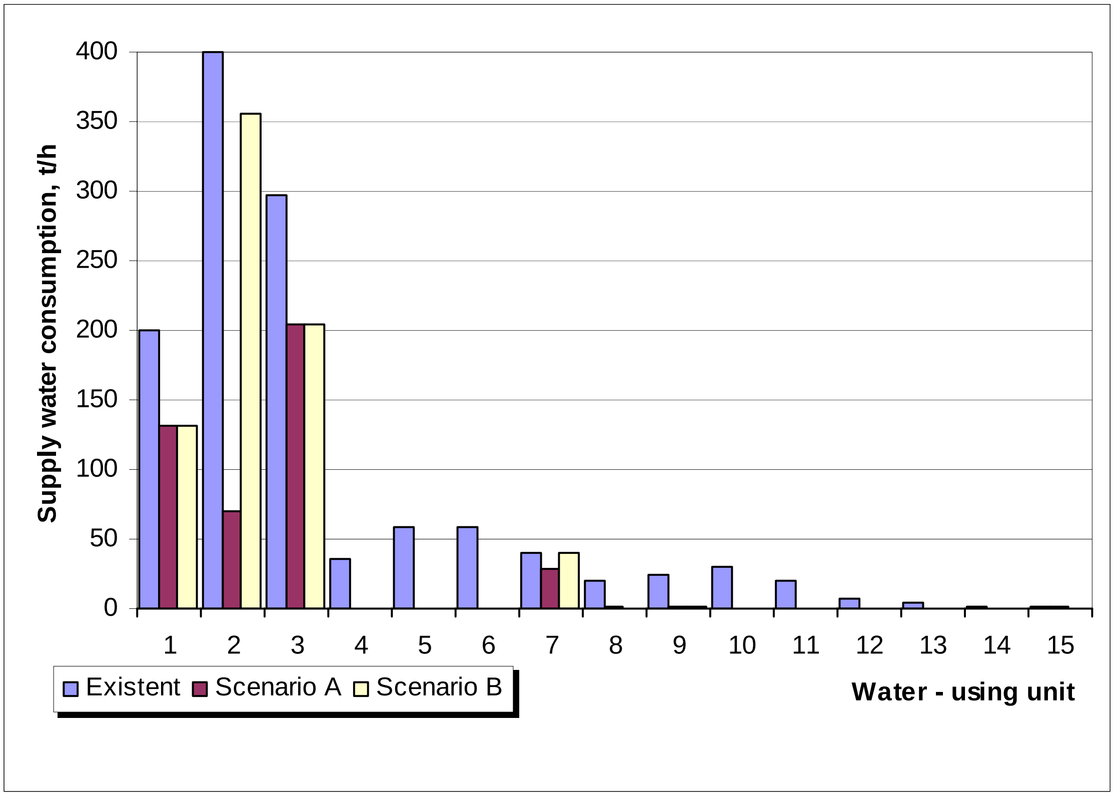


Figure 3. 27 Minimum water flowrate for Existing vs Scenarios A & B– Fcrt criterion

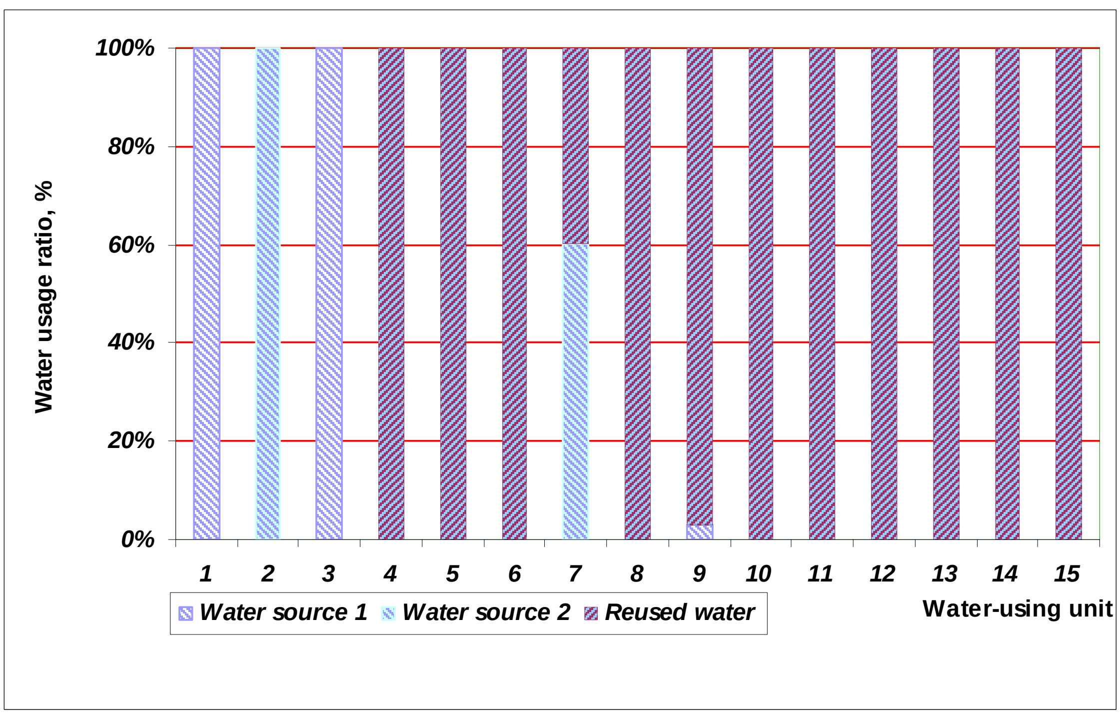


Figure 3. 28 Water usage ratio for Scenario B (Water sources S1 & S2) – Fcrt criterion

and units U2 and U7 receive water from S2. Units U6, U8, U10, U11, U12, U14 and U15 send wastewater to treatment unit. I represent in Fig. 3.27, for each water-using unit supply water consumption for scenarios A and B, compared to existing case. Units U1 and U3 have each same water consumption in both scenarios as they use only S1. As units U2 and U7 use contaminated water from S2, the consumption is much increased compared to scenario A, approaching the value of existing case (but still smaller). U9 has very small supply flowrate from S1, compared to Existing case, in both scenarios.

Comparison of results between scenarios A and B is relevant. Scenario B has the most important increase of supply water flowrate due to supply source S2. The flowrate for unit U2 increases by 6.6 times related to Scenario A. The excess of water is then sent to different units as reused water, no wastewater is sent by this unit in this scenario. Unit U7 uses also source S2, but the increase is just by 1.4 times. The number of units using supply water is reduced dramatically from 9 units in Scenario A to just five units in Scenario B. Most water-using units are fed with reused water, as I represent in Fig. 3.28. Reused water flowrate increases by 6.2 times for Fcrt and 5.2 times for Lcrt in Scenario B compared to Scenario A. The potential of water reuse is increased in scenario B because the flowrate of reused water streams is higher for each unit. The total active pipes length decreases slightly in Scenario B (there is smaller for Fcrt ranking criterion, ℓ_{Fcrt}= 57,690 m vs. ℓ_{Lcrt}= 57,710 m). Consequently from this point of view the Fcrt topology is a solution to consider (Fig.3.29). As in Scenario A, more significant results are expected if more comprehensive optimisation function, as economic optimisation criteria is used. This can support better the decision to choose the most appropriate topology. I resume this scenario in next chapter.

3.7.4.3. Optimisation Scenario C: Water sources S1, S2 & S3

a) Ranking of water network and allocation of water-supply sources

For this scenario three water sources are taken into account to satisfy network water demand. Ranking of units is slightly changed, According to my original representation of water network (Fig. 3.4), there are 3 clusters of water sources to group the units, according to Fcrt and Lcrt ranking criteria, as I presented in Table 3.20:

S1 cluster ={U1, U3, U9, U13}

S2 cluster ={U2, U5, U6, U7, U8, U11, U12, U14, U15}

S3 cluster ={U4, U10 }

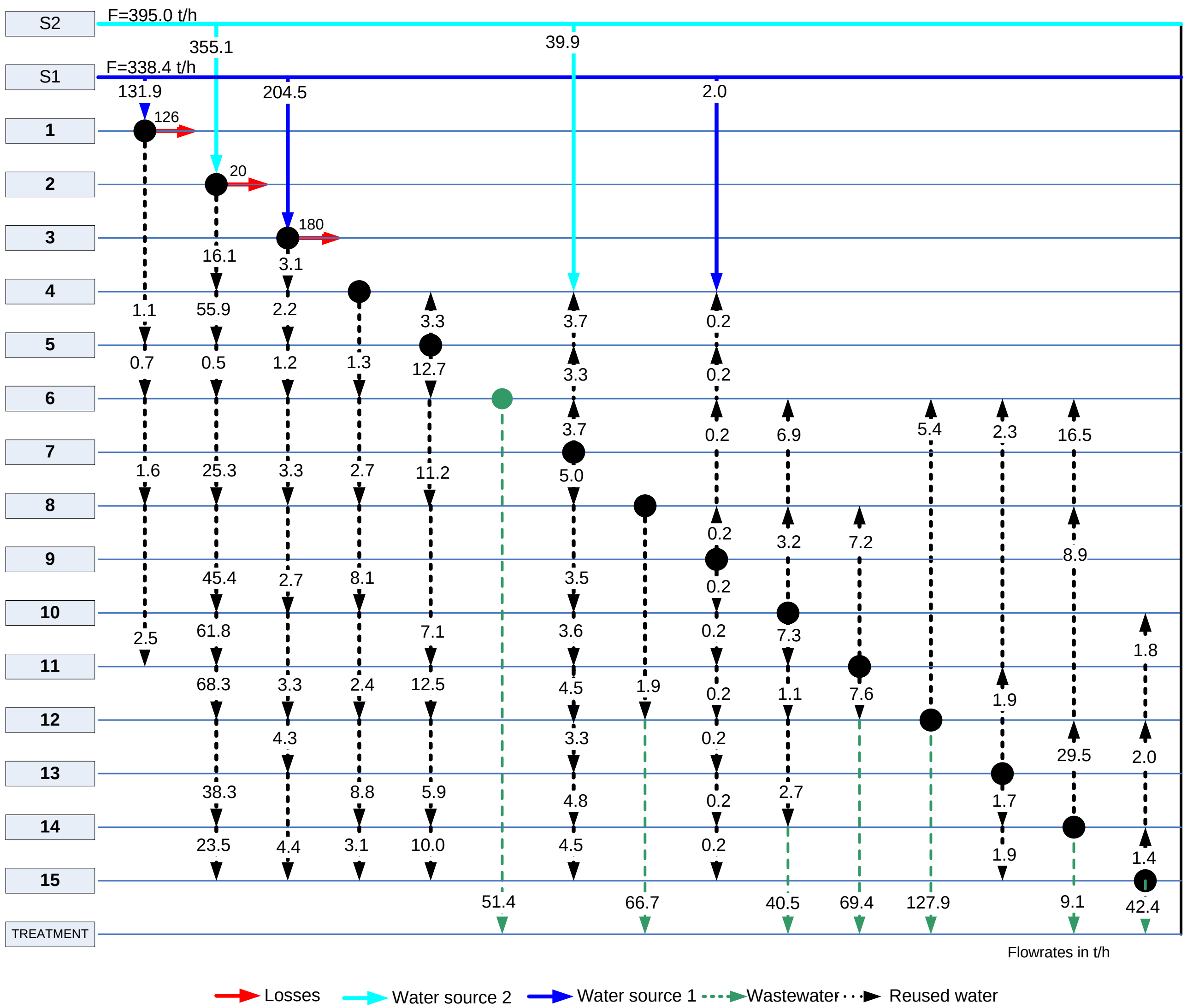


Figure 3. 29 Optimal water network topology: Scenario B (Water sources S1 & S2) – Fcrt criterion

Table 3.20 Allocation of water sources for ranking water network: Scenario C (Water sources S1, S2&S3)

Original water unit		Fcrt		Lcrt	
		Ranking water units	Allocated water source	Ranking water units	Allocated water source
U1		U1	S1	U1	S1
U2		U2	S2	U2	S2
U3		U3	S1	U3	S1
U4		U7	S2	U7	S2
U5		U9	S1	U9	S1
U6		U10	S3	U10	S3
U7		U 5	S2	U8	S2
U8	**corresponds to**	U13	S1	U13	S1
U9		U4	S3	U12	S2
U10		U15	S2	U6	S2
U11		U11	S2	U14	S2
U12		U14	S2	U11	S2
U13		U8	S2	U15	S2
U14		U12	S2	U4	S3
U15		U6	S2	U5	S2

I notice that each criterion produced different water-using units ranking, but there are minor differences compared to Scenarios B: just unit U10 moved slightly. The results of optimisation methodology described in paragraph 3.5 are presented below.

b) Total supply water

Table 3.21 Minimum water source flowrate per water-using units: Scenario C (Water sources S1&S2&S3)

Water-using unit	Minimum flowrate Source 1 (t/h)		Minimum flowrate Source 2 (t/h)		Minimum flowrate Source 3 (t/h)	
	Fcrt	Lcrt	Fcrt	Lcrt	Fcrt	Lcrt
U1	131.9	131.9	0.0	0.0	0.0	0.0
U2	0.0	0.0	355.1	355.1	0.0	0.0
U3	204.5	204.5	0.0	0.0	0.0	0.0
U4	0.0	0.0	0.0	0.0	0.0	0.0
U5	0.0	0.0	0.0	0.0	0.0	0.0
U6	0.0	0.0	0.0	0.0	0.0	0.0
U7	0.0	0.0	39.9	39.9	0.0	0.0
U8	0.0	0.0	0.0	0.0	0.0	0.0
U9	2.0	2.0	0.0	0.0	0.0	0.0
U10	0.0	0.0	0.0	0.0	7.3	7.3
U11	0.0	0.0	0.0	0.0	0.0	0.0
U12	0.0	0.0	0.0	0.0	0.0	0.0

U13	0.0	0.0	0.0	0.0	0.0	0.0
U14	0.0	0.0	0.0	0.0	0.0	0.0
U15	0.0	0.0	0.0	0.0	0.0	0.0
Total flowrate (t/h)	**338.4**	**338.4**	**395.0**	**395.0**	**7.3**	**7.3**

Source S3 has a small effect, supplying a small flowrate just to unit U10. Consequently total supply water flowrate has just a small increase (7.3 t/h) compared to Scenario B. Flowrates from S1 and S2 are unchanged.

c) Total wastewater flowrate

Table 3.22 Wastewater flowrate per water-using units: Scenario C (Water sources S1, S2 & S3)

Water-using unit	**Minimum wastewater flowrate (t/h)**	
	Fcrt	**Lcrt**
U1	0.0	0.0
U2	0.0	28.4
U3	0.0	3.0
U4	2.8	84.4
U5	0.0	101.6
U6	133.9	28.7
U7	0.0	3.7
U8	62.1	11.6
U9	0.0	0.4
U10	0.0	2.3
U11	57.7	7.0
U12	119.0	51.2
U13	0.0	0.0
U14	0.0	28.2
U15	39.2	64.2
Total flowrate (t/h)	**414.7**	**414.7**

In this scenario wastewater increases with same value as supply water (7.3 t/h).

d) Total reused water flowrate

Table 3. 23 Reused water flowrate for each water-using unit: Scenario C (Water sources S1, S2 & S3)

Water-using unit	**Reused water flowrate (t/h)**	
	Fcrt	**Lcrt**
U1	0.0	0.0
U2	0.0	0.0

U3	0.0	0.0
U4	12.8	90.0
U5	25.5	101.6
U6	133.8	45.1
U7	0.0	0.0
U8	62.1	62.0
U9	0.0	0.0
U10	0.2	0.0
U11	72.1	76.8
U12	121.1	56.3
U13	11.0	0.0
U14	65.8	47.0
U15	57.4	65.3
Total flowrate (t/h)	**561.8**	**544.1**

Flowrate of reused water decreases compared to Scenario B.

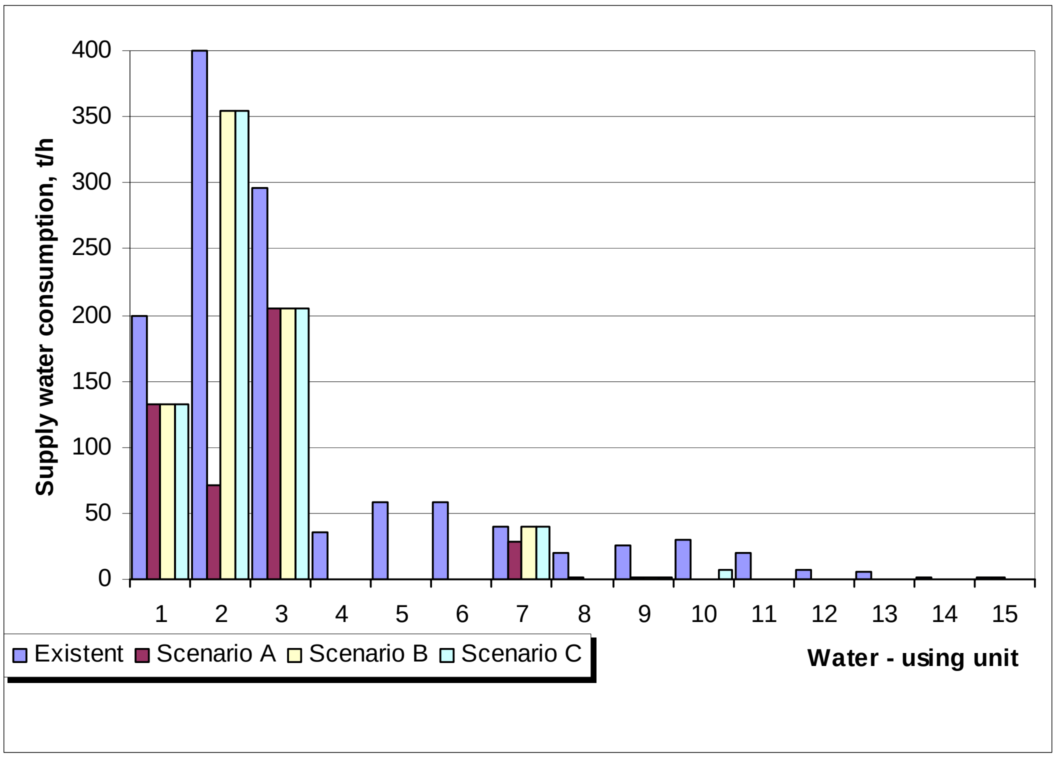


Figure 3. 30 Minimum water flowrate for Existing vs Scenarios A, B & C - Lcrt criterion

e) Savings of supply water

When contaminated water Source S3 is also considered, the optimisation algorithm gives no important modification in water supply savings, compared to Scenario B. The minimum supply water flowrate is 338.4 t/h from Source S1, 395.0 t/h from Source S2 and 7.3 t/h from Source S3. The distribution of supply water is similar to Scenario B, the only difference is that unit U10 is supplied with water from Source S3.

Comparison between existing case and scenarios A, B, respectively C for minimum supply water to each water-using unit is presented in Fig. 3.30. Distribution of supply water and reused water per each water-using unit is presented in Fig. 3.31. The flexibility reduced compared to Scenario A because all units have mainly one type of water at the entrance (either supply water or reused water). Just unit U10 makes a small difference.

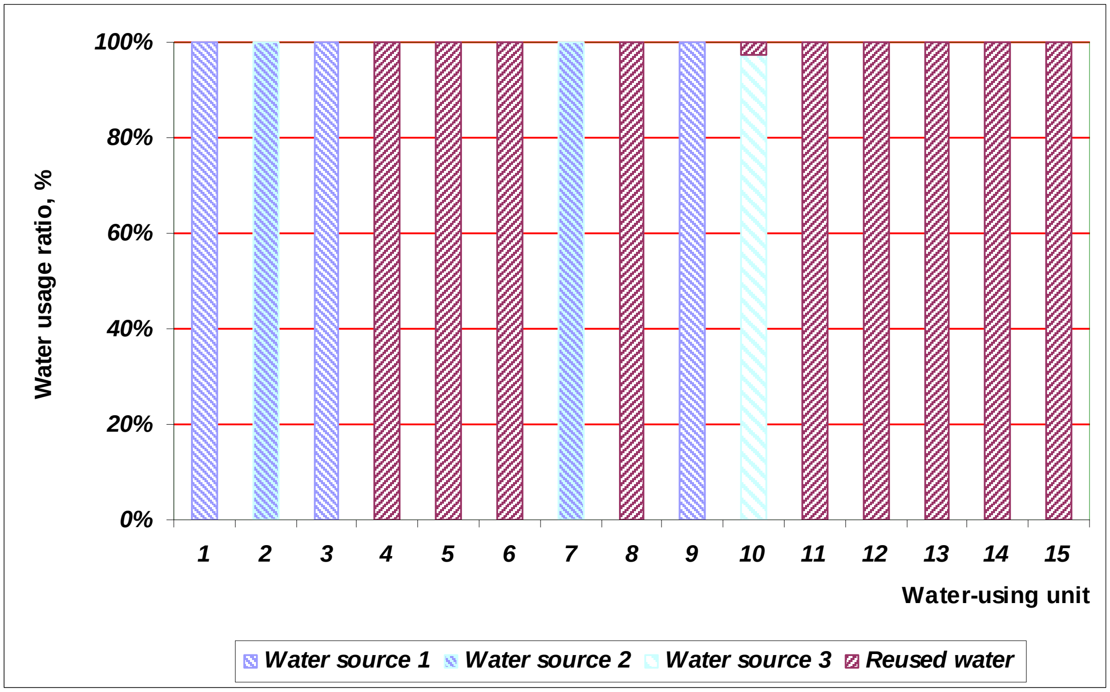


Figure 3. 31 Water usage ratio for Scenario C (Water sources S1, S2 & S3) - Lcrt criterion

f) Water network topology

There are some topological modifications between scenarios B and C, especially regarding the distribution of reused water between different water-using units. Supply water is provided to units U1 and U3 from S1, U2 and U7 from S2 and U10 from S3. Water demands for units U4, U5, U6, U8, U11-U15 is satisfied by reused water only, Fig. 3.31. Considering the total active pipe length, the topology obtained for Lcrt criterion provides a similar value as Fcrt criterion (ℓ_{Fcrt}=56.900 m vs. ℓ_{Lcrt}=55.850 m).

This result is just slightly different of Scenario B. The topology for Lcrt criterion is represented in Fig.3.32. This scenario is resumed in Chapter 4 when an economic based objective function is used for optimisation process. Results comparison for both objective functions provides a better decision support for plant managers regarding the selected solution for water network on this big site.

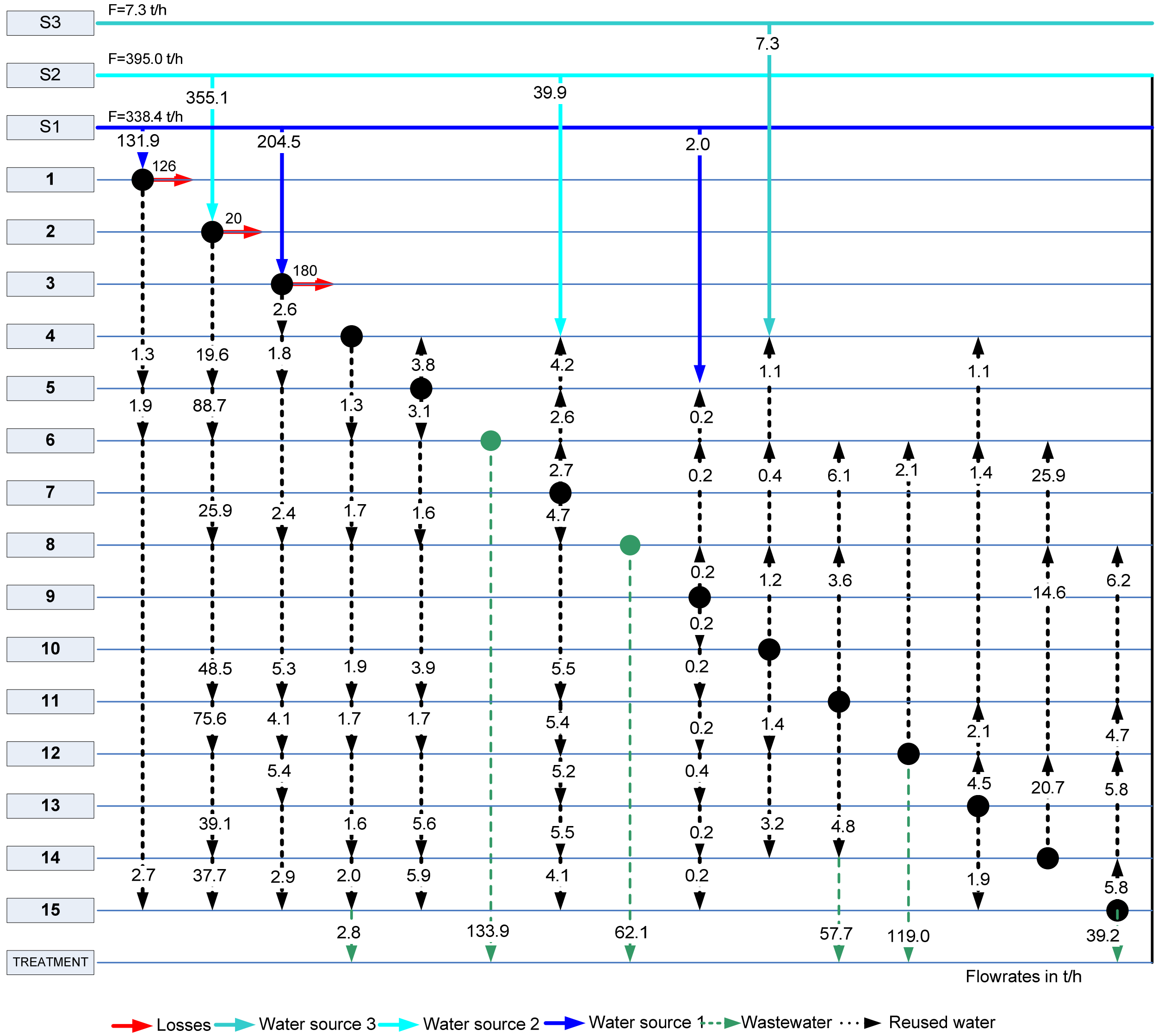


Figure 3. 32 Optimal water network topology: Scenario C (Water sources S1, S2 & S3) - Lcrt criterion

3.7.4.4. Optimisation Scenario D: Water sources S1, S2, S3 & S4

a) Ranking of water network and allocation of water-supply sources

In this scenario four water sources (Source S1 – freshwater, Source S2 – slightly contaminated, Source S3 – very contaminated and Source S4 - contaminated) are allocated to units, as I present in Table 3.24. For each water source a cluster of water using units can be allocated, as explained in paragraph 3.5 for ranking procedure:

S1 cluster ={U1, U3,U9,U13}

S2 cluster ={U2, U7 }

S3 cluster ={U4,U10 }

S4 cluster ={U5,U6, U8,U11, U12, U14,U15 }.

Table 3. 24 Allocation of water sources for water network: Scenario D (Water sources S1, S2, S3 & S4)

Original water unit		Fcrt		Lcrt	
		Ranking water units	Allocated water source	Ranking water units	Allocated water source
U1	Corresponds to	U1	S1	U1	S1
U2		U2	S2	U2	S2
U3		U3	S1	U3	S1
U4		U7	S2	U7	S2
U5		U8	S4	U8	S4
U6		U9	S1	U9	S1
U7		U10	S3	U10	S3
U8		U11	S4	U11	S4
U9		U5	S4	U13	S1
U10		U13	S1	U12	S4
U11		U4	S3	U6	S4
U12		U15	S4	U14	S4
U13		U14	S4	U15	S4
U14		U12	S4	U4	S3
U15		U6	S4	U5	S4

I notice that each criterion produced different water-using units ranking. The results of optimisation methodology described in paragraph 3.5 are presented below.

b) Total supply water flowrate

Table 3.25 Minimum water source flowrate per water-using units: Scenario D (Sources S1, S2, S3 & S4)

Water-using unit	Minimum flowrate Source 1 (t/h)		Minimum flowrate Source 2 (t/h)		Minimum flowrate Source 3 (t/h)		Minimum flowrate Source 4 (t/h)	
	Fcrt	Lcrt	Fcrt	Fcrt	Lcrt	Lcrt	Fcrt	Lcrt
U1	131.9	131.9	0.0	0.0	0.0	0.0	0.0	0.0

U2	0.0	0.0	355.1	355.1	0.0	0.0	0.0	0.0
U3	204.5	204.5	0.0	0.0	0.0	0.0	0.0	0.0
U4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
U5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
U6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
U7	0.0	0.0	39.9	39.9	0.0	0.0	0.0	0.0
U8	0.0	0.0	0.0	0.0	0.0	0.0	35.9	35.9
U9	2.0	2.0	0.0	0.0	0.0	0.0	0.0	0.0
U10	0.0	0.0	0.0	0.0	7.3	7.3	0.0	0.0
U11	0.0	0.0	0.0	0.0	0.0	0.0	6.6	6.6
U12	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
U13	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
U14	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
U15	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Total flowrate (t/h)	**338.4**	**338.4**	**395.0**	**395.0**	**7.3**	**7.3**	**42.5**	**42.5**

I notice that compared to Scenario C, supply sources S1, S2 and S3 provide same flowrate. The difference is that additional 42.5 t/h is provided by S4 which represent an increase of about 5% of supplied water flowrate. Same saving of freshwater (from source S1) is to notice as in Scenarios B and C.

c) Total wastewater flowrate

Table 3.26 Wastewater flowrate per water-using units: Scenario D (Water sources S1, S2, S3 & S4)

Water-using unit	**Minimum wastewater flowrate (t/h)**	
	Fcrt	**Lcrt**
U1	0.0	1.2
U2	0.0	53.5
U3	0.0	3.3
U4	90.3	106
U5	90.8	123.7
U6	112.9	35.3
U7	0.0	6.5
U8	0.0	5.3
U9	0.0	0.0
U10	0.0	0.0
U11	1.1	1.2
U12	72.9	60.4
U13	0.0	0.0
U14	80.9	0.0

U15	8.3	60.8
Total flowrate (t/h)	**457.2**	**457.2**

Total supply water increase involves wastewater flowrate with same amount.

d) Total reused water flowrate

Table 3. 27 Reused water flowrate per water-using unit: Scenario D (Water sources S1, S2, S3 & S4)

Water-using unit	**Reused water flowrate (t/h)**	
	Fcrt	**Lcrt**
U1	0.0	0.0
U2	0.0	0.0
U3	0.0	0.0
U4	100.6	109.8
U5	95.6	123.7
U6	112.9	53.2
U7	0.0	0.0
U8	0.0	0.0
U9	0.0	0.0
U10	0.0	0.0
U11	0.0	0.0
U12	79.1	79.3
U13	23.5	0.0
U14	82.7	59.3
U15	89.5	63.3
Total flowrate (t/h)	**583.9**	**485.6**

Water reuse has a contradictory evolution compared to Scenario C: Fcrt gives and increase in water reuse of about 3.7 % and Lcrt gives a reduction in water reuse of about 12 %. These variations can be explained by units matching restrictions for water reuse. Specific units ranking produced by each ranking criterion determine particular connectivity.

e) Savings for supply water

When considering all four water sources for water network optimisation, no improvement in water saving is obtained. S1, S2 and S3 keep same flowrate and additional 42.5 t/h are added from S4 to be used by two water-using units (U8 and U11). Units U1, U2, U3 (cooling towers) use biggest amount of water.

f) Water network topology

Water network topology is slightly modified compared to Scenario C especially for units using small amount of water, as I present in Fig. 3.35. This is normal due to new connectivity possibilities offered by introduction of source S4. Water network total active length is smaller compared to Scenario C (ℓ_{Fcrt}=50,990 m, ℓ_{Lcrt}=49,850 m). U3 has five connections for reused water compared to Scenario C where there are 7 connections. U4 has four connections in this scenario compared to 7 connections in previous scenario. U9 has a very simplified connectivity (one connection vs. 9 connections). Instead, U8 has seven connections compared with none in scenario C (where does not reuse water just is sending 62.1 t/h to treatment). U10, U12, U13 and U15 have similar number of connections in both scenarios. U11 and U14 have less connections in Scenario D. This scenario is resumed in Chapter 4 performing optimisation with an economic based objective function. Results comparison for both objective functions provides a better decision support as many other criteria cannot be taken into account by these objective functions.

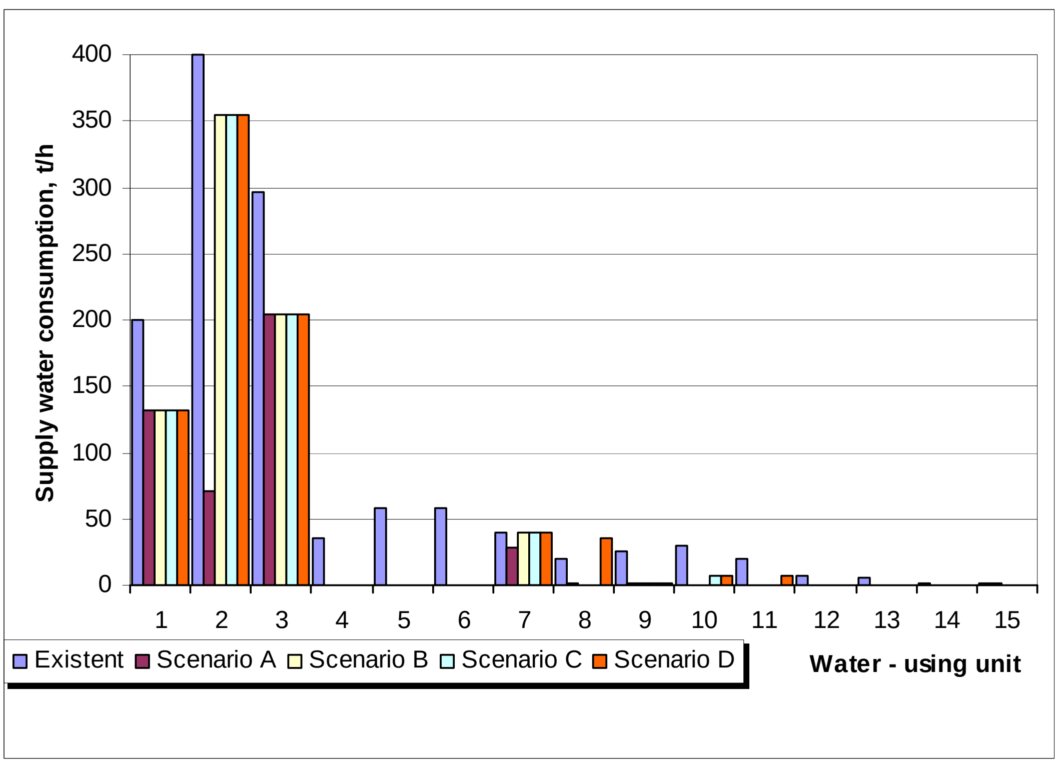


Figure 3. 33 Minimum water flowrate for Existing vs Scenarios A&B&C&D – Fcrt criterion

Existent network uses 1,198.8 t/h freshwater. The purpose of these scenarios is to identify the optimal network topology and the best allocation of water sources to have minimum supply water consumption. Comparing the results obtained for all scenarios

(A, B, C and D), it can be assessed that Scenario B is more attractive solution from supply water flowrate point of view. In scenario B total supply water consumption is 733.4 t/h (338.4 t/h from Source S1 and 395.0 t/h from Source S2. If other decision criterion indicate as more attractive Scenario A, it can be stressed that using many water sources is recommended when source S1 has limited capacity. Total reused water flowrate in Scenario B is 607.7 t/h for Fcrt criterion and 585.5 t/h for Lcrt criterion. Lcrt criterion is chosen and the topology is slightly less complex.

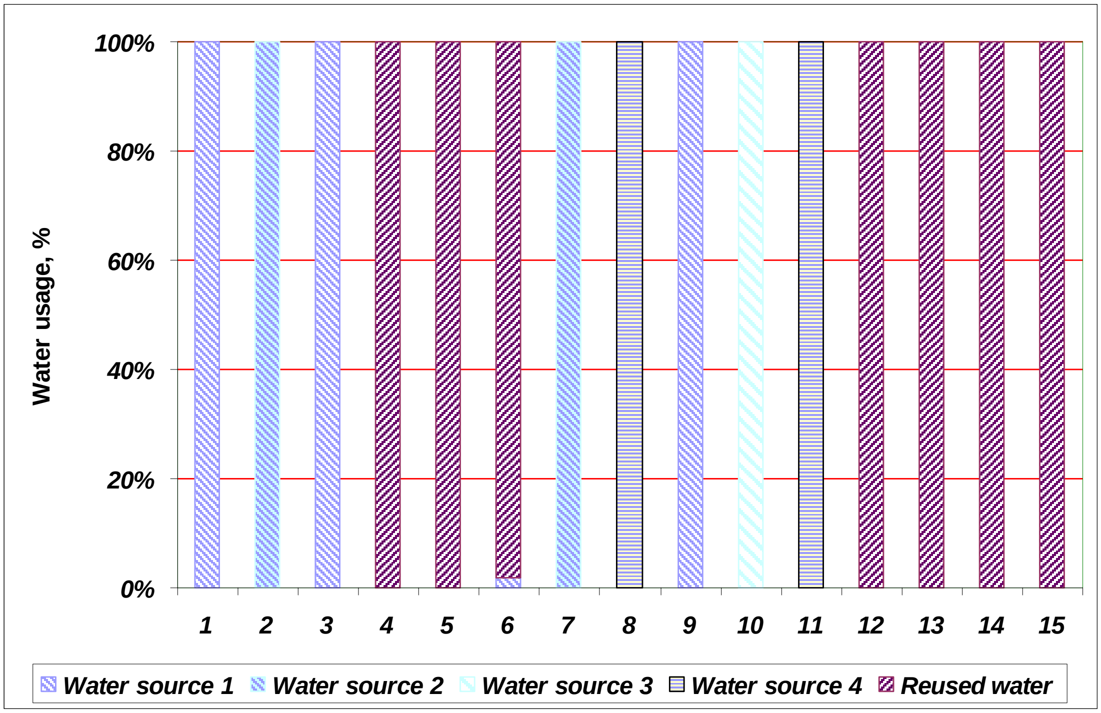


Figure 3. 34 Water usage ratio for Scenario D (Water sources S1, S2, S3 & S4) – Fcrt criterion

Table 3.28 Final results

Scenario	Supply water flowrate (t/h)		Fresh (S1) water flowrate (t/h)		Reused water flowrate (t/h)		Waste-water flowrate (t/h)	
	Fcrt	Lcrt	Fcrt	Lcrt	Fcrt	Lcrt	Fcrt	Lcrt
Existing	1198.8	1198.8	1198.8	1198.8	0.0	0.0	872.8	872.8
A	442.1	452.8	442.1	452.8	97.8	112.2	116.1	126.8
B	733.4	733.4	338.4	338.4	607.7	585.5	407.4	407.4
C	740.7	740.7	338.4	338.4	561.8	544.1	414.7	414.7
D	783.2	783.2	338.4	338.4	583.9	457.2	457.2	457.2
Selected solution	**733.4**	**733.4**	**338.4**	**338.4**	**607.7**	**585.5**	**407.4**	**407.4**

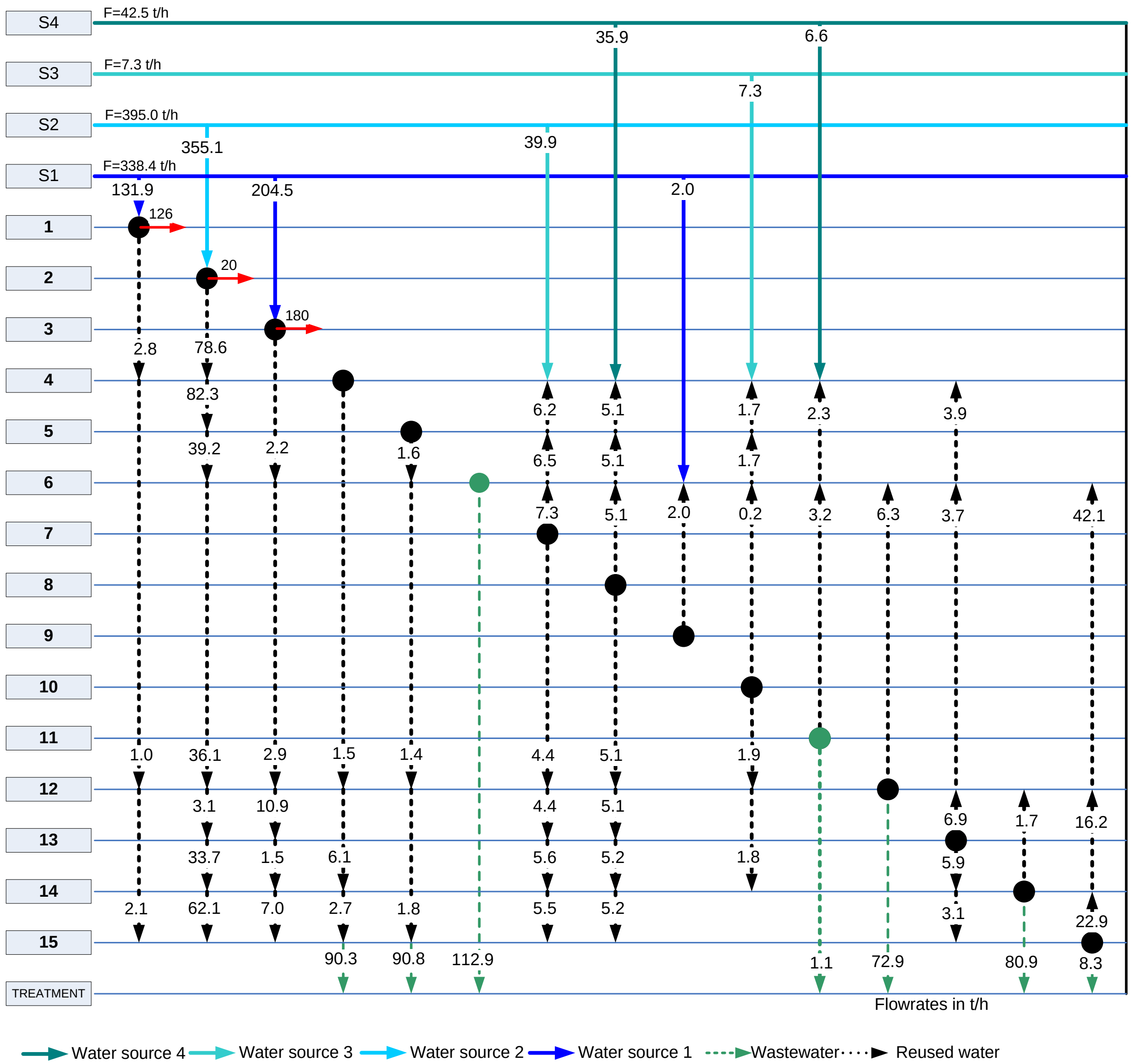


Figure 3. 35 Optimised water network topology: Scenario D (Water sources S1, S2, S3 & S4) – Fcrt criterion

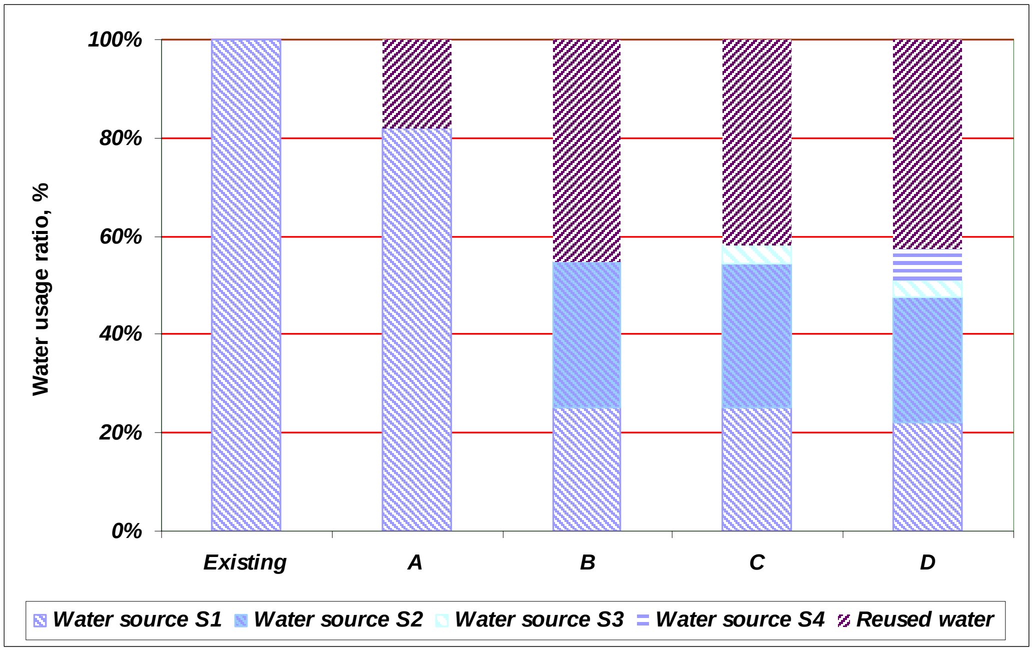


Figure 3. 36 Final results: Water using ratio Existing vs A,B,C,D Scenarios

3.8. Conclusions

In this chapter, I propose a process integration methodology to design optimal water network with more supply water external sources for a water minimisation type problem. Original physical and mathematical models are developed. The objective function used in optimisation is water supply flowrate. Solving technique is based on GA optimisation algorithm. Main achievements and original contributions in this chapter are summarised below:

a. Physical model for water network is based on oriented graph topology where water using units are knots and water streams are arches.
   - Water using units are considered perfectly mixed vessels. Process streams transfer to water stream a certain mass load of contaminants in each unit.
   - Equipartition of driving force principle is considered for taking advantage of the oriented graph nature of the water network. All the units are ranked by two criteria: ‘‘by load’’ and ‘‘by fresh water’’.
   - Supply water sources have different degrees of contamination. Water using units are grouped in clusters (according to their contaminant concentration constraints at the entrance) associated to each water source. This is an original concept introduced in my paper Lavric et al., 2005.

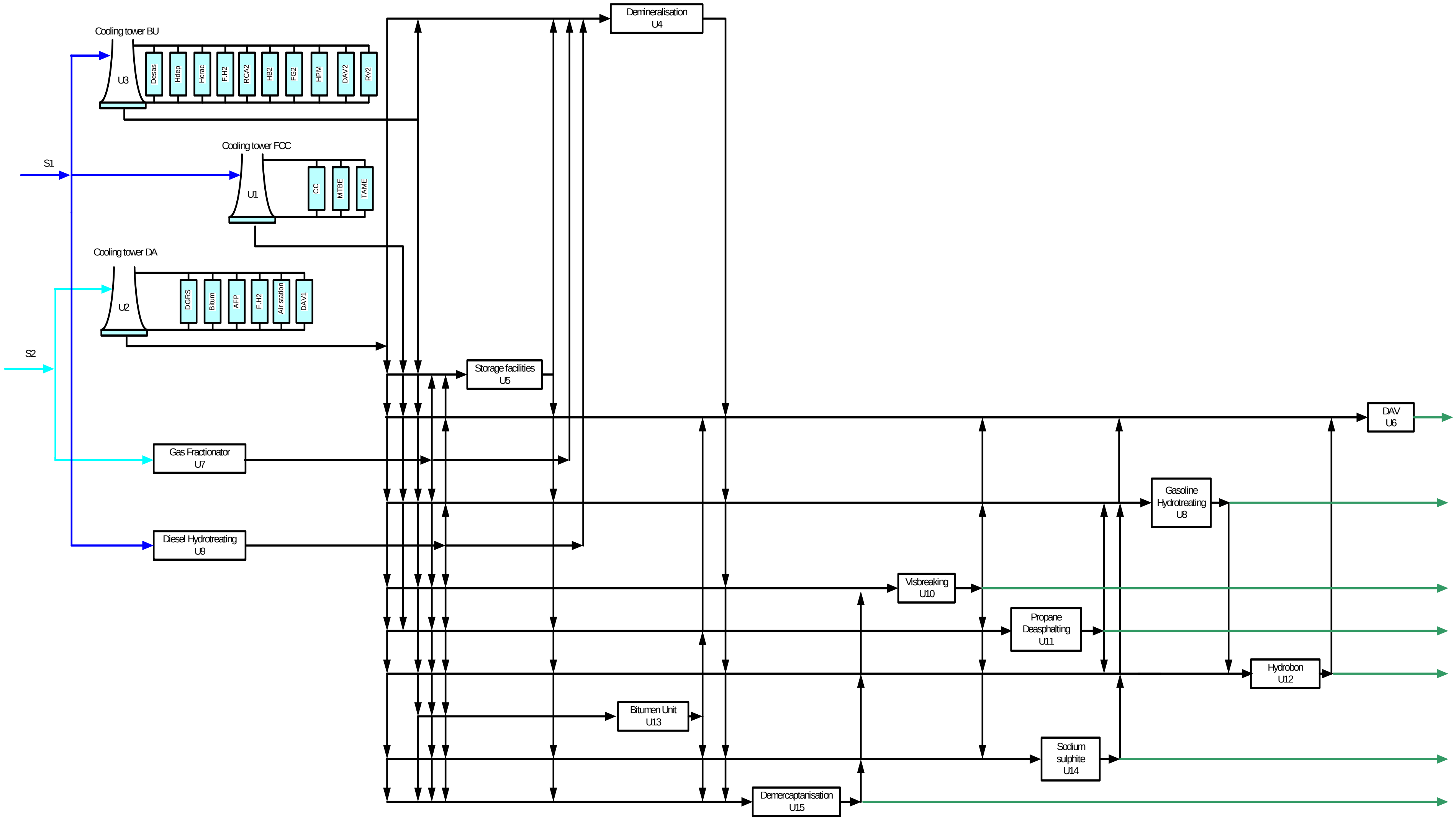


Figure 3. 37 Optimised water network

- Water recycling is not taken in consideration to observe the "equipartition of driving force" principle.

b. Mathematical model for water-using units is based on total and partial (for contaminants) mass balances. Associated constraints based on *Limiting Water Profile* concept in terms of input and output maximum allowable contaminants concentration are taken into account. Objective function is based on supply water flowrate. As a consequence a new NLP formulation for water network mathematical model is proposed. This approach is different of usual approaches in literature, where mathematical models are based on superstructures associated to water network. My development allows to get important results for solving practical problems :
   - Numerous contaminants and big number of water using units can be handled very easy.
   - The integration of streams is based on water reusing strategy (regeneration is not yet considered).

c. Hybrid modified GA solving technique is used for NLP mathematical model. Internal flowrates are independent variables, allowing to calculate model dependent variables and water network topology design, observing the imposed inlet and outlet constraints for each unit.

d. I propose a new graphical form for water network topology visualisation. The units are classified in water sources and water sinks and the streams are the links between them. Each water unit can be a **source** of reused water and/or wastewater and/or a **sink** for supply water and/or reused water. Water flowrates are also represented, creating to user an easy instrument to check mass balances.

e. A literature test case (ten water-using units, three contaminants and one supply water source) is used to proof the capacity to solve better the problem with GA optimisation technique proposed. Applied to a case study proposed by Savelsky (Savelsky et al,. 1999), his solution is classified as a local optimum, because in my approach a better solution is obtained.

f. A more complex water network case study (ten water-using units, six contaminants and four supply water sources) is solved to demonstrate that such problems are not yet tackled in literature. A problem of this dimension cannot be solved using superstructure-based algorithms. Using GA optimisation technique optimal solution and also the correspondingly water network topology for both ranking criteria is obtained. The influence of contamination level of water sources is studied in four scenarios to find the best water network.

g. A large scale case study from an oil refinery is develop to take advantage of this methodology. Fifteen water-using units, six contaminants, four available water sources (with different level of contamination) and a treatment unit are considered. To design the optimal water network topology with the minimum fresh water consumption, for each water using unit there is imposed the maximum allowable pollutant input concentration and the maximum allowable pollutant output concentration. Four particular scenarios (A-one water source, B- two water sources, C-three water sources and D-four water sources) are analysed using both units ranking criteria (Lcrt and Fcrt). The influence of available water sources on topology and on optimal solution is considered. Using different conditions for available water sources, following results are obtained:
   - The most attractive solution is obtained when simultaneously freshwater (source S1) with slight contaminated water (source S2) are used. Topology for optimised water network is presented in Fig. 3. 37.
   - The other combinations of water sources give only the modification of topology, neither freshwater supply savings nor involving important changes in water reuse.
   - 24 % savings from Source S1 is made applying this process integration methodology using simultaneously water source S1 (freshwater) with water source S2 (slightly contaminated).

For practical situations decision should be supported by more performance indexes as objective function. An important option is to use indexes based on economic considerations. Such an approach is developed in next chapter, considering as objective function water network annualised total cost or topological index.

The solution technique, based on GA algorithm, developed in this work is able to give all information to engineer regarding water network design (minimum supply water source flowrate, the best combination of supply water sources, the most recommended topology of water network) for minimum supply water source flowrate. The new representation of water network topology is simple and clear with good visual properties.

Chapter 4

Water network optimisation considering economical aspects

4.1. Introduction and motivation

Water is the universal utility, both in domestic and industrial domains. The demand never ceases to increase due to the rapid development at the global scale. Freshwater from natural sources is pre-treated to be used by industrial sites. After the contact with different process streams results effluents mainly as: process water, steam and wash water. Important quantities are used as cooling water (once-through or in recirculation system). Meteorological phenomena determine formation of rain water from process and/or non-process areas. The water deficit will increase in future, generating very serious social, economic and environmental problems at local and global scales. Supplied water quality tends to decrease as a result of global pollution and depletion of water sources as natural phenomena. Therefore, the water policy should be re-evaluated together with the improvement of the water management, usage and protection strategies. Special attention has to be focused on water consumption reduction, recycling and reuse as acceptable solutions. Modelling and optimisation based on economical aspects can include many of such situations.

Due to the high costs associated with the freshwater supply and wastewater treatment, the research over the past decades was devoted to the new techniques for optimal water network design aimed to minimise these costs (Wang & Smith, 1994a; Mann & Liu, 1999). Bagajewicz identified in a review (Bagajewicz, 2000) two approaches for the design of water-use networks, namely conceptual/graphical methods and mathematical programming. Papalexandri & Pistikopoulos, 1996 proposed a design procedure, based upon the generalised modelling framework concept, developing a systematic representation of process units and process structures, using superstructure rules such as splitting, mixing and bypassing. El-Halwagi & Manousiouthakis, 1990 developed a methodology, based on a MILP transshipment formulation that allows synthesis of the mass exchange network (MENs). The minimisation of the corresponding total annualised network cost is performed through two design targets: the cost of mass separation agents required to handle the exchangers' duty; the number of mass exchangers implying the minimum utility costs. Also, El-Halwagi et al., 1995 improved this methodology, proposing a procedure calculating the total minimum cost for heat-induced separation networks. Gupta and Manousiouthakis, 1996 introduced another model for the MEN, considering that streams target compositions are allowed to vary in a closed interval. The optimisation task was to determine the minimum mass separating agent cost needed for the transfer of a single component from rich to lean streams. The feasibility and the capacity of MEN may increase relaxing a little bit the outlet conditions lowering the outlet compositions of some lean streams above their upper bounds. This reduction translates into the minimisation of utility costs and allows greater recovery from the rich streams at no additional cost. Streams decomposition helps transforming the MINLP formulation into a LP formulation, without changing the solution. They applied successfully their methodology to two water minimisation case studies. Alva-Argaez et al., 1998 proposed an integrated methodology for the design of an industrial water system which combines water pinch analysis and mathematical programming tools. The objective function includes terms for operating cost of the network (fresh water costs) and capital costs (cost of piping and investments for treatment units). The MINLP problem is later decomposed into a sequence of MILP problems, fixing the outlet concentrations at their maximum level for the "limiting contaminants" (Alva-Argaez et al., 1999). Suh & Lee, 2002, developed a robust optimal design strategy, considering the uncertain parameter variations in both economic and technical aspects. The objective function is the net present cost, consisting of the network piping and pumps cost and the freshwater usage cost. Feng & Chu, 2004 developed a methodology for assessing the economic performance of wastewater re-usage system which has as components water utilisation system, wastewater regeneration system and wastewater treatment reuse. Reusing significant quantities of water, typically involves regeneration/treatment of resulted wastewater to cope quality requirements of water reusing units. The authors demonstrate the importance of trade-off between competing cost factors (freshwater and wastewater disposal costs vs wastewater regeneration/treatment cost), which depend on post-regeneration/post-treatment contaminant concentration. The optimisation procedure can minimise the total cost of wastewater reuse system with either wastewater regeneration reuse or wastewater treatment reuse.

4.2. Problem statement

In this chapter, I propose to determine the optimum topology considering a cost-based objective function, which takes into account the on-field geometry of the network, (through the matrix of the distances between units). Additional original contribution, compared with literature presented approaches (Lavric et al., 2005), is that water system pipes have optimum economic diameters, computed to minimise friction losses due to fluid flow and investment for piping system (piping and pipe's fittings). The calculation of optimum diameter, as presented in Bratu, 1984 and Peters et al., 2003, results from combination of principles of fluid dynamics with cost evaluation.

However, to keep the computations as simple as possible, still preserving the main characteristics of the problem at hand, no adjacent costs are included in the objective function for network optimum topology (effluent disposal charges based on volume and/or contaminant loading, or on-site treatment costs to upgrade the water quality of the effluent for reuse). Those cost components do not affect significantly my considerations as they are not influenced by independent variables (flowrates between water-using units). Proposed cost function includes main characteristics of optimal topology water network: design for minimum supply water consumption with minimum cost of new pipes implementation.

When reliable direct cost function cannot be formulated, I propose an optimisation function which represents indirect economic criteria, related to active network lengths (for which below is defined the topological index of water network). The function is defined as a linear combination between the normalised supply water consumption and the topological index (Iancu et al., 2006).

Problem statement is similar with formulation given in paragraph 3.2. A water using unit is defined as in Fig. 3.6., characterised by following elements:

$U = \{u_i \mid i = 1,2,...,N\}$ the set of water-using units associated in clusters of water sources

$S = \{s_j \mid j = 1,2,...,NS\}$ the set of supply water sources

$C = \{c_k \mid k = 1,2,...,K\}$ the set of contaminants

$M = \{m_{i,k} \mid i = 1,2,...,N,\ \ k = 1,2,...,K\}$ the set of mass load of contaminant k transferred in water-using unit $u_{i,}$ [g/h]

$L = \{L_i \mid i = 1,2,...,N\}$ the set of streams representing water losses.

$\mathscr{L} = \{\ell_{ij} \mid i = 0,1,2,...,N, j = 1,2,...,N+1\}$ set of pipes length between sources and water-using units, between water-using units and between water-using units and treatment units.

As in Chapter 3, each water-using unit is defined by maximum inlet/outlet concentration and the mass load of the contaminants to be transferred from process streams to water streams. The water network can be fed by one or more supply water sources with different levels of contamination and can produce effluents sent to treatment unit. I define the water network as oriented graph, illustrated in Fig.3.3 and Fig.3.4, using the same ordering criteria: “by freshwater consumption” criterion (*Fcrt*) and ”by mass load” criterion (*Lcrt*). In next paragraphs, the mathematical model is formulated, considering main components of water network. For this reason, in formulation of cost function is not taken into account deposit and treatment facilities. This can be developed in other kind of model, possible to be tackled in future.

Optimisation problem is solved using a procedure based on GA as presented in Chapter 3. Methodology applicability is illustrated presenting two case studies:

- Design of optimal water network topology for minimum total annualised cost (underlying the influence of supply water sources in four scenarios) (Lavric et al., 2005; Lavric et al., 2007a)

- Design of optimal water network topology for weighted objective function based on supply water flowrate and topological index (underlying the role of objective function components) (Iancu et al., 2006).

4.3. Mathematical model

I formulate a similar mathematical model as in paragraph 3.2., for the general case, applicable to the problem tackled in this chapter (Eqs.3.1 - 3.8). The objective functions are formulated in next paragraph for a design problem. Steady state operation and perfectly mixed vessels for water-using units are considered.

4.3.1. Optimal pipe diameter

In the case of cost based objective function, to get more economic influence on water network topology, I propose an original approach based on optimal pipe diameter. This calculation is adapted from literature (Bratu, 1984; Peters et al., 2003) to fit water network mathematical model already mentioned.

Pipe diameter cost-based optimisation is a trade-off between a generic investment term and a basic plant/installation/unit operation and maintenance term, gathered into a standard economic objective function. In design process of an optimum water network topology, the simplest and yet sufficiently accurate economic objective function to be considered should be *the sum of the fixed charges for investment and maintenance in the piping system* (the generic investment term) and *the pumping costs* (the basic network operating term).

The total annualised cost of the pipe unit length is a sum of pumping costs and fixed charges for piping system (Peters & Timmerhaus, 2003).

$$\mathscr{C}_{ij} = \left([\mathscr{C}]_{pumping} + [\mathscr{C}]_{pipe} \right)_{ij} \tag{4. 1}$$

The investment term includes also the cost of specific equipment (water pumps and fittings). The piping cost per unit length per year includes annual fixed charges (as return of investment and maintenance) expressed as a function of initial cost for the completely install pipe. This cost depends on the pipe diameter D_{ij}, being expressed reported to reference diameter D_r.

$$[\mathscr{C}]_{pipe,ij} = (1+f) \cdot T \cdot \left(\frac{D_{ij}}{D_r} \right)^n \cdot G_F \tag{4. 2}$$

Pumping cost depends on the cost of energy for overcoming frictional losses due to pipe flow and fittings, efficiency of motors and pumps and pipe diameter. The exponents of the pumping term depend upon the flow regime and the relationship chosen to express χ Fanning friction factor. For new and smooth steel pipes this relation has following form :

$$\chi = A \cdot Re^{-\gamma} \tag{4. 3}$$

So, apart from some variations which could be regarded as relatively small, the overall network pressure drop remains the same, which means that the number and composition of the pumps' network could be seen as fixed.

For water piping system, the pumping cost per pipe length depends on pressure drop on pipe, characteristics of fluid and efficiency of motors and pumps:

$$[\mathscr{C}]_{pumping}\Big|_{ij} = \varepsilon \cdot \frac{H_y}{E} \cdot \frac{X_{ij}}{\rho} \cdot \Delta p_{ij} \cdot (1+J) \tag{4. 4}$$

for Δp_{ℓ} expressed by Fanning type equation, the pumping cost per pipe length is:

$$[\mathscr{C}]_{pumping}\Big|_{ij} = A' \cdot \varepsilon \cdot \frac{H_y}{E} \cdot (1+J) \cdot \frac{X_{ij}^{3-\gamma} \cdot \mu^{\gamma}}{D_{ij}^{5-\gamma} \cdot \rho^2} \tag{4. 5}$$

Consequently, the explicit form of total annualised cost of pipe unit length is:

$$\mathscr{C}_{ij} = A' \cdot \varepsilon \cdot \frac{H_y}{E} \cdot (1+J) \cdot \frac{X_{ij}^{3-\gamma} \cdot \mu^{\gamma}}{D_{ij}^{5-\gamma} \cdot \rho^2} + (1+f) \cdot T \cdot \left(\frac{D_{ij}}{D_r} \right)^n \cdot G_F \tag{4. 6}$$

The specific variable is only pipe diameter D_{ij}. Function given by Eq. 4.6 is always positive and its minimum can be obtained when its derivative with respect with pipe diameter D_{ij} vanishes. Solving for pipe diameter, the optimum value $\mathscr{D}_{ij}$ is obtained.

Corresponding to the flow regime, following expressions can be deduced:

Turbulent : $$\mathcal{D}_{ij} = \left[\frac{6.04 \cdot 10^{-4} \cdot D_r^n \cdot X_{ij}^{2.84} \cdot \mu^{0.16} \cdot \varepsilon \cdot (1+J) \cdot H_y}{n \cdot (1+f) \cdot T \cdot E \cdot G_F \cdot \rho^2}\right]^{1/(4.84+n)} \tag{4.7}$$

Laminar : $$\mathcal{D}_{ij} = \left[\frac{0.1628 \cdot D_r^n \cdot X_{ij}^{2} \cdot \mu \cdot \varepsilon \cdot (1+J) \cdot H_y}{n \cdot (1+f) \cdot T \cdot E \cdot G_F \cdot \rho^{1.16}}\right]^{1/(4+n)} \tag{4.8}$$

Optimal pipe diameter can be calculated specifically considering the values of factor n for steel pipes, typically used in water networks:

$$n = \begin{cases} 1.5 & \text{if } \mathcal{D}_{ij} \geq D_r \\ 1.0 & \text{if } \mathcal{D}_{ij} < D_r \end{cases} \tag{4.9}$$

Eqs 4.7 and 4.8 take following forms:

Turbulent and $\mathcal{D}_{ij} \geq D_r$ $$\mathcal{D}_{ij} = \frac{X_{ij}^{0.448}}{\rho^{0.316}} \cdot \mu^{0.025} \left[\frac{1.63 \cdot 10^{-6} \cdot \varepsilon \cdot (1+J) \cdot H_y}{(1+f) \cdot T \cdot E \cdot G_F}\right]^{0.158} \tag{4.10}$$

Turbulent and $\mathcal{D}_{ij} < D_r$: $$\mathcal{D}_{ij} = \frac{X_{ij}^{0.487}}{\rho^{0.343}} \cdot \mu^{0.027} \left[\frac{1.53 \cdot 10^{-5} \cdot \varepsilon \cdot (1+J) \cdot H_y}{(1+f) \cdot T \cdot E \cdot G_F}\right]^{0.171} \tag{4.11}$$

Laminar and $\mathcal{D}_{ij} \geq D_r$: $$\mathcal{D}_{ij} = \frac{X_{ij}^{0.364}}{\rho^{0.364}} \cdot \mu^{0.182} \left[\frac{4.39 \cdot 10^{-4} \cdot \varepsilon \cdot (1+J) \cdot H_y}{(1+f) \cdot T \cdot E \cdot G_F}\right]^{0.182} \tag{4.12}$$

Laminar and $\mathcal{D}_{ij} < D_r$: $$\mathcal{D}_{ij} = \frac{X_{ij}^{0.4}}{\rho^{0.4}} \cdot \mu^{0.2} \left[\frac{4.14 \cdot 10^{-3} \cdot \varepsilon \cdot (1+J) \cdot H_y}{(1+f) \cdot T \cdot E \cdot G_F}\right]^{0.2} \tag{4.13}$$

Eqs. 4.10 - 4.13 can be simplified by substituting average numerical values for some of the less critical terms applicable for industrial conditions (Peters & Timmerhaus, 2003): J=35%, H_y=8760 hours/year, E=50%, f=1.4, G_F=1.2, T=2.43$/m for a D_r=0.0254m steel pipe, ε=0.05$/kWh.

Consequently, following simplified equations are obtained:

Turbulent and $\mathcal{D}_{ij} \geq D_r$: $$\mathcal{D}_{ij} = \frac{0.363 \cdot X_{ij}^{0.45} \cdot \mu^{0.025}}{\rho^{0.32}} \tag{4.14}$$

Turbulent and $\mathcal{D}_{ij} < D_r$: $$\mathcal{D}_{ij} = \frac{0.49 \cdot X_{ij}^{0.49} \cdot \mu^{0.027}}{\rho^{0.35}} \tag{4.15}$$

Laminar and $\mathcal{D}_{ij} \geq D_r$: $$\mathcal{D}_{ij} = \frac{0.863 \cdot X_{ij}^{0.36} \cdot \mu^{0.18}}{\rho^{0.36}} \tag{4.16}$$

Laminar and $\mathscr{D}_{ij} < D_r$: $$\mathscr{D}_{ij} = \frac{1.33 \cdot X_{ij}^{0.4} \cdot \mu^{0.2}}{\rho^{0.4}} \quad (4.\ 17)$$

4.3.2. General formulation

Water network optimisation based on economic considerations mathematical model proposed in this Thesis represents a highly nonlinear NLP problem. Similar original approach for different variables categories is considered as in Chapter 3.

The independent variables are same as in the case of minimum supply water flowrate problem, presented in paragraph 3.2, X_{ij} $(i=1,2,...,N\text{-}1,\ j=2,...,N)$, the flowrates of streams connecting different units, observing the oriented nature of graph for water network.

Problem parameters are:

N number of water using units

K number of contaminants

NS number of water sources

$M = \{m_{ki} \mid i = 1,2,...,N,\ k=1,2,...,K\}$ set of mass load per unit and contaminant

$L = \{L_i \mid i = 1,2,...,N\}$ set of water losses from each unit

$C^s = \{C_k^s \mid k = 1,2,...,K,\ s = 1,2,...,NS\}$ set of contaminants concentration for each water supply source

$C^{in,max} = \{C_{ki}^{in,max} \mid k = 1,2,...,K,\ i = 1,2,...,N\}$ set of inlet limiting concentration per contaminant and unit

$C^{out,max} = \{C_{ki}^{out,max} \mid k = 1,2,...,K,\ i = 1,2,...,N\}$ set of outlet limiting concentration per contaminant and unit.

$\mathscr{L} = \left\{\ell_{ij} \mid i = 0,1,2,...,N, j = 1,2,...,N+1\right\}$ set of pipes length between sources and water-using units, between water-using units and between water-using units and treatment unit.

$\rho,\ \mu$ physical properties of water.

The dependent variables of the problem are calculated from model equations :

$F^s = \{F_i^s \mid i = 1,2,...,N\}$ set of water supply flowrate for each u_i

$W = \{W_i \mid i = 1,2,...,N\}$ set of wastewater flowrate for each u_i

$C^{in} = \{C_{ki}^{in} \mid i = 1,2,...,N\ ;\ k = 1,2,...,K\}$ set of concentration of contaminant k at the entrance of u_i

$C^{out} = \{C_{ki} \mid i = 1,2,...,N \; ; \; k = 1,2,...,K\}$ set of concentration of contaminant k at the exit of u_i

$\mathcal{D} = \{\mathcal{D}_{ij} \mid i = 0,1,2,...,N, j = 1,2,...,N+1\}$ set of pipes optimal diameter for entire water network calculated as in paragraph 4.3.1.

$\mathcal{C} = \{\mathcal{C}_{ij} \mid i = 0,1,2,...,N, j = 1,2,...,N+1\}$ set of total annualised cost of the pipe unit length optimised with respect to $\mathcal{D}_{ij}$.

The total number of dependent variables of this problem is:

$\dim(W) + \dim(F^s) + \dim(C^{in}) + \dim(C^{out}) + \dim(\mathcal{D}) + \dim(\mathcal{C})$ = N + N + NK + NK +N(N-1)/2+N(N-1)/2= 2N + 2NK+N(N-1) variables.

Water flowrate from supply sources for each water-using unit, F_i^s, is calculated in the same manner as presented in paragraph 3.4.2., based on Limiting Water Profile concept and feasibility criteria (Wang & Smith,1994a). Based on F_i^s values, the wastewater flowrates W_i are calculated from total mass balance around unit u_i (Eqs.3.1). Then the inlet and outlet concentrations C^{in}, C^{out}, using Eqs. 3.4 and pipes optimal diameter $\mathcal{D}_{ij}$, using Eqs. 4.14-4.17 are calculated. Finally the total annualised cost (Eqs.4.6) is calculated for each pipe of the water network.

The total number of equations can be evaluated as follows: *N* equations for F_i^s, *N* equations for W_i, $N{\cdot}K$ equations for C^{in}, $N{\cdot}K$ equations for C^{out}, *N(N-1)/2* equations for $\mathcal{D}$ and *N(N-1)/2* equations for $\mathcal{C}$, so, *2N + 2NK+N(N-1)* equations.

4.4. Design criteria

4.4.1. Minimum total annualised cost

In formulation of optimisation problem, it is considered the cost of pumps as essentially invariant with pipe diameter. This simplifying assumption is based upon analysis of data from different industrial water networks. Network throughput water flowrate always tends to stabilise in the vicinity of the minimum supply, already available from classical network optimisation. In this respect, I propose (Lavric et al., 2005, Lavric et al., 2007a) as objective function to minimise the total annualised cost of pipes given by network topology (as a sum of cost of pipes between sources and units, cost of pipes between units and cost of pipes between units and treatment unit). It is important to stress that unit cost set has an original form developed in my work : optimised with respect to pipes diameter.

$$\min C_{total} = \min\left[\underbrace{\sum_{j=1}^{N} \mathcal{C}_{0,j}\cdot \ell_{0,j}}_{\text{Supply network pipes}} + \underbrace{\sum_{i=1}^{N-1}\sum_{j=i+1}^{N} \mathcal{C}_{i,j}\cdot \ell_{i,j}}_{\text{Internal network pipes}} + \underbrace{\sum_{j=1}^{N} \mathcal{C}_{j,N+1}\cdot \ell_{j,N+1}}_{\text{To treatment pipes}}\right] \tag{4. 18}$$

In objective function defined by Eq.4.18 the optimum economic pipes diameter is a key parameter with important influence. This, in turn, depends upon the flowrate through the pipe, i.e. the minimum total cost of the network piping system implies low values for the supply water flowrate. There are cases in which these values are slightly increased than the minimum supply water consumptions as I demonstrated in Chapter 3, minimising supply water flowrate for multiple water sources. This could happen only when the flow regime is in the proximity of the critical Reynolds number for some pipes. To get a lower economic pipe diameter, during the application of optimisation algorithm a slightly higher value is chosen for the actual flowrate, if it is the case, to pass from the laminar to the turbulent regime (Lavric et al., 2005, Lavric et al., 2007a). Always, the closest diameter to Pipe Standard (Bratu,1984) is chosen to keep, of course, the same flowing regime.

4.4.2. Minimum topological index of water network

When data regarding the costs related to pipes, pumping energy and pumps are not available, unreliable or could undergo large fluctuations, I propose another optimisation objective function related to the *minimum active water network length*, including both the internal topology and the supply&discharge piping systems.

4.4.2.1 Topological index of water network

As an original contribution, I define topological index τ the ratio between *total active lengths* (length of pipes used for transportation of supply water, reused water and effluents) and *total lengths of piping system* (overall length of pipes between sources and units, pipes between different units and pipes between units and treatment unit), as I presented in Iancu et al., 2006. The topology of water network has a major influence on this factor, as it measures the degree of network topology modification by installing / removing pipes.

As optimisation criterium I formulate an objective function based on topological index, avoiding the explicit use of any economic term/criterium. I propose this approach because it is known that economic factors strongly depend upon the market conditions. Sometimes correct economic figures and/or trends are hard to estimate, thus affecting the confidence level of results. It is obvious that the topological index has implicit economic value as water network cost strongly depends on total active pipes length.

$$\tau = \frac{\sum\limits_{\substack{j=1 \\ F_j^S>0}}^{N} l_{0,j} + \sum\limits_{i=1}^{N-1} \sum\limits_{\substack{j=i+1 \\ X_{i,j}>0}}^{N} l_{i,j} + \sum\limits_{\substack{j=1 \\ W_j>0}}^{N} l_{j,N+1}}{\sum\limits_{j=1}^{N} l_{0,j} + \sum\limits_{i=1}^{N-1} \sum\limits_{j=i+1}^{N} l_{i,j} + \sum\limits_{j=1}^{N} l_{j,N+1}} \tag{4. 19}$$

4.4.2.2 Weighted objective function

To combine the effect of more factors, I define also a weighted objective function, as is a linear combination between the normalised supply water flowrate and topological index (Iancu et al., 2006). Weighting factor is denoted by ω, underlining the relative role of objective function components.

$$\min \mathscr{J} = \min\left(\omega \, \frac{\sum\limits_{i=1}^{N} \max\left(F_{i,in}^{s,min}, F_{i,out}^{s,min}\right)}{\sum\limits_{i=1}^{N} \max\limits_{k} \left(\frac{m_{ki}}{C_{ki}^{out,max} - C_{ki}^{in,max}} \right)} + (1-\omega)\,\tau \right) \tag{4. 20}$$

When ω = 1 supply water flowrate is minimised. When ω = 0 topological index is minimised. For $0<\omega<1$ different influences of each component function on the weighted objective function is obtained. Knowing these influences, in practical situations, specific values for ω factor can be chosen.

4.5. The optimisation algorithm

The optimisation algorithm used to solve mathematical model subjected to an economical objective function, topological index based objective function or weighted objective function (given by Eq. 4.20) is a hybrid variant of a classical GA (Raducan et al., 2004). The benefits of using this GA variant are proven solving with better results a number of difficult problems as I present in Chapter 3 and I already published (Lavric et al., 2004 a,b,c, Lavric et al., 2005). It is worth mentioning two important improvements implemented into this GA variant, making it to have better convergence (Raducan et al., 2004):

1. When the part of the population disregarded from interbreeding using one-point crossover method has frequencies which are too low, corresponding to badly fitted individuals, the new population is completed applying cloning to randomly selected individuals from the better fitted part of the old population.
2. When elitism is envisaged (the best individual is cloned throughout all generations), the rest of the new population not borne throughout crossover is generated randomly around this best fitted individual, using a standard deviation which shrinks with each passing of generations.

The computation of the objective function (Eq.4.18 or Eq.4.20) involves the availability of an internal water flow distribution *X* through the network, encoded in a chromosome, which is an individual from a population of feasible solutions. The feasibility implies only that each individual flowrate (for internal water streams) observes the restrictions of water-using units. The algorithm of optimisation (GA) generates with random mechanism an initial population $\{X_o\}$, each individual observing all imposed restrictions related to upper bound as presented in Eq. 3.15. If a internal flowrate in the network does not cope the imposed restrictions, the chromosome is eliminated. The fitness functions gives a major for each individual X how far is from the best-so-far one. After ranking all individuals according their fitness performance, a new population is generated, applying crossover, cloning and mutation. For the new population, if internal network flowrates do not observe imposed restrictions, that chromosome is eliminated. In the case of cost based objective function, for best chosen chromosome, pipe optimum diameter is computed with Eqs. 4.14 to 4.17, then the total annualised cost is computed with Eq.4.18, as described in my papers Lavric et al, 2005 and Lavric et al., 2007a.

4.6. Design of optimal water network topology for minimum total annualised cost

Water network optimisation is possible for minimum supply water flowrate using the methodology I describe in Chapter 3. Important savings are obtained when a real water network is optimised with minimum supply water as objective function, considering water network ranked as an oriented graph.

For both ranking criteria (Fcrt and Lcrt) good solutions are obtained, but it is obvious that an objective function based on economic considerations could be a better support for decision to choose the best water network topology.

Table 4. 1 Matrix of pipes length (m)

$\mathscr{D}_{ij}$ (mm)	S1	S2	S3	S4	U1	U2	U3	U4	U5	U6	U7	U8	U9	U10	U11	U12	U13	U14	P15	T
S1	x	x	x	x	1,280	1,530	450	300	1400	370	420	430	450	370	580	600	1,460	1,130	760	x
S2	x	x	x	x	650	900	650	820	770	270	290	310	330	270	750	780	830	500	130	x
S3	x	x	x	x	1,820	1,350	540	315	4,100	730	240	340	550	730	880	690	1,640	1,210	960	x
S4	x	x	x	x	750	880	570	495	920	375	920	180	400	260	550	890	430	450	250	x
U1	x	x	x	x	x	50	550	1,580	500	500	480	460	450	500	600	650	600	100	100	540
U2	x	x	x	x	x	x	50	1,830	250	650	630	610	600	500	550	600	500	75	75	410
U3	x	x	x	x	x	x	x	750	1,220	420	500	550	570	420	480	70	1,430	800	400	900
U4	x	x	x	x	x	x	x	x	1,700	670	650	630	620	670	880	900	1,760	1,430	1,060	170
U5	x	x	x	x	x	x	x	x	x	920	790	850	870	920	1,390	1,460	320	250	700	2,150
U6	x	x	x	x	x	x	x	x	x	x	130	180	200	20	470	540	1,100	700	340	1,450
U7	x	x	x	x	x	x	x	x	x	x	x	50	70	70	600	670	1,050	650	340	950
U8	x	x	x	x	x	x	x	x	x	x	x	x	20	20	650	720	1,020	630	390	970
U9	x	x	x	x	x	x	x	x	x	x	x	x	x	20	670	740	1,000	600	410	940
U10	x	x	x	x	x	x	x	x	x	x	x	x	x	x	470	540	1,100	700	340	810
U11	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	70	1,570	1170	840	450
U12	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	1,600	1320	850	640
U13	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	350	770	1,800
U14	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	420	1,700
U15	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	X	1,550
T	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	X

In this paragraph I develop a case study with four scenarios to illustrate the importance of using total annualised cost as objective function for optimal water network design, when more water sources are available. I compare the results with those obtained for the case study developed in paragraph 3.7, when total water supply flowrate objective function is used. I already gave in Chapter 3 paragraph 3.7.3 a detailed description of the industrial site (integrated oil refinery). Same data is used in this case study. For such large water network, the total annualised cost is important decision factor to implement an optimal solution for water network as it stands for more components : investment, maintenance and operation. As I present in paragraph 3.7.3, I consider fifteen water using processes, four water sources and six contaminants, as in my paper Iacob et al., 2004, with specific data given in Table 3.9 and Table 3.10. Additionally, for calculation of piping system length, the distances between different water supply sources, water-using units and treatment unit are given in Table 4.1. The existing water network system does not include water reuse, as I present in Fig. 3.23. The complete procedure of water supply sources allocation according to units restrictions (clusters) encourage to use contamined source, as water cost is lower. Nevertheless, when using a cost-based objective function, both the piping and pumping costs from the water source can play an important role to allocate particular unit to a source. It could happen that a source matches the inlet restrictions of a water-using unit, but the distance between the source and the unit could be so big that the algorithm disregards selecting that source.

The first step in designing an optimal topology for water network with minimum annualised total cost, in agreement with the methodology I propose in paragraph 4.5, is to order the water-using units according one of ranking criteria described in Chapter 3 and published in my paper Lavric et al., 2005 : water network ordered by freshwater flowrate needed by (Fcrt) or ordered by mass load of transferred contaminant (Lcrt). Both criteria conforme to the principle of equipartition of the driving force, which ensures smaller entropy generation. The order thus established represents the starting point for the iterative process to find the optimal network topology as oriented graph. Next, I discuss in terms of topology differences, the results obtained when using contaminant-free supply water (Scenario A), then two, three of four water supply sources (Scenarios B-D). I am interested to select the water network topology with lower total annualised cost, as given by Eq. 4.18. To show the importance of using cost-based objective function same scenarios are compared to results obtained for supply water flowrate objective function presented in paragraph 3.7.4. Relevant results are presented in common tables with case study developed in Chapter 3 paragraph 3.7.4 to underline the relative importance of using each objective function. The above methodology, representing an original contribution in my Thesis, allows to calculate all dependent variables, from which some are particularly considered in following analyses:

- F^s water supply flowrate for each water-using unit
- $\mathscr{D}$ set of optimal pipes diameters for entire water network
- $\mathscr{C}$ set of total annualised cost of pipe unit lenght for optimised pipe diameters set
- $[\mathscr{C}]_{pumping}$ total annualised operating cost
- $[\mathscr{C}]_{piping}$ total annualised investment cost
- $\mathscr{L}$ set of active pipes lenghts

4.6.1. Optimisation Scenario A: Freshwater source (S1)

In this scenario I perform optimisation of a water network using a single supply water source S1 – uncontaminated water (freshwater). For this reason source S1 has higher price than the other three sources (which have different degrees of contamination). But the great influence in this scenario comes from optimal diameter for each new pipe installed into the system. Units ranking is presented in paragraph 3.7.4.1.

a) Total supply water flowrate

For both criteria I noticed that the minimum total supply water flowrate is slightly increased compared to Chapter 3 paragraph 3.7.4.1 results, the difference is due to the trade-off between minimum freshwater consumption and minimum total annualised cost. The solution obtained in this paragraph has lower cost. The water flowrate for units which need bigger water flowrate is close for both objective functions.

Table 4. 2 Supply water flowrate per water-using units: Scenario A (Freshwater source only, S1)

Water unit	Supply Water Flowrate objective function		Total Annualised Cost objective function	
	Minimum supply water flowrate (t/h)		Minimum supply water flowrate (t/h)	
	Fcrt	Lcrt	Fcrt	Lcrt
U1	131.9	131.9	131.9	131.9
U2	70.5	69.9	68.1	69.9
U3	204.5	204.5	204.5	204.5
U4	0.0	0.0	0.0	0.0
U5	0.0	0.0	0.0	0.0
U6	0.0	4.7	33.1	0.0

U7	28.5	30.9	31.9	31.9
U8	1.7	5.7	9.2	10.3
U9	2.0	2.0	2.0	2.0
U10	0.0	0.4	0.0	0.0
U11	0.7	0.0	0.0	0.0
U12	0.0	1.3	7.8	13.3
U13	0.0	0.8	0.0	0.0
U14	0.4	0.7	0.0	0.0
U15	1.9	0.0	5.1	0.0
Total flowrate (t/h)	**442.1**	**452.8**	**493.6**	**463.8**

b) Total wastewater flowrate

The flowrate of wastewater streams have the close value to results from Chapter 3 as I present in Table 4.3. This variable is not very important to select the best water network topology.

Table 4. 3 Wastewater flowrate per water-using units: Scenario A (Freshwater source only, S1)

Water unit	Supply Water Flowrate objective function		Total Annualised Cost objective function	
	Wastewater flowrate (t/h)		Wastewater flowrate (t/h)	
	Fcrt	Lcrt	Fcrt	Lcrt
U1	0.0	0.0	0.0	0.0
U2	51.0	20.5	52.4	34.1
U3	0.0	0.0	0.0	0.0
U4	0.4	17.0	0.6	3.6
U5	0.0	8.9	0.4	3.5
U6	40.1	35.0	30.6	34.6
U7	0.2	30.4	33.9	30.0
U8	0.1	0.1	11.1	0.0
U9	0.0	0.0	0.0	0.0
U10	1.6	0.2	7.7	0.7
U11	3.9	2.5	7.0	11.7
U12	17.2	0.0	17.0	1.6
U13	0.3	0.2	1.8	0.3
U14	1.0	2.5	5.1	6.4
U15	0.3	9.5	0.0	11.3
Total flowrate (t/h)	**116.1**	**126.8**	**167.6**	**137.8**

Table 4. 4 Matrix of standardised of pipes optimum diameter : Scenario A (Freshwater source only, S1) – Fcrt criterion

$\mathscr{D}_{ij}$ (mm)	S1	U1	U3	U9	U5	U13	U4	U15	U10	U11	U14	U8	U7	U12	U6	U2	T
S1	x	155.50	210.00	26.00	-	-	-	41.25	-	-	-	52.50	105.50	52.50	105.50	130.00	-
U1	x	x	-	-	-	-	21.25	-	21.25	21.25	21.25	-	-		21.25	-	-
U3	x	x	x	-	15.75	26.00	35.75	-	26.00	35.75	35.75	21.25	-	52.50	15.75	-	-
U9	x	x	x	x	-	-	-	-	-	-	-	-	26.00	-	-	-	-
U5	x	x	x	x	x	-	-	-	-	-	-	-	-	-	-	-	15.75
U13	x	x	x	x	x	x				15.75	-	-	-	-	-	-	26.00
U4	x	x	x	x	x	x	x		21.25	21.25	-	-	-	21.25	-	-	21.25
U15	x	x	x	x	x	x	x	x	35.75	12.25	21.95	15.75	-	-	-	-	-
U10	x	x	x	x	x	x	x	x	x	21.95	-	-	-	-	-	-	52.50
U11	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-	-	52.50
U14	x	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-	41.25
U8	x	x	x	x	x	x	x	x	x	x	x	x	-	-	-	-	52.50
U7	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-	-	105.50
U12	x	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-	67.00
U6	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	35.75	105.50
U2	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	105.50
T	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x

x- forbidden matches due to the oriented graph, -no pipes between units

c) Optimum pipe diameter

After optimisation, the solution is to install new pipes between water-using units. Optimal pipes diameters $\mathscr{D}_{ij}$, are calculated with Eqs. 4.14 - 4.17 then are addapted to observe Pipe Standard (Bratu,1984). For minimum total annualised cost objective function, the optimum pipe diameters set for Fcrt criterion is presented in Table 4.4. This variable influences both components of cost objective function : investment cost and operation cost.

d) Total annualised cost of water network

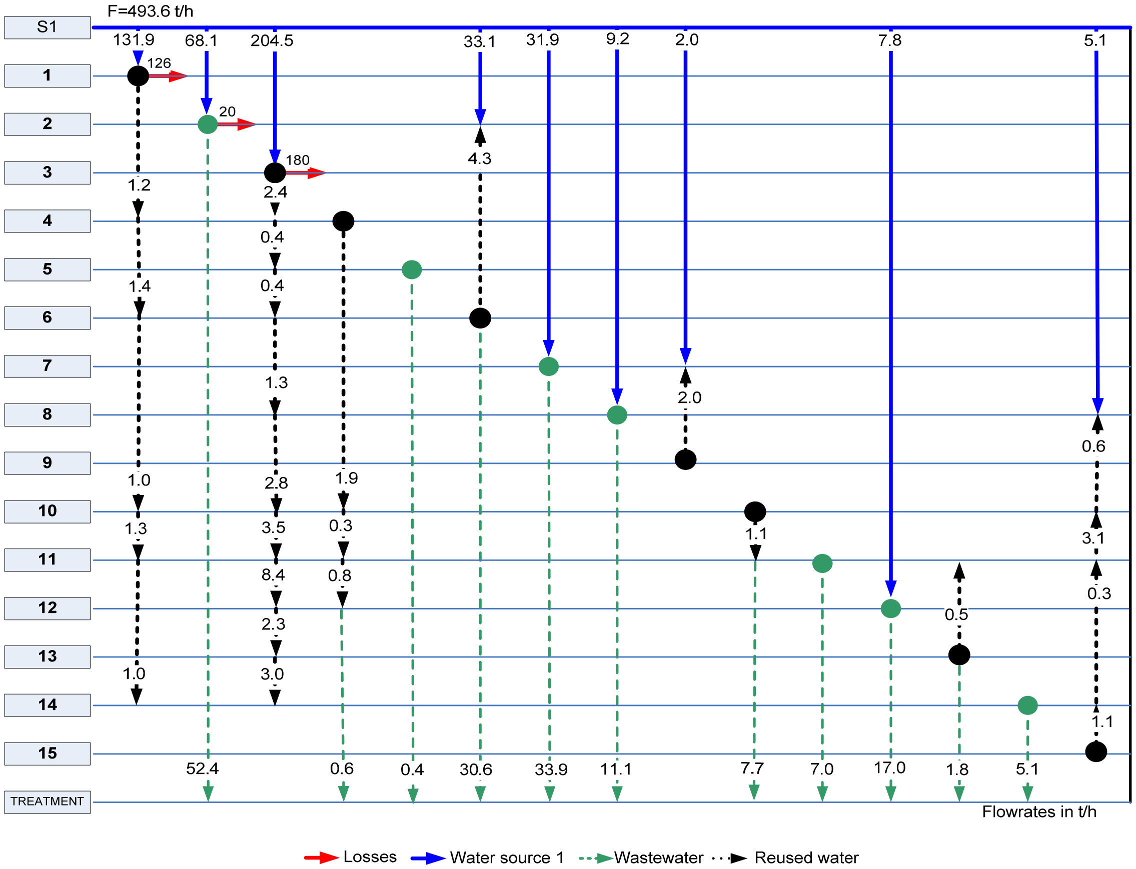
I present in Table 4.5 data calculated to select optimal topology obtained with both optimisation objective functions (supply water flowrate and total annualised cost) for both rsnking criteria (Fcrt and Lcrt). Comparing these results, I conclude that the most attractive solution is for the total annualised cost optimisation criterium (914,390 $/year).

Table 4. 5 Total annualised cost: Scenario A (Freshwater source only, S1)

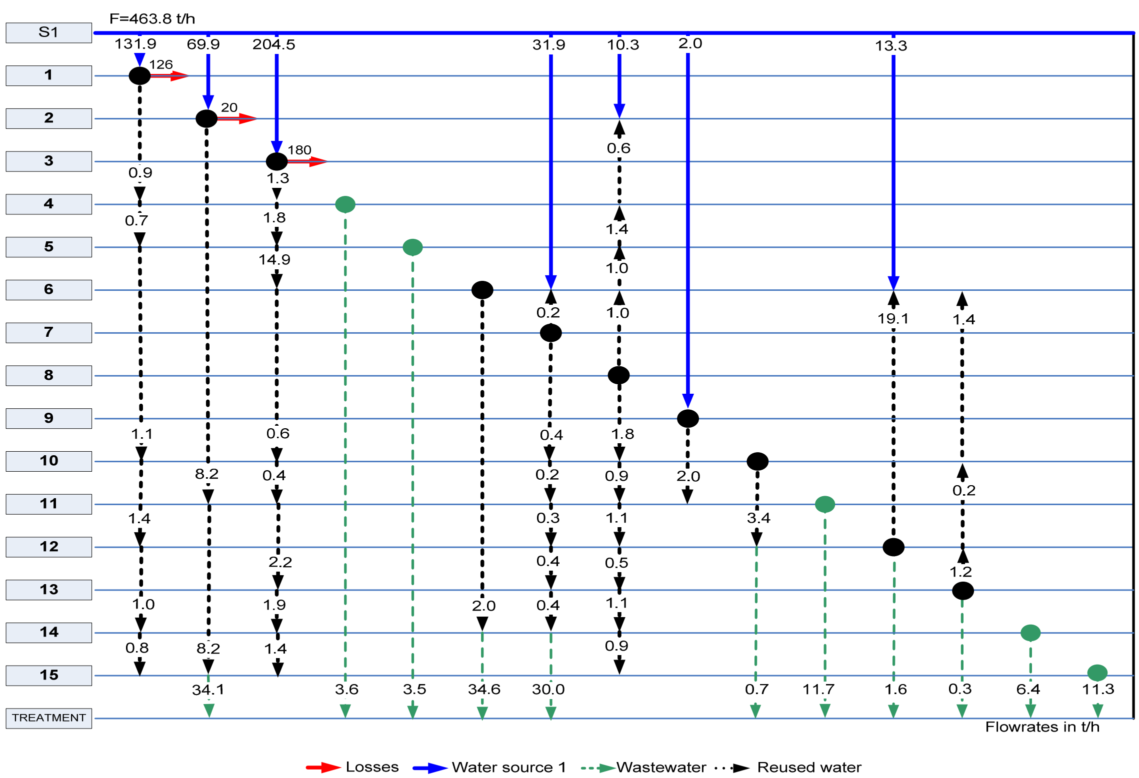
Cost type	Supply Water Flowrate objective function		Total Annualised Cost objective function	
	Fcrt	Lcrt	Fcrt	Lcrt
Source S1 flowrate, t/h	442.10	452.80	493.60	463.80
Reused water flowrate, t/h	98.30	112.70	46.40	87.10
Length of all pipes, m	51,630	53,555	34,360	40,375
Operating cost, $/year	235,240	247,709	168,158	195,346
Investment cost, $/year	690,420	801,615	746,232	781,384
Total Annualised Cost, $/year	**925,660**	**1,049,324**	**914,390**	**976,730**

e) Water network topology

In Fig. 4.1, I draw the optimal topology of water network from economical point of view, when only a freshwater source (S1) is considered. The topology is drawn for both both ranking criteria. They look more simplified compared to topologies presented in paragraph 3.7.4.1, Fig. 3.26, for supply water flowrate optimisation. For this reason, the total lenght of piping system is reduced by ~33% for Fcrt, respectivelly ~25% for Lcrt. For Fcrt presented in Fig. 4.1 a) all units have less connections compared to similar topology presented in Fig. 3.26 a) e.g. : unit U1 has five connections in Fig. 4.1 a) vs nine connections in Fig. 3.26 a), U5 has just connection to treatment unit vs 3 connections, U7-U14 have just connection to treatment or at most one additional connection vs more than two connections and one additional to treatment. For Lcrt the topology presented in Fig. 4.1 b) remains quite complicated compared to Fig. 4.1 a), however simplified compared to Fig. 3.26 b). Pipes length is bigger for Lcrt compared to Fcrt, as presented in Table 4.5.



a) Fcrt criterion topology



b) Lcrt criterion topology

Figure 4. 1 Total annualised cost optimised network topology: Scenario A (Freshwater source, S1)

4.6.2. Optimisation Scenario B: Water sources S1 & S2

In Scenario B, two water sources (S1 and S2) are considered to supply water network. Ranking water-using units is same as in Chapter 3, paragraph 3.7.4.2

a) Minimum supply water flowrate

Using two available water sources: S1 without contaminants and S2 slightly contaminated, for total annualised cost objective function, the total flowrate of supply water and distribution on water-using units remain unchanged, as in paragraph 3.7.4.2 :

S1 cluster = {U1, U3, U9, U13}

S2 cluster = {U2, U4, U5, U6, U7, U8, U10, U11, U12, U13, U14, U15}

Optimisation results are presented in Table 4.6 to compare both case studies. It is remarkable that total supply water flowrate is unchanged, 733.4 t/h distributed like in Chapter 3 case study : 338.4 t/h from S1 and 395 t/h from S2. Both ranking criteria gave same results. Allocation of water per units is identical for both case studies. Losses represent 326 t/h. Compared to Scenario A the total flowrate increased substantially eg for Fcrt from 493.6 t/h to 733.4 t/h. Water flowrate from S1 decreased from 493.6 t/h to 338.4 t/h, ie ~ 31%.

Table 4. 6 Supply water flowrate per water-using units: scenario B (Water sources S1 & S2)

Water unit	Supply Water Flowrate objective function		Total Annualised Cost objective function	
	Minimum Supply water flowrate (t/h)		Minimum Supply water flowrate (t/h)	
	Fcrt	Lcrt	Fcrt	Lcrt
U1	131.9	131.9	131.9	131.9
U2	355.1	355.1	355.1	355.1
U3	204.5	204.5	204.5	204.5
U4	0.0	0.0	0.0	0.0
U5	0.0	0.0	0.0	0.0
U6	0.0	0.0	0.0	0.0
U7	39.9	39.9	39.9	39.9
U8	0.0	0.0	0.0	0.0
U9	2.0	2.0	2.0	2.0
U10	0.0	0.0	0.0	0.0
U11	0.0	0.0	0.0	0.0
U12	0.0	0.0	0.0	0.0
U13	0.0	0.0	0.0	0.0
U14	0.0	0.0	0.0	0.0
U15	0.0	0.0	0.0	0.0
Total flowrate (t/h)	**733.4**	**733.4**	**733.4**	**733.4**

Source S1 is used as supply water in units U1, U3 and U9 and Source S2 is used only for units U2 and U7.

b) Total wastewater flowrate

For this case study slight differences are to notice compared to case study presented in paragraph 3.7.4.2. The wastewater flowrate is the same. The distribution on water-using units is quite different, as presented in Table 4.7. In the case study presented in Chapter 3, Scenario B seven units produce wastewater. In current Scenario B ten units produce wastewater if ranked upon Fcrt and seven units produce wastewater for ranking upon Lcrt. These differences can be explained as consequence of redistribution of internal reused water streams in the network for different conditions of optimisation.

Table 4. 7 Wastewater flowrate per water-using units: scenario B (Water sources S1 & S2)

Water unit	Supply Water Flowrate objective function		Total Annualised Cost objective function	
	Minimum wastewater flowrate (t/h)		Minimum wastewater flowrate (t/h)	
	Fcrt	Lcrt	Fcrt	Lcrt
U1	0.0	0.0	0.0	0.0
U2	0.0	0.0	0.0	0.0
U3	0.0	43.5	0.0	0.0
U4	0.0	0.0	4.4	154.9
U5	0.0	0.0	0.4	146.3
U6	51.4	98.8	169.7	41.7
U7	0.0	25.5	0.0	0.0
U8	66.7	52.9	15.4	6.1
U9	0.0	0.0	0.0	0.0
U10	40.5	71.1	7.2	0.7
U11	69.4	0.0	9.9	12.4
U12	127.9	42.8	166.0	26.4
U13	0.0	72.8	11.9	8.7
U14	9.1	0.0	13.4	1.7
U15	42.4	0.0	9.1	8.5
Total flowrate (t/h)	**407.4**	**407.4**	**407.4**	**407.4**

c) Optimum pipe diameter

During optimisation procedure at each iteration once calculated the flowrate of internal stream X_{ij} using Eqs. 4.14 - 4.17 optimal diameter $\mathcal{D}_{ij}$ is calculated. When optimisation process is finished final standardised values (Bratu,1984) are reported.

Table 4. 8 Matrix of standardised pipes optimum diameter: Scenario B (Water sources S1 & S2) – Fcrt Criterion

$\mathcal{D}_{ij}$ (mm)	S1	S2	U1	U2	U3	U7	U9	U5	U13	U4	U15	U10	U11	U14	U8	U12	U6	T
S1	x	x	155.50	-	210.00	-	26.00	-	-	-	-	-	-	-	-	-	-	-
S2	x	x	-	275.00	-	105.00	-	-	-	-	-	-	-	-	-	-	-	-
U1	x	x	x	-	-	-	-	21.25	-	21.25	-	21.25	-	-	-	21.25	21.25	-
U2	x	x	x	x	-	-	-	-	-	-	-	-	-	-	41.25	210.00	210.00	-
U3	x	x	x	x	x	-	-	35.75	41.25	-	-	-	35.75	52.50	-	-	-	-
U7	x	x	x	x	x	x	-	35.75	35.75	26.00	52.50	35.75	35.75	35.75	53.50	15.75	35.75	-
U9	x	x	x	x	x	x	x	8.75	-	8.75	12.25	12.25	12.25	12.25	12.25	12.25	12.25	-
U5	x	x	x	x	x	x	x	x	21.25	21.25	12.25	26.00	26.00	-	-	-	-	12.25
U13	x	x	x	x	x	x	x	x	x	-	-	-	-	-	-	-	-	67.00
U4	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-	-	-	35.75
U15	x	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-	-	52.50
U10	x	x	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-	41.25
U11	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-	-	-	52.50
U14	x	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-	-	67.00
U8	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-	67.00
U12	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	21.25	210.00
U6	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	210.00
T	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x

x- forbidden matches due to the oriented graph, -no pipes between units

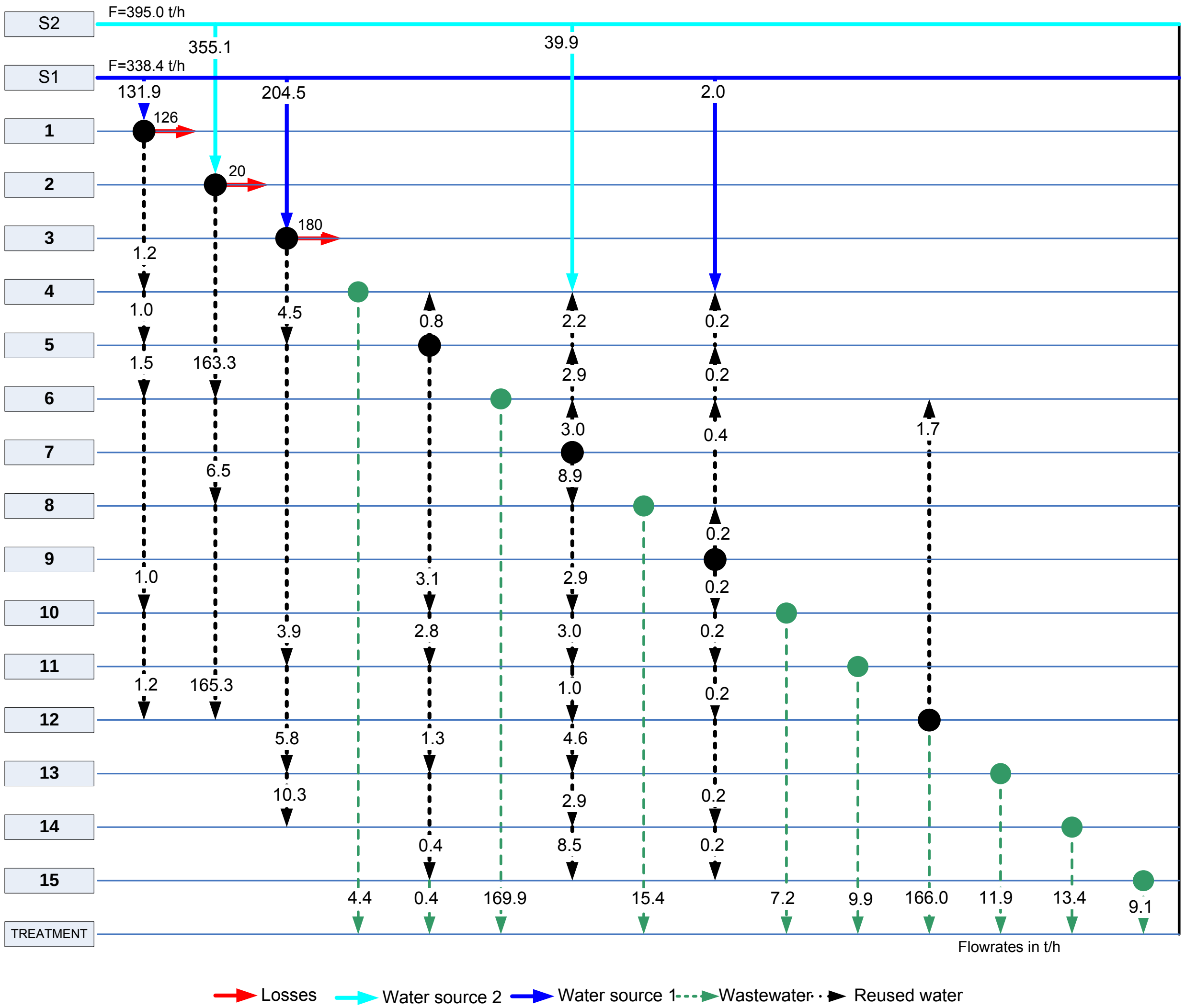


Figure 4. 2 Total annualised cost optimised network topology: Scenario B (Water sources S1 & S2) – Fcrt criterion

These final optimal values for pipe diameters are presented in Table 4.9. For unit U2, the pipe coming from source S2 has the biggest diameter. The diameter of pipes going from units to treatment unit are generally bigger as internal pipes.

d) Total cost of water network

Data related to calculation of total annualised cost of water network is given in Table 4.9, to compare results for both objective functions and both ranking criteria. The results obtained show that both objective functions search for minimium supply water flowrate, but after this step in the case of total annualised cost objective function the search continues to find improved topology with shorter pipes length and better allocation of reused water between units. It can be noticed that minimising the total annualised cost the topology is rationalised. To have a complete comparison between both case studies, costs are calculated as well for the topology obtained with supply water flowrate. The lowest total annualised cost is obtained as expected for the current case study. Fcrt ranking criterium gives lowest total annualised cost, 1,487,064 $/year sugesting the most attractive solution for this scenario.

Table 4. 9 Total annualised cost: Scenario B (Water sources S1 & S2)

Cost type	Supply Water Flowrate objective function		Total Annualised Cost objective function	
	Fcrt	Lcrt	Fcrt	Lcrt
Source S1 flowrate, t/h	338.40	338.40	338.40	338.40
Source S2 flowrate, t/h	395.00	395.00	395.00	395.00
Reused water flowrate, t/h	607.70	585.50	417.50	427.10
Length of all pipes, m	57,690	57,710	39,030	40,850
Operating cost, $/year	296,442	301,094	206,529	219,623
Investment cost, $/year	1,615,234	1,734,653	1,280,535	1,431,584
Total Annualised Cost, $/year	**1,911,676**	**2,035,747**	**1,487,064**	**1,651,207**

e) Water network topology

For this scenario, the topology is very much simplified when total annualised cost objective function is considered. In this respect, the total length of the pipes between the processes, between sources and processes and between processes and treatment unit is reduced globally with ~ 32 %. Compared to the topology obtained in Scenario A the pipes total length is quite close. The optimal topology for this scenario is presented in the Fig. 4.2. Units U1, U2, U3, U5, U7 and U9 produce reuse water streams. For the other units (U4, U6, U8, U10, U11, U13, U14 and U15 quite simple topology is obtained i.e. connection direct to treatment unit. Total reused water flowrate is 417.5 t/h representing a reduction of ~31% compared to case study based on supply water flowrate objective function Scenario B (604.4 t/h) presented in paragraph 3.7.4.2. This is another proof of more simplified topology obtained for cost based objective function.

4.6.3. Optimisation Scenario C: Water sources S1 & S2 &S3

In this scenario a very contamined source is added, so the water network has now three sources : S1, S2 and S3. The cost of water is smallest because this is most polluted of four sources, as presented in Table 3.9. Network units are ranked in clusters associated to each source, as presented in paragraph 3.7.4.3 and Table 3.20

S1 cluster ={U1, U3, U9, U13}

S2 cluster ={U2, U5, U6, U7, U8, U11, U12, U14, U15}

S3 cluster ={U4, U10 }

The objective function is total annualised cost as defined in paragraph 4.4.1 with original contribution to consider in cost evaluation optimal pipe diameter. The results of optimisation are presented in following sections.

a) Minimum supply water flowrate

The optimal water supply flowrate is not changed too much compared to Scenario B, source S3 is selected for just one unit (U10). In Table 4.12 I make a comparative presentation with case study developed din paragraph 3.6.4.3 for water supply flowrate objective function. For both case studies same sources distribution is obtained.

Table 4. 10 Supply water flowrate per water-using units: scenario C (Water sources S1 & S2 & S3)

Water unit	Supply Water Flowrate objective function		Total Annualised Cost objective function	
	Minimum Supply water flowrate (t/h)		Minimum Supply water flowrate (t/h)	
	Fcrt	Lcrt	Fcrt	Lcrt
U1	131.9	131.9	131.9	131.9
U2	355.1	355.1	355.1	355.1
U3	204.5	204.5	204.5	204.5
U4	0.0	0.0	0.0	0.0
U5	0.0	0.0	0.0	0.0
U6	0.0	0.0	0.0	0.0
U7	39.9	39.9	39.9	39.9
U8	0.0	0.0	0.0	0.0
U9	2.0	2.0	2.0	2.0
U10	7.3	7.3	7.3	7.3
U11	0.0	0.0	0.0	0.0
U12	0.0	0.0	0.0	0.0

U13	0.0	0.0	0.0	0.0
U14	0.0	0.0	0.0	0.0
U15	0.0	0.0	0.0	0.0
Total flowrate (t/h)	**740.7**	**740.7**	**740.7**	**740.7**

b) Total wastewater flowrate

In this scenario wastewater is produced by only six units. Comparing to Scenario B (Table 4.6) the total flowrate is slightly increased. Compared to same scenario presented in the case study developed in paragraph 3.7.4.3 the distribution of wastewater per units is different (Table 4.10), obtaining an important concentration of wastewater production. I can explain this behaviour as determined by the distribution of internal effluents, specific for each situation. Despite the fact that the distribution of wastewater effluents is different the total flowrate is the same for both case studies.

Table 4. 11 Wastewater flowrate per water-using units: Scenario C (Water sources S1 & S2 & S3)

Water unit	Supply Water Flowrate objective function		Total Annualised Cost objective function	
	Minimum wastewater flowrate (t/h)		Minimum wastewater flowrate (t/h)	
	Fcrt	Lcrt	Fcrt	Lcrt
U1	0.0	0.0	0.0	0.0
U2	0.0	28.4	0.0	0.0
U3	0.0	3.0	0.0	0.0
U4	2.8	84.4	2.2	3.0
U5	0.0	101.6	0.8	378.6
U6	133.9	28.7	366.0	3.0
U7	0.0	3.7	0.0	0.0
U8	62.1	11.6	16.6	0.0
U9	0.0	0.4	0.0	0.0
U10	0.0	2.3	0.0	0.0
U11	57.7	7.0	0.8	3.8
U12	119.0	51.2	15.3	10.3
U13	0.0	0.0	0.4	0.0
U14	0.0	28.2	5.7	7.7
U15	39.2	64.2	6.9	8.3
Total flowrate (t/h)	**414.7**	**414.7**	**414.7**	**414.7**

c) Optimum pipe diameter

For each value of internal streams flowrate, X_{ij}, is calculated the optimal diameter, $\mathscr{D}_{ij}$, with Eqs. 4.14 - 4.17 then similar procedure is used in calculation as described above. Pipes optimum diameter for this scenario are presented in Table 4.12.

The water Source S3 is used only in water-using unit 10 and the flowrate is very small, compared to other water supply flowrates. Source S1 is used as supply water in units U1, U3 and U9 and sources S2 is used only for units U2 and U7. The optimal diameter pipes are different for each internal streams.

d) Total cost of water network

A cost analysis of this scenario is presented in Table 4.11. The best solution is with 1,320,472 $/year for Total Cost optimisation and Fcrt, as in Table (4.13).

Table 4. 12 Total annualised cost: Scenario C (Water sources S1 & S2 & S3)

Cost type	Supply Water Flowrate objective function		Total Annualised Cost objective function	
	Fcrt	Lcrt	Fcrt	Lcrt
Source S1 flowrate, t/h	338.40	338.40	338.40	338.40
Source S2 flowrate, t/h	395.00	395.00	395.00	395.00
Source S3 flowrate, t/h	7.30	7.30	7.30	7.30
Reused water flowrate, t/h	561.80	544.10	430.00	422.00
Length of all pipes, m	56,900	55,850	23.420	23,560
Pumping cost, $/year	289,928	293,867	138.769	143,518
Investment cost, $/year	1,542,992	1,742,765	1,181,703	1,297,542
Total Annualised Cost, $/year	**1,832,920**	**2,036,632**	**1,320,472**	**1,441,060**

e) Water network topology

The GA algorithm applied to a mathematical model considering three water sources (freshwater, slightly contaminated water and contaminated water) and minimum of investment cost as optimisation criterion, the network topology is very simplified. Almost all the process send their effluents to unit U6 and from this process a huge amount is sent to treatment unit. For this reason the network of pipes is not very complicated and the total length of pipes is at half as in the similar case.

4.6.4. Optimisation Scenario D: Water sources S1 & S2 & S3 & S4

In this scenario four sources are considered : S1, S2, S3, and S4. Data relevant for these sources are given in Table 3.9. Water using units are grouped in clusters associated to each water source as presented in paragraph 3.7.4.4

S1 cluster ={U1, U3, U9, U13}

S2 cluster ={U2, U7 }

S3 cluster ={U4, U10 }

S4 cluster ={U5, U6, U8, U11, U12, U14, U15 }.

Table 4. 13 Matrix of standardised pipes optimum diameter: Scenario C (Water sources S1 & S2 & S3) – Fcrt criterion

$\mathscr{D}_{ij}$ (mm)	S1	S2	S3	U1	U2	U3	U7	U9	U10	U5	U13	U4	U15	U11	U14	U8	U12	U6	T
S1	x	x	x	155.50		210.0		26.00	-	-	-	-	-	-	-	-	-	-	-
S2	x	x	x	-	275.0	-	105.0	-	-	-	-	-	-	-	-	-	-	-	-
S3	x	x	x	-	-	-	-	-	52.50	-	-	-	-	-	-	-	-	-	-
U1	x	x	x	x	-	-	-	-	-	-	-	-	-	-	-	-	-	41.25	-
U2	x	x	x	x	x	-	-	-		15.75	26.00	26.00	41.25	41.25	41.25	67.00	80.25	265.0	-
U3	x	x	x	x	x	x	-	-	-	-	-	-	-	-	-	-	-	80.25	-
U7	x	x	x	x	x	x	x	-	-	-	-	-	-	-	-	-	-	105.5	-
U9	x	x	x	x	x	x	x	x	-	-	-	-	-	-	-	-	-	26.00	-
U10	x	x	x	x	x	x	x	x	x		-	-	-	-	-	-	-	52.50	-
U5	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-	-	-	-	15.75
U13	x	x	x	x	x	x	x	x	x	x	x	-	-	-	-	21.25	-	-	15.75
U4	x	x	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-	-	26.00
U15	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-	52.50
U11	x	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-	-	41.25	21.25
U14	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-	-	41.25
U8	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-	67.00
U12	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	41.25	67.00
U6	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	320.0
T	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x

x- forbidden matches due to the oriented graph, -no pipes between units

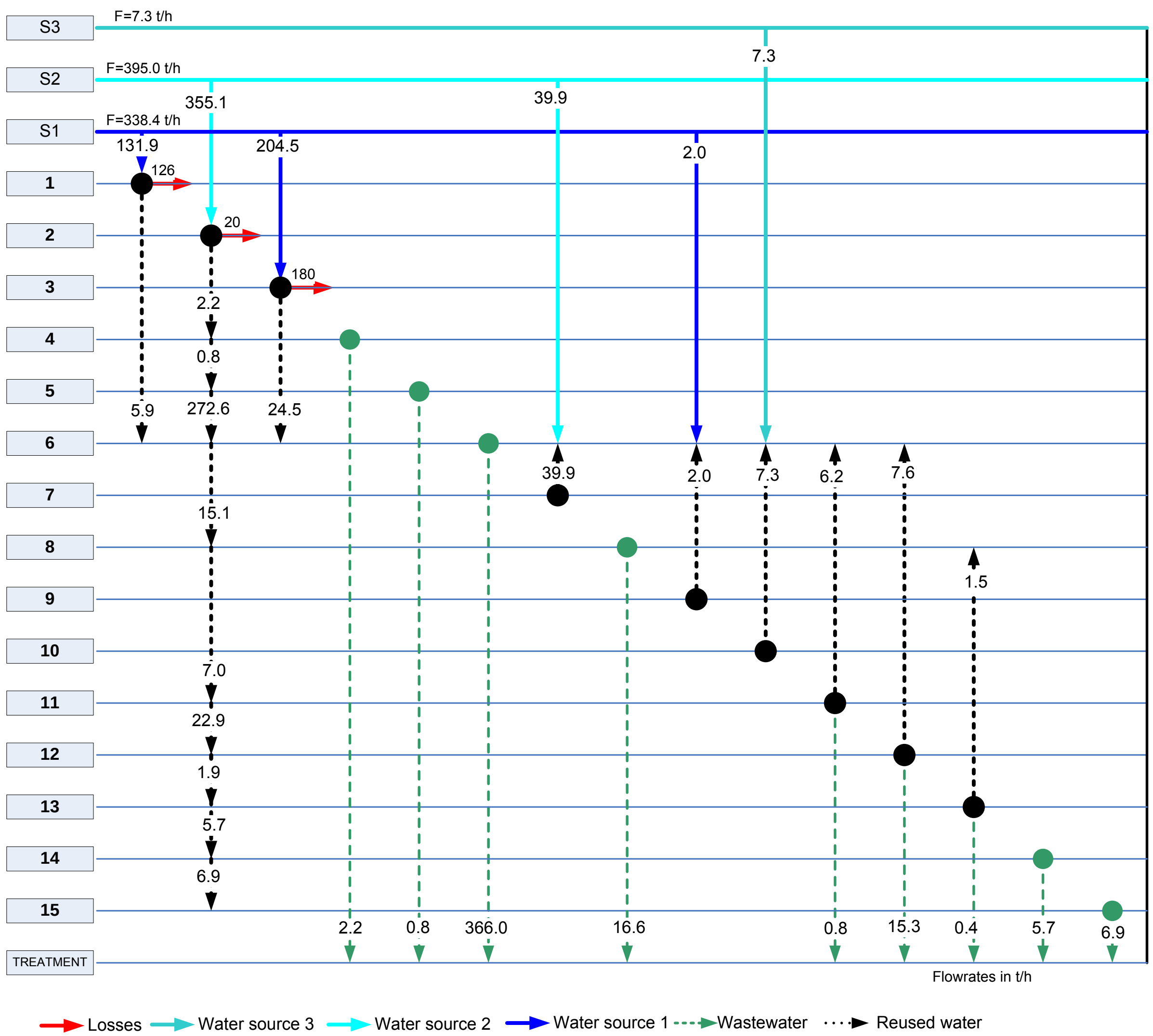


Figure 4. 3 Total annualised cost optimised network topology: Scenario C (Water sources S1 & S2 & S3) – Fcrt criterion

The objective function for optimisation is total annualised cost described in paragraph 4.4.1. In following tables the results are presented to be compared to the case study developed in Chapter 3 when water source flowrate objective function is used. Both ranking criteria (Fcrt and Lcrt) are considered in data analysis.

a) Minimum supply water flowrate

In Table 4.15 I present minimum supply water flowrate allocation to water-using units. It is interesting to notice that no change is recorded for the two objective functions. Compared with Scenario C, Source S4 is connected to units U8 and U11, increasing source flowrate from 740.7 t/h to 783.2 t/h. The other three sources keep same connectivity and flowrates. There are no differences between results obtained for ranking criteria.

Table 4. 14 Supply water flowrate per water-using units: Scenario D (Water sources S1 & S2 & S3 & S4)

Water unit	**Supply Water Flowrate objective function**		**Total Annualised Cost objective function**	
	Minimum Supply water flowrate (t/h)		**Minimum Supply water flowrate (t/h)**	
	Fcrt	**Lcrt**	**Fcrt**	**Lcrt**
U1	131.9	131.9	131.9	131.9
U2	355.1	355.1	355.1	355.1
U3	204.4	204.4	204.4	204.4
U4	0.0	0.0	0.0	0.0
U5	0.0	0.0	0.0	0.0
U6	0.0	0.0	0.0	0.0
U7	39.9	39.9	39.9	39.9
U8	35.9	35.9	35.9	35.9
U9	2.0	2.0	2.0	2.0
U10	7.3	7.3	7.3	7.3
U11	6.6	6.6	6.6	6.6
U12	0.0	0.0	0.0	0.0
U13	0.0	0.0	0.0	0.0
U14	0.0	0.0	0.0	0.0
U15	0.0	0.0	0.0	0.0
Total flowrate (t/h)	**783.2**	**783.2**	**783.2**	**783.2**

b) Total wastewater flowrate

The same amount of wastewater is discharged to treatment unit for both case studies. As I present in Table 4.14, the distribution of wastewater effluents is quite different when cost-based objective function is considered. The ranking criteria produce quite different results for internal production of wastwwater effluents. There are eight water-using units producing wastewater effluents in this case study.

Table 4. 15 Wastewater flowrate per water-using units: Scenario D (Sources S1 & S2 & S3 & S4)

Water unit	Supply Water Flowrate objective function		Total Annualised Cost objective function	
	Minimum wastewater flowrate (t/h)		Minimum wastewater flowrate (t/h)	
	Fcrt	Lcrt	Fcrt	Lcrt
U1	0.0	1.2	0.0	0.0
U2	0.0	53.5	0.0	0.0
U3	0.0	3.3	0.0	0.0
U4	90.3	106.0	22.8	156.5
U5	90.8	123.7	23.3	186.3
U6	112.9	35.3	227.5	41.4
U7	0.0	6.5	0.0	4.0
U8	0.0	5.3	0.0	0.0
U9	0.0	0.0	0.0	0.0
U10	0.0	0.0	0.0	0.0
U11	1.1	1.2	6.6	6.6
U12	72.9	60.4	133.4	30.1
U13	0.0	0.0	12.1	8.5
U14	80.9	0.0	19.5	17.2
U15	8.3	60.8	12.0	6.6
Total flowrate (t/h)	**457.2**	**457.2**	**457.2**	**457.2**

c) Optimum pipe diameter

For each value of internal streams flowrate, X_{ij}, the optimal diameter $\mathcal{D}_{ij}$ is calculated with Eqs. 4.14 - 4.17, then standardised diameters are chosen (Bratu, 1984) as presente din Table 4.16. The water source S4 is used only in water-using units U8 and U11 and the flowrate is quite small, compared to with other water supply flowrates. Source S1 is used as supply water in units U1, U3 and U9 and source S2 is used for units U2 and U7. Source S3 is used just for U10. Pipes optimal diameter has large variations for internal streams from 21.25 mm to 210 mm.

d) Total cost of water network

In Table 4.15 comparative data is presented to allow cost analysis for Scenaria D in both case studies. It was evaluated the cost for supply water flowrate as well to allow comparison of costs. From this point of view as it is obvious cost optimisation gives best results. For this scenario the solution to be chosen is obtained for Total Annualised Cost objective function Fcrt ranking criterion, **1,613,001** $/year. The network has minimum pipies length, 32.6 km and reused water flowrate is nearly minimum, 456.3 t/h.

Table 4. 16 Total annualised cost: Scenario D (Water sources S1 & S2 & S3 & S4)

Cost type	Supply Water Flowrate objective function		Total Annualised Cost objective function	
	Fcrt	Lcrt	Fcrt	Lcrt
Source S1 flowrate, t/h	338.40	338.40	338.40	338.40
Source S2 flowrate, t/h	395.00	395.00	395.00	395.00
Source S3 flowrate, t/h	7.30	7.30	7.30	7.30
Source S4 flowrate, t/h	42.50	42.50	42.50	42.50
Reused water flowrate, t/h	583.90	485.60	456.30	454.90
Length of all pipes, m	50,990	49,850	32,590	37.560
Operating cost, $/year	274,612	265,368	186,314	212.279
Investment cost, $/year	1,763,880	1,642,749	1,426,687	1,580,056
Total Annualised Cost, $/year	**2,038,492**	**1,908,117**	**1,613,001**	**1,792,335**

d) Water network topology

When all four water resources are used to feed water network the topology changes as illustrated in Fig. 4.4 compared to Scenario C, Fig. 4.3. In current scenario four units have more than 2 reused water streams to connect other units. In Scenario C just one unit have more than 2 connections. This I can explain by the fact that Source S4 (with relative low contamination degree) determines important reuse of water inside the network. Consequently this scenario is less attractive than Scenario C. Compared to Scenario D described in paragraph 3.4.7.4 (summarised in Table 4.15) the topology is simplified obviously due to continuation of optimisation process. After finding the minimum water supply flowrate the search process continues to simplify the topology. As a proof the total pipes length decreases from about 60 km in Scenario D described in paragraph 3.4.7.4 to 32.6 km in current scenario. The number of units with more than two connection streams for reused water decreases from ten units to just four units.

4.7. Design of optimal water network topology for minimum topological index

In paragraphs 3.7.4 and 4.6, I present two case studies based on a large scale water network for design strategy considering two objective functions: supply water flowrate and respectively total annualised cost. I analyse for both cases the effect of using more supply water sources.

Table 4. 17 Matrix of standardised pipes optimum diameter : Scenario D (Water sources S1 & S2 & S3 & S4) – Lcrt criterion

$\mathscr{D}_{ij}$ (mm)	S1	S2	S3	S4	U1	U2	U3	U7	U8	U9	U10	U11	U5	U13	U4	U15	U14	U12	U6	T
S1	x	x	x	x	155.5	-	210.0	-	-	26.00			-	-	-	-	-	-	-	-
S2	x	x	x	x	-	275.0	-	105.5	-	-	-	-	-	-	-	-	-	-	-	-
S3	x	x	x	x	-	-	-	-	-	-	52.5	-	-	-	-	-	-	-	-	-
S4	x	x	x	x	-	-	-	-	105.5	-	-	41.25	-	-	-	-	-	-	-	-
U1	x	x	x	x	x	-	-	-	-	-	-	-	21.25	-	21.25	-	21.25	21.25	26.00	-
U2	x	x	x	x	x	x	-	-	-	-	-	-	-	-	-	-	-	155.5	210.0	-
U3	x	x	x	x	x	x	x	-	-	-	-	-	-	41.25	26.00	67.00	-	-	35.75	-
U7	x	x	x	x	x	x	x	x	-	-	-	-	52.50	35.75	52.50	-	67.00	26.00	35.75	-
U8	x	x	x	x	x	x	x	x	x	-	-	-	52.50	26.00	52.50	-	52.50	52.50	15.75	-
U9	x	x	x	x	x	x	x	x	x	x	-	-	-	-	21.25	-	-	-	26.00	-
U10	x	x	x	x	x	x	x	x	x	x	x	-	26.00	-	-	-	-	-	35.75	-
U5	x	x	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-	-	-	80.25
U13	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-	-	67.00
U4	x	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-	-	-	-	80.25
U15	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-	-	-	67.00
U11	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-	-	41.25
U14	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	-	-	80.25
U12	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	41.25	210.0
U6	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	210.0
T	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x	x

x- forbidden matches due to the oriented graph, -no pipes between units

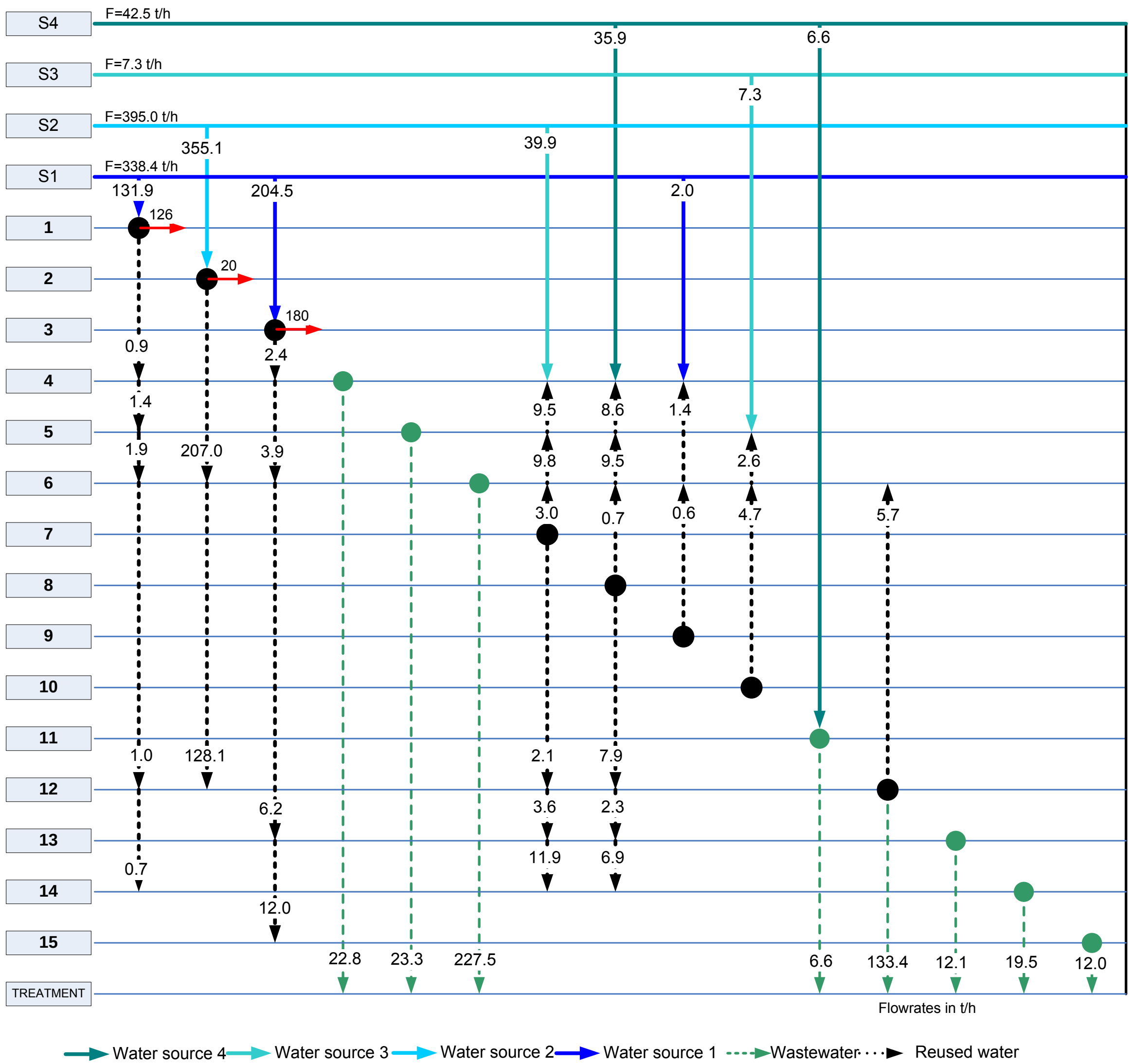


Figure 4. 4 Total annualised cost optimised network topology: Scenario D (Water sources S1 & S2 & S3 & S4) – Fcrt criterion

However, when cost data is not available on the site to calculate the total annualised cost, the topological index is a criterion to take into account for decision basis. As I present in paragraph 4.4.2 search for recommended topology can also be made considering a weighted objective function (a linear combination between supply water flowrate and network topological index). The relative influence of each of these two criteria is given by weighting factor ω as defined in my paper Iancu et al., 2006.

In this paragraph I continue the analysis of same site water network using the above described weighted objective function. The influence of each component is underlined optimising for different values of ω factor, as follows:

- ω = 0 gives comparable results with the economic criteria strategy
- ω = 1 gives same results with the supply water criteria strategy
- ω = 0.5 to prove that the GA optimisation tool gives intermediate results with the supply water flowrate criterion mixed with topological index criterion.

A combination of both components is useful when the results should have quite reduced supply water flowrate and reasonable complex water network topology. The optimal topology found using this weighted objective function is compared against each other and also with the best topology acquired using total annualised costs. Results of this analysis are presented in Table 4.18 for different values of ω. If the water network is supplied only with freshwater (most expensive source), Scenario A, the results for total annualised cost and supply water flowrate (ω = 1) objective functions are already known and discussed.

Table 4. 18 Results for different objective functions

Scenario	Ranking criteria	Objective function: Total annualised cost		Supply water flowrate ω = 1		Weighted objective function ω = 0.5		Topological index ω = 0	
		Flowrate (t/h)	Pipes length (km)	Flowrate (t/h)	Pipes length (km)	Flowrate (t/h)	Pipes length (km)	Flowrate (t/h)	Pipes length (km)
A	Fcrt	493.6	34.36	442.1	51.63	490.1	42.06	529.3	38.99
	Lcrt	463.8	40.38	452.8	53.55	456.3	44.14	504.4	42.55
B	Fcrt	733.4	39.03	733.4	57.69	733.4	52.62	742.7	49.45
	Lcrt	733.4	40.85	733.4	57.71	733.4	53.59	742.7	50.74
C	Fcrt	**740.7**	**23.42**	**740.7**	56.90	**740.7**	**49.06**	**740.7**	**39.96**
	Lcrt	**740.7**	**23.56**	**740.7**	55.85	**740.7**	**48.32**	**740.7**	**41.15**
D	Fcrt	783.2	32.59	783.2	50.99	783.2	46.08	784.9	38.57
	Lcrt	783.2	37.56	783.2	49.85	784.1	45.62	784.4	40.55

It is remarkable the supply water flowrate bigger with ~10% and total pipes length reduced with 30%. When topological index is considered alone (ω = 0), supply water flowrate increases with ~20% compared to $\omega = 1$ but the pipe length is very close to cost based objective function results (~13.5% for Fcrt vs 5% for Lcrt). It is very interesting however that for weighted objective function ($\omega = 0.5$) water supply flowrate is very close to results for total annualised cost and total pipes length is not very different as well (~22% for Fcrt vs ~10% for Lcrt). So, using a quite simple weighted objective function for this scenario, the results are encouraging.

In Scenario B when two supply water sources are considered it is to underline that total supply water flowrate increases compared to Scenario A, but Source S1 flowrate is reduced, as presented in paragraphs 3.7.4.2 and 4.6.2. However, same flowrate is obtained i.e.733.4 t/h but quite different topologies i.e. total pipes length reduces 32% for total annualised cost compared to supply water flowrate ($\omega = 1$) objective functions. For topological index objective function ($\omega = 0$), supply water flowrate is slightly modified and topology is less complicated that $\omega = 1$ (total pipes length reduces ~14%). When weighted objective function is considered $\omega = 0.5$, water flowrate has same value: 733.4 t/h and total pipes length is reduced with ~9% compared to $\omega = 1$. In this Scenario topological index objective function usage is benefice giving results quite satisfactory comparing to total annualised cost objective function.

Data obtained for optimised water network in Scenario C and Scenario D keep same trend i.e. total suply water flowrate is practically the same for all objective functions, while total pipes length increases for weighted objective function from ~30% for $\omega = 0$ to ~43% for $\omega = 1$ compared to value obtained for total annualised cost objective function.

Comparing data for all four scenarios, most attractive results are obtained for Scenario C. As a consequence, in Fig. 4.5 optimised topology for this scenario is compared to three different values of ω factor to draw a conclusion on using weighted objective function. It is obvious that the topology for $\omega=1$ is most complicated while for $\omega=0$ is quite simple. It is interesting that for $\omega=0.5$ the topology is closer to topology obtained when $\omega=0$.

This case study allows me to draw the conclusion that using weighted objective function is benefice. For $\omega=0.5$ quite attractive results are obtained. When detailed cost data are not available, I recommend to use a weighted objective function rather then a simple one, as mutual influences of component functions affect favourably the results (supply water flowrate component tends to keep low flowrate while topological index component tends to keep topology quite simple).

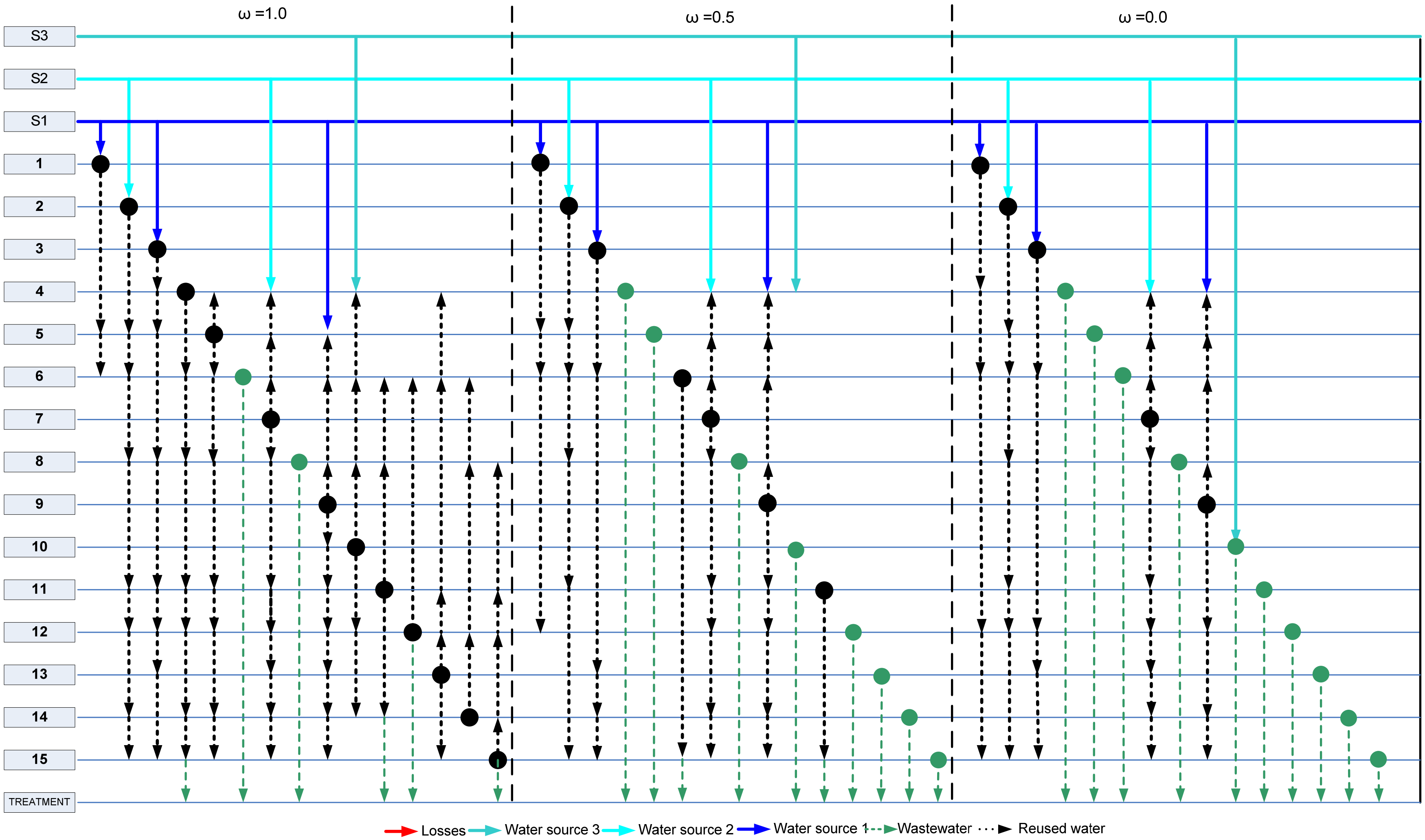


Figure 4. 5 Influence of optimisation criteria on topology of water network for Scenario C

4.8. Conclusions

In this chapter water network problem modelling and optimisation is formulated as original approach to take into account objective functions based on economic considerations. Total annualised cost objective function is calculated in original manner accounting for optimal pipes diameter. Minimum total annualised cost for pumping and fixed charges provides basis for minimum pipes diameter calculation with Eqs. 4.10-4.13. This approach is not reported in literature. The value of optimal diameter can be obtained by combining the principle of fluid dynamics with cost considerations. Solution of water network NLP mathematical model is made using GA optimisation tool. An original objective function is taken into account based on water network topological index. Despite the fact that it does not include explicitly economic variables, the water network cost strongly depends on total active pipes length is the weighted objective function obtained as linear combination of water supply flowrate and topological index. My analysis encourages to use it when there is scarce economic data.

As illustration of new methodology for total annualised cost objective function an industrial large scale case study is solved. 15 water-using units, 6 contaminants and four water sources with different degree of contamination, as described in Iacob et al., 2004 are taken into account. Such complex case study is not yet reported in literature. The topology of water network allows for maximum internal reuse of the water. The influence of using simultaneously more water sources is considered in four scenarios as developed in Chapter 3. Ranking water-using units by freshwater needs, the units less restrictive are placed at the end of the oriented graph, and are fed with internal streams only, provided that the input restrictions are coped with. Case study results published in my paper Lavric et al., 2007a are compared with same approach developed in Chapter 3.

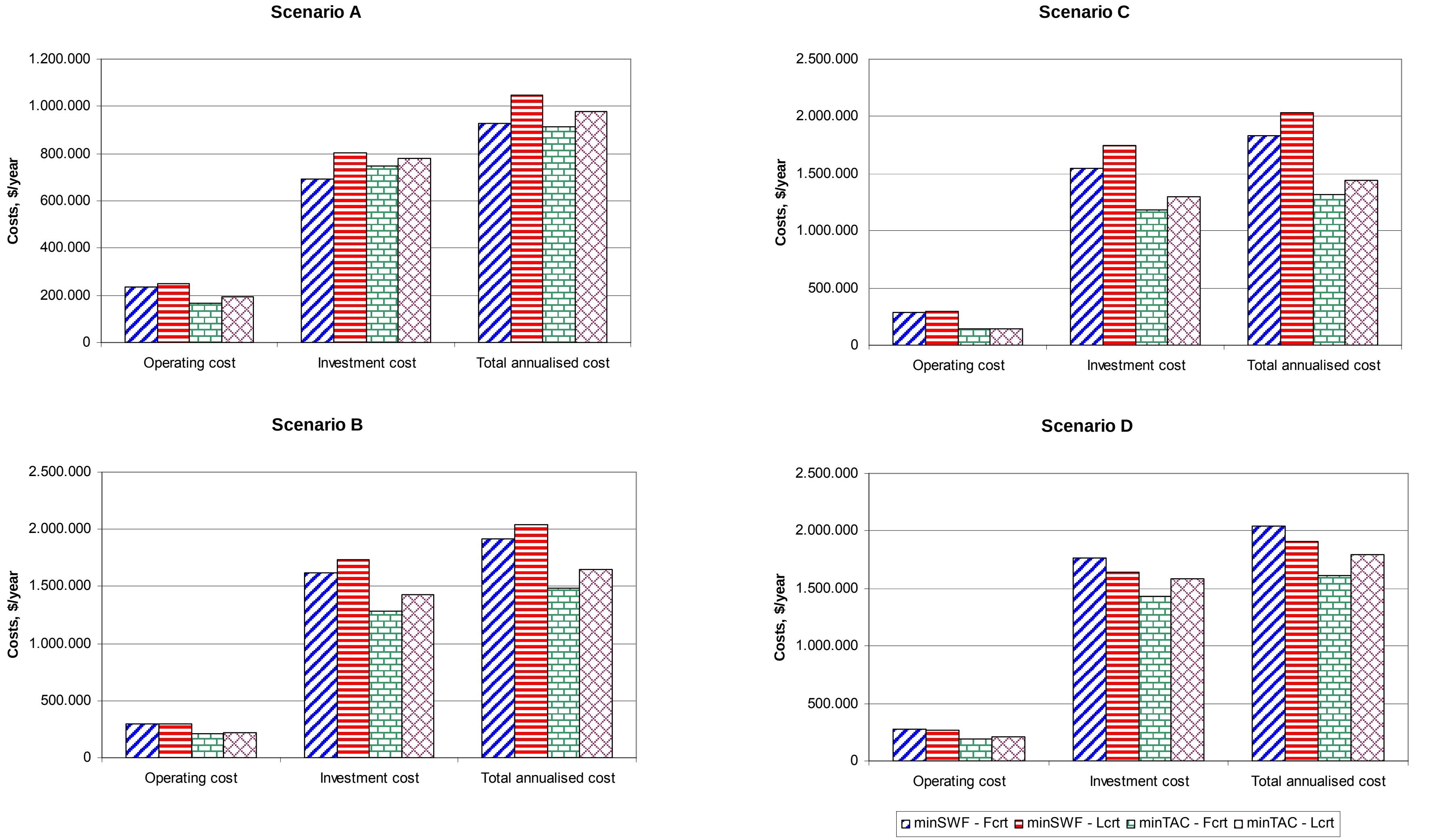
Scenario A: network is optimised for one water source: freshwater (very restrictive limiting data, no contamination). Compared to the case study developed in Chapter 3 same scenario, the minimum flowrate of supply water is a little bit increased but the total annualised cost (investment and operating costs) are reduced drastically. These aspects have important influence on water network topology, total length of piping system is reduced.

In Scenarios B, C and D simultaneous use of more supply water sources is taken into account. The flowrate of freshwater (the expensive water source) is reduced but the difference is given by an increased flowrate supplied by the other source(s). For the same value of total water flowrate, total annualised cost is lower for the scenarios of this case study compared with results obtained in Chapter 3. Significant differences in water network topology are also to notice. Consequently pipes length reduces when cost based objective function is used for optimisation, compared to supply water flowrate objective function. This can be explained by search mechanism to find optimum. When using water supply flowrate as objective function, search process stops after finding minimum flowrate, no attempts being made to reduce the pipes length. When using an economic based objective function, finding the minimum supply water throughput flow is accomplished in a first step, afterwards the search for better combinations of internal streams continues to find water network topology simplification as much as possible. A summary of results is presented in Table 4.19. Operating cost and investment cost are interesting to be compared. From data analysis I notice that the maximum degree of freedom exists only for non-contaminated supply water. Remarkably, when using combination of water sources the water throughput flowrate is the same for both objective functions. I noticed that reused water flowrate reduces in the case of cost based objective function. Comparing results from Table 4.19, the most attractive solution depends on optimisation criterion.

Table 4. 19 Water network design costs result summary

Scenario	Ranking criterium	Objective function					
		Minimum Supply Water Flowrate			Minimum Total Annualised Cost		
		Operating cost	Investment cost	Total annualised cost	Operating cost	Investment cost	Total annualised cost
		$/year	$/year	$/year	$/year	$/year	$/year
A	Fcrt	235,240	690,420	925,660	168,158	746,232	914,390
	Lcrt	247,709	801,615	1,049,324	195,346	781,384	976,730
B	Fcrt	296,442	1,615,234	1,911,676	206,529	1,280,535	1,487,064
	Lcrt	301,094	1,734,653	2,035,747	219,623	1,431,584	1,651,207
C	Fcrt	289,928	1,542,992	1,832,920	**138,769**	**1,181,703**	**1,320,472**
	Lcrt	293,867	1,742,765	2,036,632	143,518	1,297,542	1,441,060
D	Fcrt	274,612	1,763,880	2,038,492	186,314	1,426,687	1,613,001
	Lcrt	265,368	1,642,749	1,908,117	212,279	1,580,056	1,792,335

- For supply water flowrate objective function, water network most attractive solution with more water sources is given by Scenario B (733.4 t/h), when sources S1 and S2 are used for Fcrt ranking criterion. However, for this case the total annualised cost is **1,911,676 $/year**.



minSWF - minimum supply water flowrate; min TAC - minimum total annualised cost

Figure 4. 6 Water network Total Annualised Cost for different objective functions

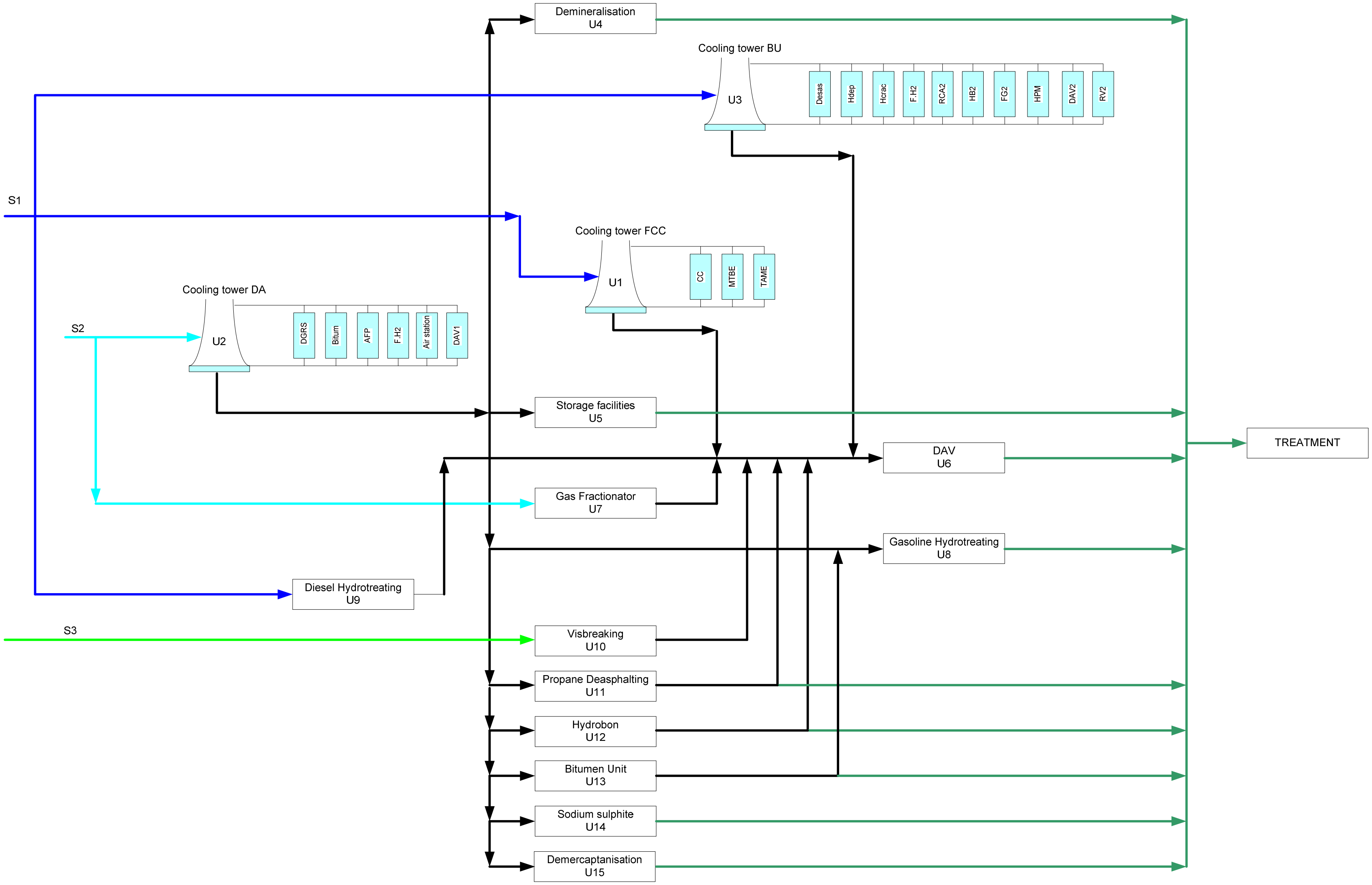


Figure 4. 7 The optimal water network flowsheet for oil refinery case study

- For minimum total cost annualised objective function, the optimal solution is using Scenario C (740.7 t/h), when total annualised cost is **1,320,472 $/year**, when three sources (S1, S2 and S3) are used and water network is ranked by Fcrt. Some results of this study are also published in my paper Lavric et al., 2005.

In Fig. 4.6 variation of operating cost, investment cost and total annualised cost is illustrated for different scenarios and objective functions. Operating cost decreases when different water sources are used, as water flowrate increases if the contamination of water source increases but water is cheaper (when comparing Scenarios B, C and D). Investment cost increases when more water sources are considered (eg scenario A vs scenario B). Minimum cost is however obtained for Scenario C. This means that there is a trade off between operating cost and investment cost given by minimum of total annualised cost. The most attractive solution in my study is given in Scenario C involving also a simpler topology. While total annualised cost is **1,320,472 $/year**, the water network uses 740,7 t/h (338.4 t/h from S1, 395.0 t/h from S2 and 7.3 t/h from S3) instead of 1,198.8 t/h for the base case, that means water saving of 38.8%. As final result for both case studies developed in Chapter 3 and Chapter 4 respectively and different scenarios the proposed water network flowsheet is presented in Fig. 4.7. Piping system is modified compared to base case presented in Fig. 3.22 and total piping length is proposed 23,420 m.

In the case of scarce economic data I propose in this chapter an implicit cost based objective function, topological index, because active pipes length is implicitly related to some components of cost based objective function. But this last one is related as well to supply water flowrate. As a consequence, I propose another original objective function a weighted one as a linear combination between water supply flowrate and topological index, of factor ω. In the case study presented in paragraph 4.7 based on same industrial site water system data as presented before (paragraphs 3.7.4.2 and 4.6.2), I obtained interesting results reported as well in my paper Iancu et al., 2007. For topological index objective function quite close total pipes length to cost based objective function is obtained, but in some scenarios quite different supply water flowrate. If weighted objective function is considered (ω=0.5), mutual influence of components on the objective function is like a synergy. Consequently, Scenario C gives most attractive results compared to other scenarios for all objective functions evaluated when supply water flowrate and total pipes length are considered.

CHAPTER 5

Water network optimisation considering regeneration

5.1. Introduction

In this chapter I extend the methodologies developed in previous chapters considering water streams regeneration in a systematic approach.

Waste minimisation is a strategy and policy of reducing the amount of waste in general but in particular produced by oil refineries and petrochemical platforms (European Commission, 2003). Waste minimisation strategies classification generates the "waste minimisation hierarchy" presented in Fig. 5.1 (Wikipedia Encyclopaedia). In this figure the most effective policies and strategies are at top. Waste minimisation less effective strategy is energy recovery, than more effective are considered the so called "3R" (recycle, reuse and reduce). The most effective option is prevention. In water systems regeneration is of particular interest.

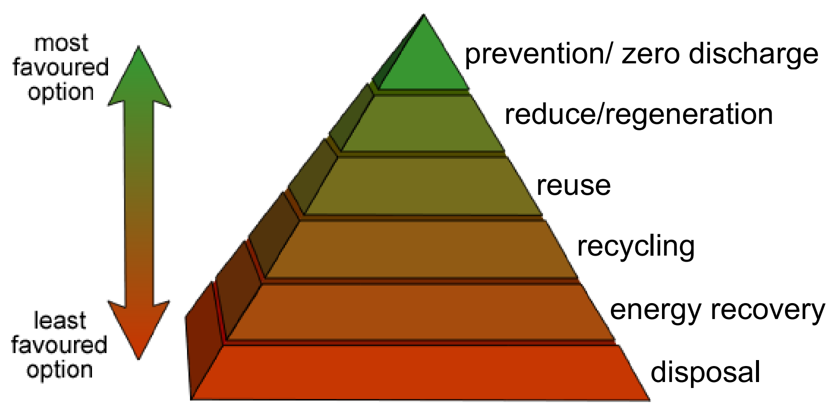


Figure 5. 1 Water and wastewater minimisation strategies

Regeneration can be a solution to reduce the water streams contamination and then to reuse them inside water network. Water regeneration and reuse is largely applied in process industries. Through partial treatment of contaminated water, a regeneration unit allows to reduce freshwater requirements and wastewater generation.

In the last few years, water networks optimisation via regeneration gained an increased interest. Several methods for the synthesis of grassroots water network design involving water regeneration are published. These methods generally fall under two main categories, i.e., the graphical-based water pinch technique and mathematical-based optimisation approaches or evolutionary methods. The former uses various heuristics as well as graphical tools to provide insights on water network synthesis, whereas the latest involves problem formulation into mathematical models to be solved via optimisation techniques, as presented in Chapter 2.

The first pinch-based water network synthesis approach using regeneration was proposed in classical papers Wang&Smith, 1994 and Kuo & Smith, 1998. In regeneration-reuse scheme, water is partially treated by water regeneration unit before reusing. The slope of limiting water profile after regeneration is the minimum flowrate of regenerated water which could be reused (Fig. 2.23). The problem of placement of regeneration unit (above or below the pinch point) was solved by Halale, 2002, which guides water streams regeneration as :

- *Regeneration above the pinch*: water streams in the region above the pinch are partially treated to achieve a composition under the pinch point
- *Regeneration below the pinch*: water streams in the region below the pinch are partially treated to achieve a composition higher as the pinch point.

Castro et co-workers in well known paper Castro et al., 1999 extended the concept of regeneration-reuse of water streams for water network with multiple pinch points. A water source diagram was used to achieve the targets for minimum utility and regenerated water. However, the network synthesised using this technique predominantly does not achieve the minimum number of target units, due to the need for stream splitting. To overcome this problem, additional freshwater is required. An improved algorithmic procedure was proposed by Gomes et al., 2005 which took into account a variety of situations, such as reuse, multiple water sources, water losses along the process, flowrate constraints, regeneration and reuse&regeneration &recycling. A numerically equivalent tabular approach known as *water cascade analysis* (WCA) was recently introduced in two interesting papers by Manan et al., 2004 and respectively by Foo, 2006 as an alternative to tedious iterative graphical approach of the *water surplus diagram*. Regeneration and process changes were also assessed, based on the principles of the water surplus diagram.

First complete mathematical optimisation approach using regeneration technique was introduced in a classical paper by Takama et al., 1980. They proposed the synthesis of a water recovery network in an oil refinery by generating a superstructure of all possible reuse and regeneration opportunities. Optimisation was then performed on the superstructure to obtain an optimal water network. Later, Alva-Argaez et al., 1998 proposed for water network a model which includes all possibilities for water reuse, regeneration-reuse and regeneration-recycling. Water network synthesised with this approach featured the minimum total annualised cost and considered process constraints such as geographical location, control and safety. Soem linear programming (LP) and mixed integer linear programming (MILP) formulations to synthesise optimum water network that considered the placement of regeneration units was proposed by Bagajewicz & Savelski, 2001. Choosing as objective function cost of placement of the regeneration unit, Feng&Chu, 2004 concluded that the total cost of a water network can be minimised after the optimum regenerator outlet concentration was determined. A new systematic methodology for water network retrofit involving the optimisation of existing regeneration units was proposed by Tan et al., 2006. The procedure begun with setting-up the minimum utility targets for water network and application of some process changes heuristics to choose the best optimisation scheme for existing regeneration units. Next, utility savings and capital investment targets were established for the chosen optimisation scheme. The existing water network was finally retrofitted to realise the economic targets.

In my Thesis I present in Chapter 3 original methodology for water network optimisation with multiple supply sources. The methodology is developed considering water network physical model, mathematical model, design criteria, optimisation algorithm and graphical representation.

In Chapter 4, I consider the economic aspects for optimisation of water network. Specific elements are added to physical and mathematical model to take into account different cost elements. When economic data are not available a weighted objective function based on water supply flowrate and topological index is found to be a good option for water network optimisation. Relevant case studies presented in both Chapter 3 and Chapter 4 support the proposed methodologies

In this chapter I present original approach on the role of regeneration unit for water network optimisation, based on the work published in my last two papers Lavric et al., 2007 and Iancu et al., 2007. Main original concepts introduced for the new methodology are: *mean availability, critical contaminant analysis, bottleneck island, Internal/external reuse quotient and partial and total regeneration*. Specific model for regeneration unit is defined. Water network physical and mathematical models are based on previous chapters' developments and new concepts. Same optimisation problem formulation and solution technique based on Genetic Algorithm (GA) are presented. Illustration of new methodology is performed in case studies for design and retrofit of industrial water networks with regeneration.

The need to drop streams concentration for one or more contaminants is satisfied by regeneration unit. Contaminant(s) removal is based on different technologies with diverse agents for regeneration, imposing the limiting inlet and outlet concentration of contaminants. Some possible techniques to regenerate water streams include pH control to ensure certain acidity/causticity, precipitation of different ions or other compounds, sedimentation to remove suspended solids, liquid-liquid extraction and stripping to remove organic compounds, etc. *In this analysis I do not consider the influence of treatment technology or removing agents.*

Some questions can be answered based on this approach:

- Where to placed the regeneration unit for an optimal water network?
- Can be obtained benefits removing only one or more or all contaminants?
- How to find which contaminant has largest influence on water network design?

In next paragraphs to these questions convenient answers are given.

5.2. Abstraction of water network and new concepts

In previous chapters water network is considered an oriented graph. The knots are water-using units and the lines are the water streams between different units.

The physical model is based on the formulation presented in previous chapters: "*The water network is considered an oriented multicomponent graph where water-using units are ordered according either to their maximum load (Lcrt criterion) or their supply water needs (Fcrt criterion), thus, any water recycling is conceptually avoided".*

In this chapter the model is developed adding an original approach to the regeneration unit, as I illustrate in Fig.5.2.

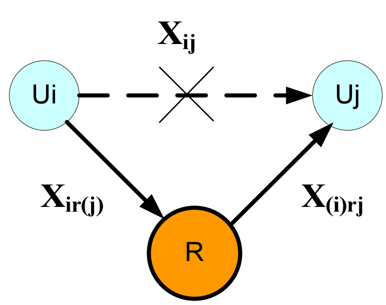


Figure 5. 2 Role of regeneration unit for the connection between water-using units u_i and u_j

Regeneration unit (denoted R) is considered as a facility where streams with high contamination level can drop contamination to observe imposed restrictions. In this manner the effluent from unit u_i can arrive to targeted water-using unit u_j with lower contamination level. As I present in Fig. 5.2, if stream X_{ij} needs regeneration, it is disconnected from unit u_j, a new stream with same characteristics (flowrate and concentrations) connects unit u_i to regeneration unit, $X_{i(j)r}$. Then, a new stream $X_{(i)rj}$ connects unit R to unit u_j. This stream has the same characteristics with X_{ij}, except the changes in contamination level for one or more contaminants (as conditions are imposed). An effluent stream is sent to regeneration unit when the concentration of one or more contaminants in internal streams X_{ij} reach the given threshold value, specific to regeneration unit inlet. As a consequence, regeneration unit removes a certain mass load of contaminant [kg/s], Δm_k^r, $k \in J_k$, where J_k is the group of contaminants to be removed by unit R. The unit u_j receives a regenerated stream with same water flowrate but lower concentration of contaminant k, specific for regeneration unit. Based on this physical model, the connections with regeneration unit can be represented for the whole water network, as illustrated schematically in Fig. 5.3.

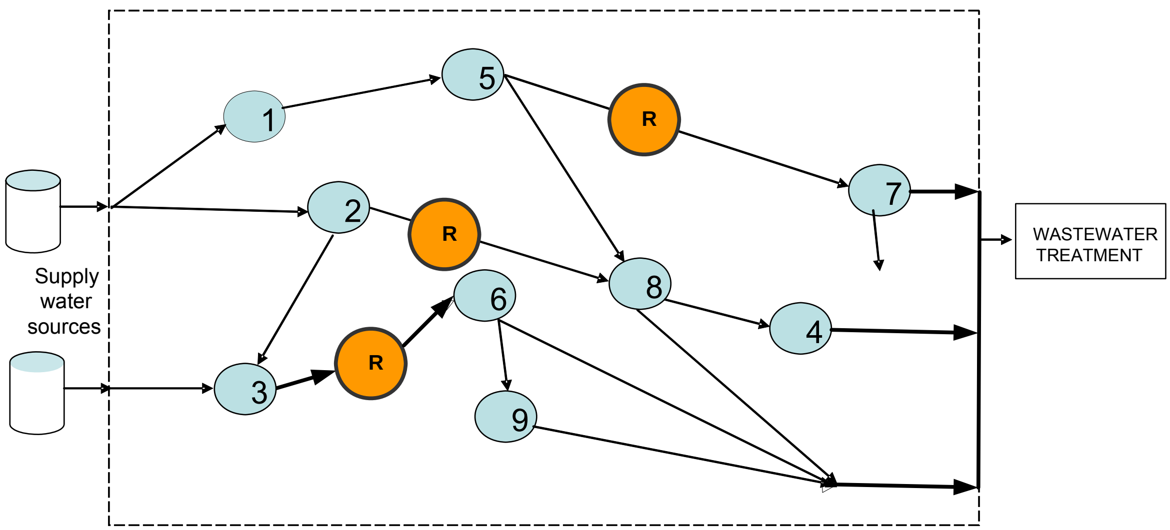


Figure 5. 3 Abstraction of water network, considering regeneration units

In development of a mathematical model to include regeneration unit as defined above some new concepts are introduced in my papers Iancu et al., 2007 and Lavric et al., 2007b:

- *Mean availability* defined as the mean of the mass transfer driving forces for a specific contaminant at the entrance and exit for all water-using units in the water network.
- *Critical contaminant regeneration*: removing only the contaminant with lower mean availability which bottlenecks the water network.
- *Bottleneck island:* group of some contaminants (considered neighbours as having close mean availability to critical contaminant) including this one as well.

This group is quite isolated from the rest of contaminants, having lowest mean availabilities.

- *Partial regeneration* : unlimited or limited removal of one or some contaminants, eventually forming a bottleneck island, from internal streams to acceptable level, once their concentration pass over an imposed threshold.
- *Total regeneration (zero discharge)* : all the contaminants are completely removed in the regeneration unit, no wastewater discharges in the environment.

- *Internal/external reuse quotient (IRQ, ERQ)* represents the ratio between flowrate of reused internal/external water streams and the flowrate of the contaminated water sent to treatment or recycled back, in zero discharge; the higher I/ERQ is the easier treatment units task should be, decreasing operating costs together with environmental impact of discharged wastewater.

The regeneration could happen more often, leading to an overall increase in the mass transfer driving force at the level of whole network; this could diminish the supply water demand.

The mathematical model is formulated in similar manner as in previous chapters. An objective function is formulated with fresh water supply flowrate. Problem restrictions are based on : mass balances around water-using units and regeneration unit, contaminants limits at entrance and at exit of water-using units, as well as regeneration unit characteristics.

5.2.1. Critical contaminant regeneration

Critical contaminant is the contaminant which determines the level of the supply water consumption and/or limits for internal reuse due to network units bottlenecking. This contaminant has the lowest mean pseudo-driving force, defined by analogy with heat transfer, as a mean of concentration differences for each contaminant k at the entrance and at the exit of each water-using unit, as illustrated in Fig. 5.4.

$$\overline{\Delta C_k} = \frac{\sum_{i=1}^{N} \frac{\left(C_{k,i}^{max} - C_{k,i}\right)_{in} + \left(C_{k,i}^{max} - C_{k,i}\right)_{out}}{2}}{N} \qquad (5.\ 1)$$

Concentration difference for contaminant k at the entrance of a water–using unit u_i is calculated between maximum concentration imposed as limiting data by different constrains (physical, technological, economical, mechanical, etc) and the current concentration in inlet water stream. The contaminant concentration difference at water–using unit exit is calculated between maximum allowable outlet concentration and current concentration unit effluents as I illustrate in Fig.5.4. I underline that the mean is just arithmetical because there are no other concentration differences to consider related to unit u_i, as it is considered perfectly mixed.

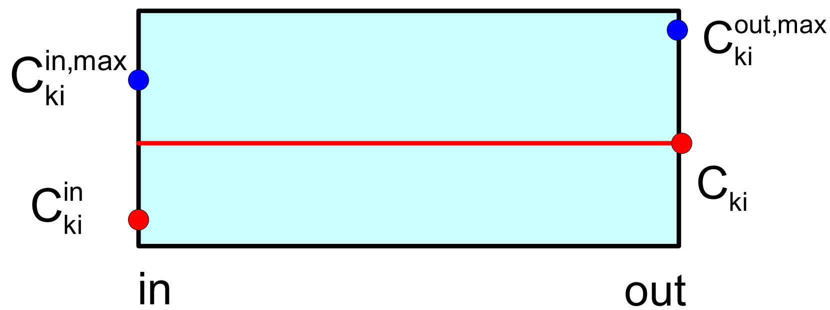


Figure 5. 4 Definition of pseudo-driving force of contaminant k

Applying this calculation to all contaminants, it is possible to find a particular one which has the lowest mean availability. This contaminant has a major influence on either supply water consumption or internal streams topology, due to mass transfer bottleneck. It is also possible that this particular contaminant attends, in the units at the first part of the oriented graph, a threshold concentration, which prevents reuse internal water streams. This contaminant should be the primary target for partial regeneration. To overcome this bottleneck, regeneration unit is introduced to water network, to clean-up all the internal streams reaching threshold concentration for the critical contaminant.

To determine the critical contaminant of water network, I propose a six steps procedure to calculate mean availability for each contaminant.

a) From problem definition (as I presented in paragraph 3.4.2), limiting data for all contaminants in each water-using unit u_i at entrance and exit are selected :

$$C^{in,max} = \left\{C_{ki}^{in,max}, k = 1,2,...,K, i = 1,2,...,N\right\}$$
$$C^{out,max} = \left\{C_{ki}^{out,max}, k = 1,2,...,K, i = 1,2,...,N\right\} \quad (5.\ 2)$$

b) From problem solving algorithm application, current data for all contaminants in each water-using unit u_i at entrance and exit is selected :

$$C^{in} = \left\{C_{ki}^{in}, k = 1,2,...,K, i = 1,2,...,N\right\}$$
$$C^{out} = \left\{C_{ki}, k = 1,2,...,K, i = 1,2,...,N\right\} \quad (5.\ 3)$$

c) Limiting composition difference at entrance for all contaminants in each water-using unit u_i is calculated :

$$\Delta C_{ki}^{in} = C_{ki}^{in,max} - C_{ki}^{in}, \quad k=1,2,...,K,\ i=1,2,...,N \quad (5.\ 4)$$

d) Limiting composition difference at exit for all contaminants in each water-using unit u_i is calculated :

$$\Delta C_{ki}^{out} = C_{ki}^{out,max} - C_{ki}, \quad k=1,2,...,K, \; i=1,2,...,N \qquad (5.\,5)$$

e) Average composition difference (as arithmetic mean) for all contaminants in each water-using unit u_i is calculated :

$$\Delta C_{ki}\Big|_{mean} = \frac{\left(\Delta C_{ki}^{out} + \Delta C_{ki}^{in}\right)}{2}, \quad k=1,2,...,K, \; i=1,2,...,N \qquad (5.\,6)$$

f) Average composition difference for each contaminant in all water using units (mean pseudo-driving force for each contaminant for the water network or mean availability) is calculated :

$$\overline{\Delta C_k} = \frac{\sum_{i=1}^{N} \Delta C_{ki}\Big|_{mean}}{N}, \quad k=1,2,..., K \qquad (5.\,7)$$

The value $\min_{k=1}^{K}\left(\overline{\Delta C_k}\right)$ gives the critical contaminant p. The contaminants having mean availability $\overline{\Delta C_k}$ close of the critical contaminant value $\overline{\Delta C_p}$, form a bottleneck island denoted J_p. Regeneration of any single contaminant from a bottleneck island does not guarantee debottlenecking network, but the regeneration of all the contaminants of the island has an important effect on the whole water network, as illustrated in case study described in paragraph 5.10.

5.2.2. Partial regeneration

In most oil refineries and petrochemical sites, wastewater is treated in a centralised system.

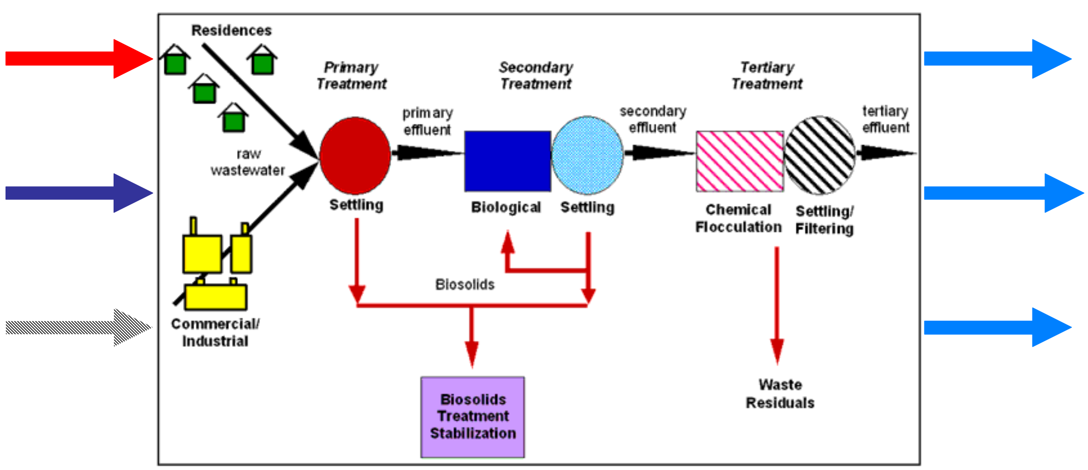


Figure 5. 5 Traditional treatment of industrial effluents

Wastewater is collected from all processes and first treated by an API separator. The purpose of this equipment is to perform the initial separation of solids from liquids and oil from water. The sludge is removed from the API separators, the water is passed on to further treatment and the oil is recycled. The wastewater effluent may be subjected to further primary treatment, then to secondary treatment (biological treatment), tertiary treatment (chemical treatment) and finally discharged to surface waters under a legislation permit, discharged to a sewing system, recycled, or impounded in a lagoon, as illustrated in Fig.5.5. As a new strategy to reduce the water supply consumption, the partial regeneration of the water streams is proposed. The regeneration unit is modelled as "black box", Fig.5.6, able to remove one contaminant, more contaminants or all contaminants, using different available treatment technologies.

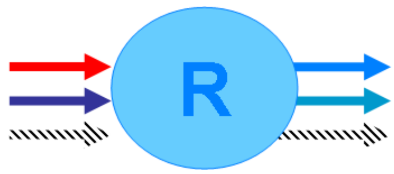


Figure 5. 6 Regeneration unit defined as a "black box"

Partial regeneration of internal streams can be performed either using some heuristic criteria or a thorough analysis and optimisation, reported to threshold concentrations beyond which each stream is cleaned-up to a certain level. In my opinion, the regeneration exit level should be an economic compromise or, when this is not possible, it should correspond to the minimum allowable input restrictions for all units, except those with contaminant free input. In this way, the regenerated water can be easily supplied to all units in water network. So, the input into the regeneration unit can produce a reasonable low concentration of contaminants. The regeneration should happen more often, leading to an overall increase in contaminants mean availability at the network level with a direct consequence reduction of supply water demand.

The *unlimited regeneration* corresponds to the case when all streams are decontaminated, while limited regeneration corresponds to the case when not all streams are regenerated from different reasons as technical availability or limited capacity of regeneration unit.

5.2.3. Total regeneration or zero discharge

The *total regeneration or zero discharge* is environmentally appealing, represents an ideal isolated system, supposed to be harmless to the environment. No supply water is needed, except for the fresh water used to compensate the technological losses, no aggression against environment is done, since no water is discharged outside the system.

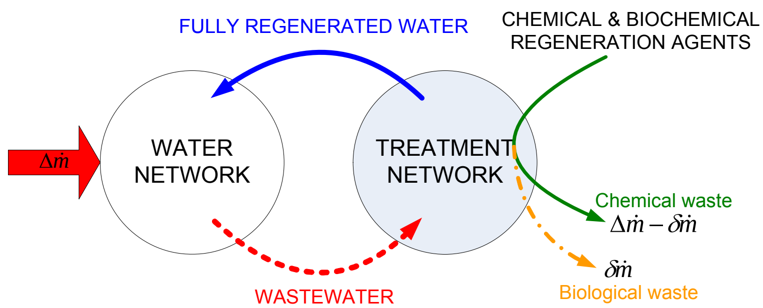


Figure 5. 7 Zero discharge concept

I wish to stress that in fact *zero discharge concept* hinders the problem of contaminants disposal as in Fig. 5.7, through the redistribution of the treatment network.

A mass flowrate $\Delta\dot{m}$ of contaminants enters the system through the water network and should leave the system, either transformed or in very concentrate state. According to the *ideal zero discharge concept*, water is a simple carrier, claiming that the pollution is reduced or even solved since no water is released into the environment. Still, the waste is there and should be disposed of, even if a part of the initial $\Delta\dot{m}$ flowrate could be converted during the treatment into environmentally harmless wastes. However, the main advantage of the *zero discharge concept* is the reduction of operating and treatment costs, since less water should be fully treated to be disposed into the environment.

5.3. Problem statement

I consider *a general water network with N water-using units, NS supply water sources and K contaminants identified to be removed by regeneration unit*.

Water network elements are defined as in Chapter 3:

$U=\{u_i \mid i=1,2,...,N\}$ set of water-using units associated in clusters related to each water source.

$S=\{s_j \mid j=1,2,...,NS\}$ set of supply water sources.

$C=\{c_k \mid k=1,2,...,K\}$ set of contaminants.

$M=\{m_{i,k} \mid i=1,2,...,N,\ \ k=1,2,...,K\}$ matrix of mass load [kg/s] of contaminant k transferred in water-using unit u_i

$L=\{L_i \mid i=1,2,...,N\}$ set of water losses streams.

The analysis is made in steady state and the water-using units are considered perfectly mixed vessels such as contaminant concentration C_{ki} in unit u_i is the same with concentration to unit exit. Regeneration unit is available to remove selected contaminant(s) having a “black box” structure. Threshold limits for contamination at entrance and exit of regeneration unit are given. Same approach is introduced as in paragraph 3.2, based on principle of driving force equipartition across the unit, the network is assimilated to an oriented graph.

The aim of this chapter is to establish which type of regeneration influences most the topology (removing one contaminant, more or all contaminants). In the same time the analysis is directed to find which contaminant(s) should be removed to obtain the best trade-off between supply water flowrate decrease and the difficulties arisen by the new topology.

5.4. Retrofit strategy

Retrofitting water network is not a trivial task since this has to be done under two major supplemental constraints: geographic and/or operational. The former implies that the network topology is stiffen (the geographic position of water sources, contamination degree and treatment units are given). The only allowed changes are the suppression or addition of some interconnections between units to achieve a desired goal such as furthermore minimisation of supply water input, among others. This involves all the internal flowrates which should be kept at a given value, due to various technological constraints.

The retrofit or revamp appears after the water/wastewater complex comes in use and represents the modifications, which can or have to be done, to cope to changed physical (changes in water supply), technological (changes in process equipment or treatment unit capacity), legislative, market (increased cost for energy or labour) conditions. During retrofit, connection between processes can be reconfigured and new equipment (as pumps) can be added. In a comprehensive review, Bagajewicz, 2000, outlined different graphical and mathematical programming techniques used to design and retrofit water networks, presenting some oil refinery case studies for one/multiple contaminants.

The approach to retrofit in this chapter is different compared to the techniques presented in literature. The originality arises, as in whole my Thesis, from different approach to water network – considered as oriented graph - and the criteria used to ensure retrofit.

- Supply water flowrate minimisation using the regeneration of one/some contaminants resulted from critical contaminant analysis.

- To keep network structure as simple as possible, considering topological index (as presented in Chapter 4).

Based on the concepts introduced in paragraph 5.2, the new topology and/or network performance are compared against the original case with respect to the topological index, contaminants mean availability and internal reuse quotient.

Retrofit implies internal water regeneration as presented in paragraph 5.3., targeting the critical contaminants from the bottleneck island or all contaminants, corresponding to zero discharge concept. The mathematical model is similar to the problem for water network considering regeneration.

5.5. Mathematical model for water network with regeneration

For the problem of water network optimisation with consideration of regeneration (presented in paragraph 5.3), mathematical model is based on overall and contaminant mass balances around water-using units and regeneration unit, together with associated constraints related to units input and output maximum allowable concentrations. The objective function is calculated as in paragraph 3.4 – minimum supply water flowrate. This objective function is chosen to get results closer to technical feasibility. When choosing cost based objective function, more factors are taken into account. If cost data are scarce weighted objective function based on supply water flowrate and topological index can be considered.

5.5.1. Mass balances for the generic water-using unit u_i

A schematic representation of generic water-using unit u_i is given in Fig. 5.8. The unit receives water from external supply sources (freshwater or slightly contaminated or contaminated) and/or at most h effluents ($h=1,2,\ldots i-1$) from units u_h placed before u_i (corresponding to water-using units ranking after one of two criteria Fcrt or Lcrt). Some of these streams can be regenerated. Mass load of contaminant k [kg/s], m_{ki} is removed from process streams into water stream in water-using unit u_i. According to their destination, water effluents of unit u_i can be:

- Reused water streams towards next j units ($j=i+1,\ldots, N$), X_{ij}
- Reused water streams satisfying the contamination condition for regeneration, $X_{ir(j)}$, towards regeneration unit (then automatically the stream goes to targeted unit u_j as stream $X_{(i)rj}$)
- Discharged stream W_i to treatment unit
- Losses stream L_i

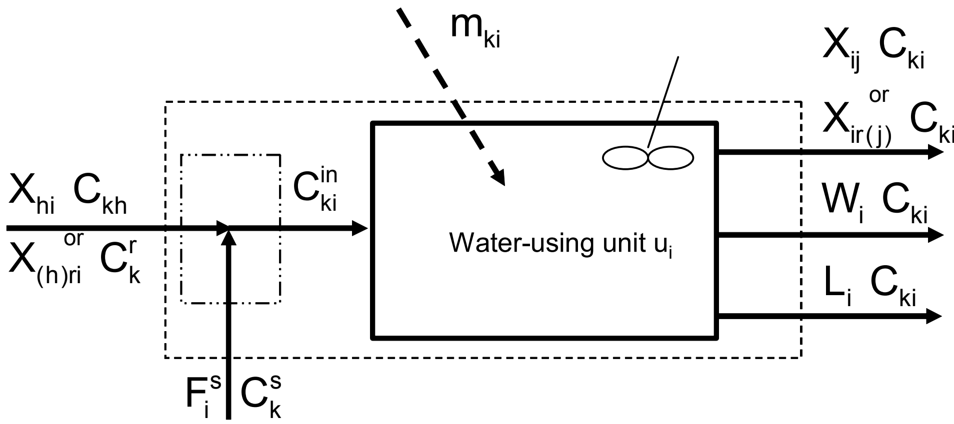


Figure 5. 8 Representation of generic water-using unit u_i

Each contaminant k is characterised by inlet and outlet concentration (C_{ki}^{in} and C_{ki}) restricted to corresponding limiting concentrations ($C_{ki}^{in,max}$ and $C_{ki}^{out,max}$). To ensure uniform notation in mass balances, following notations are introduced.

$$\chi_{hi} = \begin{cases} X_{hi} & \text{if stream comes from unit } u_h \text{ directly} \\ X_{(h)ri} & \text{if stream comes from unit } u_h \text{ via regeneration} \end{cases} \tag{5. 8}$$

$$\varsigma_{hi} = \begin{cases} C_{kh} & \text{if stream comes from unit } u_h \text{ directly} \\ C_k^r & \text{if stream comes from unit } u_h \text{ via regeneration} \end{cases} \tag{5. 9}$$

$$\chi_{ij} = \begin{cases} X_{ij} & \text{if stream comes from } u_i \text{ and goes to unit } u_j \\ X_{ir(j)} & \text{if stream comes from } u_i\text{, goes to regeneration and then to unit } u_j \end{cases} \tag{5. 10}$$

For uniformity, the concentration of effluents emerging unit u_i is denoted:

$$\varsigma_{ki} = C_{ki} \tag{5. 11}$$

5.5.2. Total mass balance around water-using unit u_i

$$\begin{aligned} & F_i^s + \sum_{h=1}^{i-1} \chi_{hi} + \sum_{k=1}^{K} m_{ki} - W_i - \sum_{j=i+1}^{N} \chi_{ij} - L_i = 0 \qquad \text{i=2,...,N-1} \\ & F_1^s + \sum_{k=1}^{K} m_{k1} - W_1 - \sum_{j=2}^{N} \chi_{1j} - L_1 = 0 \qquad \text{in particular for first unit} \end{aligned} \tag{5. 12}$$

In Eqs.5.12, the total flowrate entering in water-using unit u_i (i=2,3,…,N) is given by the flowrate of supply water F_i^s and all collected flowrates from preceding units $\sum_{h=1}^{i-1} \chi_{hi}$ (eventually some passed through regeneration unit). The effluents of unit u_i go to regeneration unit, before going to other water-using units, if the bottleneck island contaminants concentration is greater then regeneration threshold concentration.

5.5.3. Partial mass balance for contaminant k around water-using unit u_i

$$F_i^s C_k^s + \sum_{h=1}^{i-1} \chi_{hi} \varsigma_{kh} + m_{ki} - \left(W_i + L_i + \sum_{j=i+1}^{N} \chi_{ij} \right) \varsigma_{ki} = 0, \quad k = 1, 2, ..., K \qquad i=2,...,N-1$$
$$F_1^s C_k^s + m_{k1} - (W_1 + \sum_{j=2}^{N} \chi_{1j} + L_1) \varsigma_{k1} = 0 \qquad k = 1, 2, ..., K \qquad \text{in particular for first unit} \qquad (5.\ 13)$$

Eqs. 5.13 are written for the most general case, corresponding to contaminated water sources. When dealing with freshwater only, the first term of the left hand side of Eqs. 5.13 vanish.

5.5.4. Partial mass balance for contaminant k at water-using unit u_i input

$$F_i^s C_k^s + \sum_{h=1}^{i-1} \chi_{hi} \varsigma_{kh} - \left(\sum_{h=1}^{i-1} \chi_{hi} + F_i^s \right) \varsigma_{ki}^{in} = 0, \quad k = 1, 2, ..., K \qquad i=2,...,N \qquad (5.\ 14)$$

For the first unit, as there is no internal flow from other units, Eqs.(5.14) become

$$\varsigma_{k1}^{in} = \varsigma_{k1}^{s} \quad k=1,2,...,K \qquad (5.\ 15)$$

5.5.5. Set of constraints for contaminant concentration

The set of constraints for inlet/outlet contaminant concentration of water-using unit u_i are similar to those presented in paragraphs 3.3.5 and 3.3.6. These are generated by the limiting concentrations allowed by unit u_i at inlet ($C_{ki}^{in,max}$), respectively at outlet ($C_{ki}^{out,max}$). The possibility to regenerate exit streams is evaluated with reference to inlet limiting concentration for bottleneck island contaminants. In this respect, if $C_{ki} \geq C_{kr}^{in,min} \quad k \in J_p$, the effluent stream X_{ij} is sent first to regeneration, becoming stream $X_{ir(j)}$. After regeneration, is sent to initially target unit u_j, becoming stream $X_{(i)rj}$.

Mathematical model for water-using unit u_i is original due to elements of physical model, complexity of approach (as shown above, paragraph 5.2) and similarity to original elements introduced in analysis presented in Chapter 3.

5.5.6. Mass balances for regeneration unit, R

As the regeneration unit is considered perfectly mixed vessel, operating in steady state without losses (paragraph 5.2), the total mass balance is banal:

$$\sum_{j=i+1}^{N}(X_{ir(j)} - \sum_{k \in J_p} \Delta m^r_{kij}) = \sum_{j=i+1}^{N} X_{(i)rj} \tag{5. 16}$$

In agreement with paragraph 5.2 just for the connection between units u_i and u_j :

$$X_{ir(j)} - \sum_{k \in J_p} \Delta m^r_{kij} = X_{(i)rj} \tag{5. 17}$$

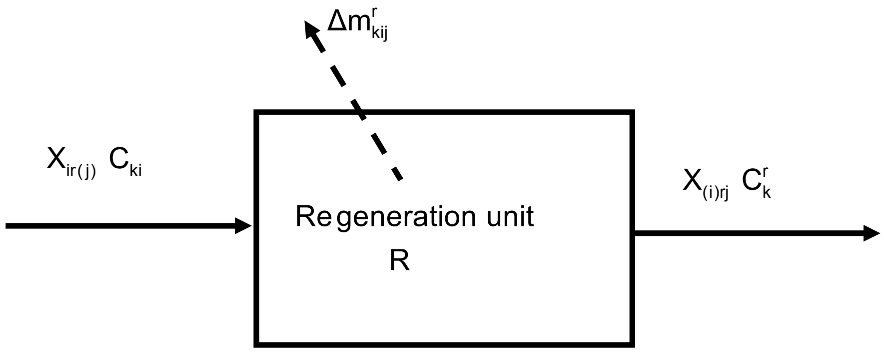


Figure 5. 9 Representation of regeneration unit R

The mass balance for regenerated contaminants:

$$\sum_{j=i+1}^{N}(X_{ir(j)}C_{ki} - \Delta m^r_{kij}) - \sum_{j=i+1}^{N} X_{(i)rj}C^r_k = 0 \quad k \in J_P \tag{5. 18}$$

Considering observation from Eq.(5.17), for the direct link between units u_i and u_j:

$$X_{ir(j)}C_{ki} - \Delta m^r_{kij} - X_{(i)rj}C^r_k = 0 \quad k \in J_P,\ j=i+1,...,N \tag{5. 19}$$

In this respect Eqs. 5.18 and 5.19 can be used to calculate mass load $\sum_{j=i+1}^{K} \Delta m^r_{kij}$ for each regenerated contaminant $k \in J_P$ originating in effluents of unit u_i, respectively Δm^r_{kij} originating in effluent of unit u_i going to unit u_j.

5.6. Design criteria

As mentioned in paragraph 3.4, the objective function to be minimised is supply water flowrate from different sources (Eq.3.9). The constraints are presented in above section, Eqs. 5.12 to 5.19, underlying the role of regeneration both in design and in retrofit problems. The optimisation problem regards water network as a whole, determining how to allocate the quality and quantity of water for each water-using unit u_i. For design problem with regeneration, the independent variables are same as in previous formulations (Chapter 3 and Chapter 4), the internal mass flowrates between water-using units: $X = \{X_{ij} \mid i = 1,2,...,N-1,\ j=2,...,N\}$.

As a consequence of considering the water network as oriented graph, the total number of independent variables is N(N-1)/2. In case of regeneration, new streams determine new variables ($X_{ir(j)}, X_{(i)rj}, C_{(i)rj}$), which can be considered auxiliary variables, they do not enlarge the dimension of the problem because there are relations for calculations.

The parameters of the problem are same as presented in paragraph 3.4.2, adding as well the limiting concentration sets for regeneration unit:

$C_r^{in,min} = \{C_{kr}^{in,min} \mid k = 1,2,...,K\}$ Limiting concentration set at regeneration unit entrance

$C_r^{out,max} = \{C_{kr}^{out,max} \mid k = 1,2,...,K\}$ Limiting concentration set at regeneration unit exit

The dependent variables of the problem are similarly considered as in paragraph 3.4.2:

$F^s = \{F_i^s \mid i = 1,2,...,N\}$ set of water supply source flowrates for each u_i

$W = \{W_i \mid i = 1,2,...,N\}$ set of wastewater flowrates from each u_i

$C^{in} = \{C_{ki}^{in} \mid i = 1,2,...,N\ ;\ k = 1,2,...,K\}$ set of concentration of contaminant k at the entrance of u_i

$C^{out} = \{C_{ki} \mid i = 1,2,...,N\ ;\ k = 1,2,...,K\}$ set of concentration of contaminant k at the exit of u_i

The flowrate of supply water for each unit u_i is also calculated with relations similar to Eqs. 3.10 to 3.14. For retrofit problem, the approach is similar, just the initial state of water network (flowrates, compositions, etc) is used to initiate calculations when regeneration unit is introduced.

5.7. Solving strategy and optimisation algorithm

The models formulated above (either design or retrofit) are highly non linear and large NLP problems. As in previous chapters, a modified variant of GA is used to find optimum solution. The internal flows X_{ij} (independent variables) compose the chromosome. The fitness function is based on the objective function in a normalised form to keep the values of independent variables in [0,1] domain, to enlarge or reduce the difference between bad and good individuals.

Same parameters of GA algorithm are kept, based on my experience (Lavric et al., 2004a, Lavric et al., 2004b, Lavric et al, 2005). The optimisation procedure to solve the design problem is presented in paragraph 3.5 (but some slight modifications are needed to evaluate the bottleneck island of the network):

1. Rank water-using units by Fcrt or Lcrt criteria.
2. Compute the minimum supply water flowrate for water-using unit u_i based on Eqs. 3.10 - 3.11 and individuals calculated by GA (calculus is cascaded).
3. Compute bottleneck island J_K based on six steps procedure given in paragraph 5.2.1, taking decision for regeneration of contaminants (one or J_K or all).
4. Compute wastewater flowrates for water-using unit u_i according to Eqs. 5.13 with specification from paragraph 3.5.
5. Compute concentrations of streams around each unit, if $C_{ki} > C_{kr}^{in,min}$ the stream is directed to regeneration unit.
6. Compute for each contaminant the regeneration mass load summing up the regeneration per stream, Eqs. 5.18-5.19.
7. Return the objective function value, summing up minimum supply water flowrate for all water-using units.

Following these steps, the optimal solution is obtained in terms of the minimum supply water flowrate. The algorithm is coded into original software, as presented in Annex 2 and published in (Lavric et al., 2004a, Lavric et al., 2004b, Lavric et al, 2005).

For retrofit problem, in steps 1-2-3, given data for water network is used to start calculations.

5.8. Graphical representation of water network topology with regeneration

Importance of water network visualisation in adequate graphical form is discussed in paragraph 3.6. Original representation given in my paper Iancu et al., 2007 offers easier access to information related to water network. This representation allows obvious integration of regeneration unit as I present in Fig. 5.10.

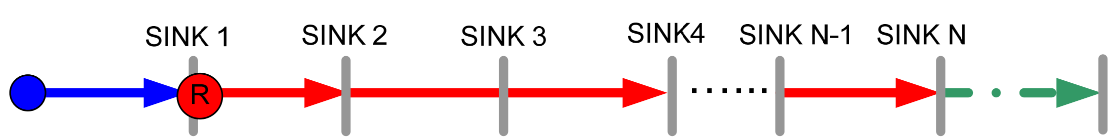


Figure 5. 10 Representation of regenerated water streams from source (regeneration unit) to sinks (water-using units)

A regenerated water stream is represented as a red arrow between source (regeneration unit) and a sink (water-using unit). If the stream does not exist there is no arrow between source and sink. Using this coding procedure for water streams, I propose to represent the water network as in Fig. 5.11.

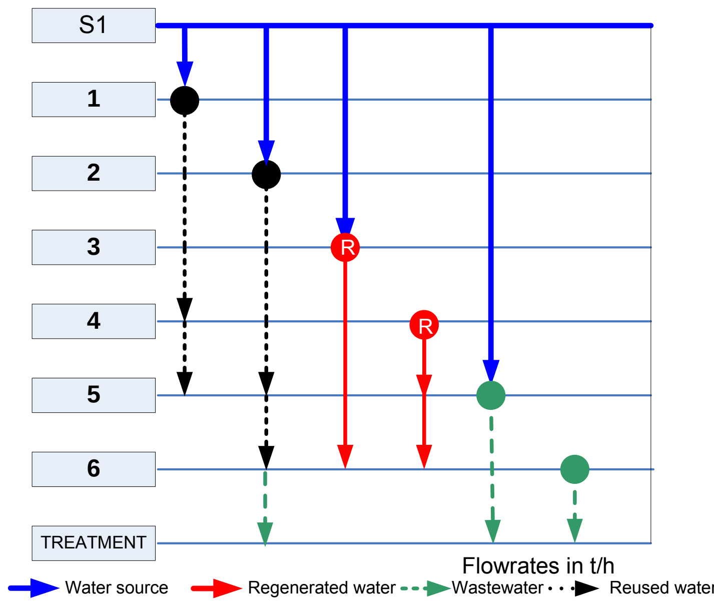


Figure 5. 11 Representation of topology for water-using network with regeneration

5.9. Water network optimisation case study with regeneration

5.9.1. Case study presentation

A case study related to a petrochemical plant, with six water-using units, one freshwater source and four contaminants is presented, to optimise the water network, considering regeneration. The procedure described in paragraph 5.2.1 allows establishing critical contaminant and network bottleneck. In Table 5.1 the limiting data for water-using units ($C^{in,max}$, $C^{out,max}$) and regeneration unit ($C_r^{in,min}$, $C_r^{out,max}$) are given. The water network has one supply source with freshwater (all contaminants vanish).

Table 5. 1 Water-using units and regeneration unit limiting data

Contami-nant	Water-using units												Regeneration unit	
	$C^{in,max}$ (ppm)						$C^{out,max}$ (ppm)						$C_r^{in,min}$ (ppm)	$C_r^{out,max}$ (ppm)
	U1	U2	U3	U4	U5	U6	U1	U2	U3	U4	U5	U6	Inlet	Outlet
C1	0	**10**	15	14	12	20	35	63	81	80	75	100	50	10
C2	0	**8**	12	18	10	23	38	49	73	78	70	95	40	8
C3	0	12	18	20	**10**	25	27	39	87	95	100	120	30	10
C4	0	15	16	15	**13**	20	32	80	102	105	110	150	50	13

Mass load of contaminants removed in each water-using unit are given in Table 5.2.

Table 5. 2 Mass load of contaminants

Mass load of contaminants m_{ki} (g/h)	Water-using units					
	U1	U2	U3	U4	U5	U6
C1	750	1,200	2,000	1,300	7,100	2,100
C2	1,100	900	1,800	2,100	3,200	3,150
C3	480	850	730	3,000	3,800	2,750
C4	150	1,300	600	1,500	3,500	2,350

The units have no water losses, as this parameter is not relevant for this analysis. I intend to keep the case study enough simple to underline the role of regeneration.

From direct analysis of this data it can be seen that the input limits are very restrictive. It is not possible to reuse neither water streams because the outlet compositions are higher that the inlet acceptable limits. Water streams reuse is possible if a regeneration unit, to reduce the contamination level of selected contaminants to an acceptable value. The output regeneration unit limits for each contaminant are given in Table 5.1 : to reduce the concentration for contaminant 1 to 10 ppm, for contaminant 2 to 8 ppm, for contaminant 3 to 10 ppm and for contaminant 4 to 13 ppm. The ratio of removing contaminants for regeneration unit is a very important variable. It is better to reduce the contamination as much as possible to decrease the costs of treatment. Also this variable can be a criterion for optimisation.

The water network is optimised for supply water flowrate as objective function, applying the methodology that I present and illustrate in Chapter 3 (just for reusing strategy). The results for both ranking criteria (Fcrt and Lcrt), total minimum supply water flowrate and distribution on water-using units is given in Table 5.3.

Table 5. 3 Minimum supply water flowrate

Water-using units	Existing case	Supply water flowrate optimisation	
	Maximum supply water flowrate (t/h)	Supply water flowrate (t/h)	
		Fcrt	Lcrt
U1	28.95	28.95	28.95
U2	31.48	21.13	19.87
U3	30.30	23.14	22.81
U4	40.00	23.02	20.92
U5	112.70	84.63	83.47
U6	43.75	23.40	26.85
Total flowrate (t/h)	**287.18**	**204.27**	**202.87**

Applying *only reusing strategy*, the water network needs about 204.27 t/h (Fcrt) or 202.87 (Lcrt) supply water flowrate as illustrated in (Table 5.3). Compared to existing situation, 28.9% saving for freshwater consumption is obtained. In optimised topology new streams appear because water is reused (i.e. $U1 \rightarrow U2, U3, U4, U5, U6$). Reused water flowrates are given in Table 5.4. Due to oriented graph model of water network, the units U5 (for Fcrt criteria) and U6 (for Lcrt criteria) collect internal streams from different other units and send effluents to treatment as I present in Table 5.4 and illustrate in Fig. 5.12. It is not possible to reuse these effluents to other units because of their high level of contamination.

Table 5. 4 Wastewater and reused water flowrate distribution per units

Water-using units	Supply water flowrate optimisation			
	Reused water flowrate (t/h)		Wastewater flowrate (t/h)	
	Fcrt	Lcrt	Fcrt	Lcrt
U1	0.0	0.0	0.0	0.0
U2	1.4	5.3	1.4	1.2
U3	3.2	5.9	21.5	27.5
U4	11.0	13.7	31.4	30.8
U5	24.1	25.9	108.8	103.3
U6	18.2	13.4	41.2	40.2
Total flowrate (t/h)	**57.9**	**64.1**	**204.3**	**202.9**

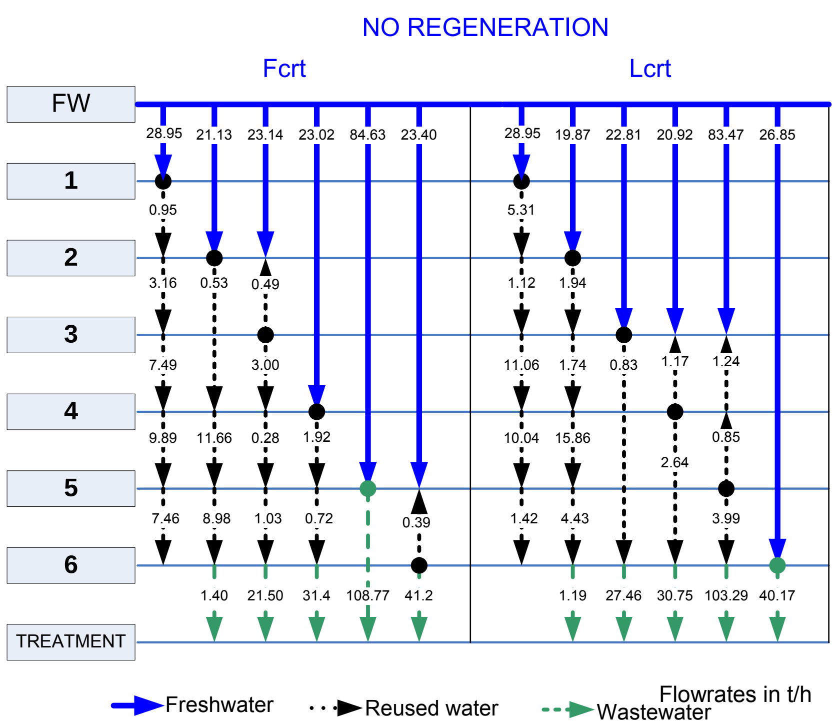


Figure 5. 12 Water network topology

The concentrations of water streams at units entrance and exit obtained after optimisation, necessary for critical contaminant analysis are presented in Table 5.5. and Table 5.6.

Table 5. 5 Contaminants composition at water-using unit entrance

$C_{k,i}\|_{in}$	U1	U2	U3	U4	U5	U6
C1	0.00	2.82	3.12	13.56	9.72	19.59
C2	0.00	3.19	4.57	15.48	9.96	19.26
C3	0.00	1.35	1.99	6.90	7.73	13.78
C4	0.00	0.73	0.62	4.13	7.89	14.94

Table 5. 6 Contaminants composition at water-using unit exit

$C_{k,i}\|_{out}$	U1	U2	U3	U4	U5	U6
C1	25.91	55.98	79.15	51.75	75.00	70.08
C2	38.00	43.06	73.00	77.16	39.38	95.00
C3	16.58	39.00	29.75	95.00	42.67	79.91
C4	5.18	58.32	23.43	48.19	40.07	71.45

Analysing optimisation data for minimum supply water flowrate, enabling just water reuse, I notice some characteristics.

- From limiting data, the network is very restricted involving rigidity in reuse of water (e.g. unit U1 accepts only freshwater).
- Ranking criteria give relatively close results.
- The optimised topology is quite complicated, units U1 and U2 sending reused water to other units, total reused water flowrate is 57.9 t/h – Fcrt , respectively 64.1 t/h – Lcrt.
- Unit U1 reuses all water (no wastewater from this unit), all other units produce wastewater.
- Reused water flowrate is relatively small compared to supply water flowrate (~30%)

In this situation, it is obvious that the possibility to use regeneration unit in water network design should be analysed. According to the algorithm I give in paragraph 5.7, critical contaminant analysis allows to decide on the regeneration strategy, computing the bottleneck island J_k (as in paragraph 5.9.2). Then, four scenarios for optimal water network design using regeneration of one or more contaminants and reuse the regenerated streams into the network are analysed (in paragraph 5.9.3). Finally, the most attractive solution is chosen.

5.9.2. Critical contaminant analysis

In agreement to solving strategy and optimisation algorithm presented in paragraph 5.7, for determination of critical contaminant I evaluate the mean availability of each contaminant per each water-using unit following the procedure presented in paragraph 5.2.1:

a) Setting-up the limiting data ($C^{in,max}$, $C^{out,max}$), for all contaminants and all water-using units (Table 5.1)

b) Setting-up the current data for all contaminants and all water-using units (Tables 5.5 and 5.6). Current situation is considered the optimised water network for minimum supply water flowrate objective function. The inlet and outlet concentrations obtained from optimisation procedure are given in Tables 5.4 and 5.5.

c) Composition difference at entrance (Eq.5.4), for all contaminants in each water-using unit u_i' (Table 5.7)

Table 5. 7 Composition difference of contaminants at each unit entrance

$\Delta C_{k,i}\big\vert_{in}$	U1	U2	U3	U4	U5	U6
C1	0.000	7.183	11.885	0.436	2.278	0.413
C2	0.000	4.812	7.432	2.523	0.041	3.744
C3	0.000	10.655	16.007	13.101	2.272	11.219
C4	0.000	14.270	15.377	10.869	5.112	5.062

d) Composition difference at exit (Eq.5.5), for all contaminants in each water-using unit u_i, (Table 5.8)

Table 5. 8 Composition difference of contaminants at each unit exit

$\Delta C_{k,i}\big\vert_{out}$	U1	U2	U3	U4	U5	U6
C1	9.091	7.023	1.850	28.254	0.000	29.917
C2	0.000	5.942	0.000	0.845	30.620	0.000
C3	10.418	0.000	57.254	0.000	57.335	40.094
C4	26.818	21.680	78.566	56.813	69.933	78.555

e) Average composition difference (Eq.5.6), for all contaminants in each water-using unit u_i (Table 5.9)

Table 5. 9 The average composition difference of contaminant for each unit

$\Delta C_{k,i}\big\vert_{mean}$	U1	U2	U3	U4	U5	U6
C1	4.546	7.103	6.868	14.345	1.139	15.165
C2	0.000	5.377	3.716	1.684	15.331	1.872
C3	5.209	5.328	36.631	6.551	29.804	25.657
C4	13.409	17.975	46.972	33.841	37.523	41.809

f) Mean availability (Eq.5.7) as average composition difference for each contaminant in all water using units (Table 5.10)

Table 5. 10 Mean availability per contaminant

$\overline{\Delta C_k}$	Mean pseudo driving-force
C1	8.194
C2	**4.663**
C3	18.196
C4	31.921

The critical contaminant can be identified as the contaminant with the lowest mean availability, (contaminant C2 has $\overline{\Delta C_2} = 4.663$). Similar conclusion can be drawn from Fig.5.13, where pseudo-driving force for each unit is represented. Applying my original approach for critical contaminant analysis to the whole water network, the contaminant C2 is able to produce bottleneck as has lowest mean availability. This contaminant limits supply water consumption or internal water reuse. Close to contaminant C2 as mean availability is contaminant C1 ($\overline{\Delta C_1} = 8.19$). As other contaminants have quite higher mean availability, there is obvious that $J_2=\{C_1,C_2\}$ is bottleneck island.

g) The final step of critical contaminant analysis is to identify the minimum supply water consumption and proving that minimum is obtained for critical contaminant.

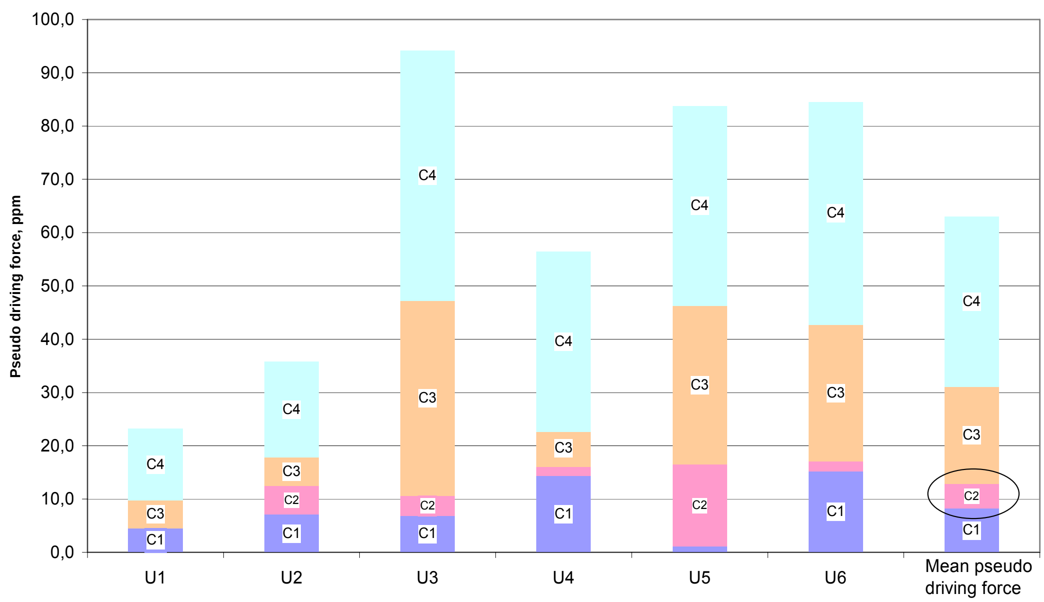


Figure 5. 13 Choosing the critical contaminant from pseudo-driving force diagram

If the procedure is used also for Lcrt optimised water network, also the contaminant C2 is identified as critical contaminant with a mean availability about 4.12 ppm. Then, the water network is optimised four times, each time one contaminant is regenerated. The results of optimisations, considering water network as oriented graph, ranked either by Fcrt and Lcrt criteria, are summarised in Table 5.11.

Table 5. 11 Supply water flowrate for critical contaminant regeneration

Optimisation criterion	Ranking criteria	Critical Contaminant Regeneration			
		C1	C2	C3	C4
Supply water flowrate (t/h)	Fcrt	194.76	**189.17**	202.96	204.16
	Lcrt	190.82	**188.35**	202.20	202.08

Minimum supply water flowrate is obtained for regeneration of critical contaminant for both ranking criteria (Fcrt and Lcrt), so, the principle of critical contaminant proved that :

Regeneration of the contaminant with minimum mean availability gives the best solution for optimisation of water network, because this contaminant is a bottleneck factor.

From this case study I can draw the conclusion that following scenarios are interesting to develop :

Scenario A – regeneration of contaminant C2 as critical contaminant

Scenario B – regeneration of bottleneck island of contaminant C2, $J_2=\{C_1,C_2\}$

Scenario C – regeneration of three contaminants {C1, C2, C3}

Scenario D – total regeneration (zero discharge) of contaminants {C1, C2, C3, C4}

Regeneration of contaminants with minimum availability is a good choice to obtain an improved water network because critical contaminant is a bottleneck factor. However, it is more advisable to regenerate the whole bottleneck island of critical contaminant as I prove below. In these scenarios, I propose a detailed analysis to determine the favourable groups of contaminants which can be removed in regeneration unit for generation of optimal water network (in terms of supply water flowrate).

5.9.3. Design optimal water network considering regeneration

It is expected that using regeneration, supply water flowrate is reduced. It is interesting to analyse which is the most convenient configuration for contaminant regeneration to have a solid support for decision making to improve water network performance. In practice, different techniques are available (keeping in mind the nature of process and contaminants) as microfiltration, greenhouse filters, sand filters, etc. There is beyond the purpose of this case study to analyse in deep these processes.

Considering the models developed in paragraph 5.5, in design I am concerned to minimise freshwater flowrate, to underline the nature of reused water (either regenerated or not), the wastewater flowrate released by each unit and network topology. No other objective function is considered in this case study. In general, to reduce further supply water consumption and wastewater generation, regenerated water can be reused by other water using unit or recycled in same unit. In this case study just the first situation is considered as is more realistic and has greater flexibility. Results obtained in scenarios described below are compared with optimised water network, when no regeneration is allowed for both ranking criteria.

5.9.3.1. Scenario A: Partial regeneration of critical contaminant

As C2 is critical contaminant, in this scenario I present the influence of partial regeneration on topology of water network. Actually, the optimisation of supply water flowrate as objective function is considered. In Table 5.12, I present the flowrates of supply water, wastewater and reused water streams for each water-using unit from water network.

Table 5. 12 Supply water, reused water, regenerated water and wastewater flowrates Scenario A: regeneration of contaminant C2

Water-using units	Fcrt				Lcrt			
	Supply water flowrate (t/h)	Reused water flowrate (t/h)	Regenerated water flowrate (t/h)	Waste water flowrate (t/h)	Supply water flowrate (t/h)	Reused water flowrate (t/h)	Regenerated water flowrate (t/h)	Waste water flowrate (t/h)
U1	28.95	0.00	0.00	0.00	28.95	0.00	0.00	0.00
U2	21.13	0.86	1.12	3.68	20.13	2.90	0.00	2.33
U3	17.05	1.05	0.00	12.08	17.34	3.58	6.34	24.57
U4	22.40	0.72	9.65	22.29	23.87	6.29	4.41	22.26
U5	74.87	25.94	11.34	112.09	75.07	15.46	13.30	100.98
U6	21.87	0.44	16.78	39.03	22.99	0.72	11.63	38.21
Total flowrate (t/h)	**204.27**	**29.01**	**38.89**	**189.17**	**188.35**	**28.95**	**35.68**	**188.35**

Internal flowrates are 67.90 t/h for Fcrt and 64.63 for Lcrt. Reused water is produced practically by U1. Compared with base case, freshwater flowrate decreased slightly (7.5% for Fcrt and 9.3% for Lcrt). Same trend has also wastewater flowrate. Comparing the topology represented in Fig. 5.14 with base case, changes are not dramatic and similar water flowrates circulate inside water network.

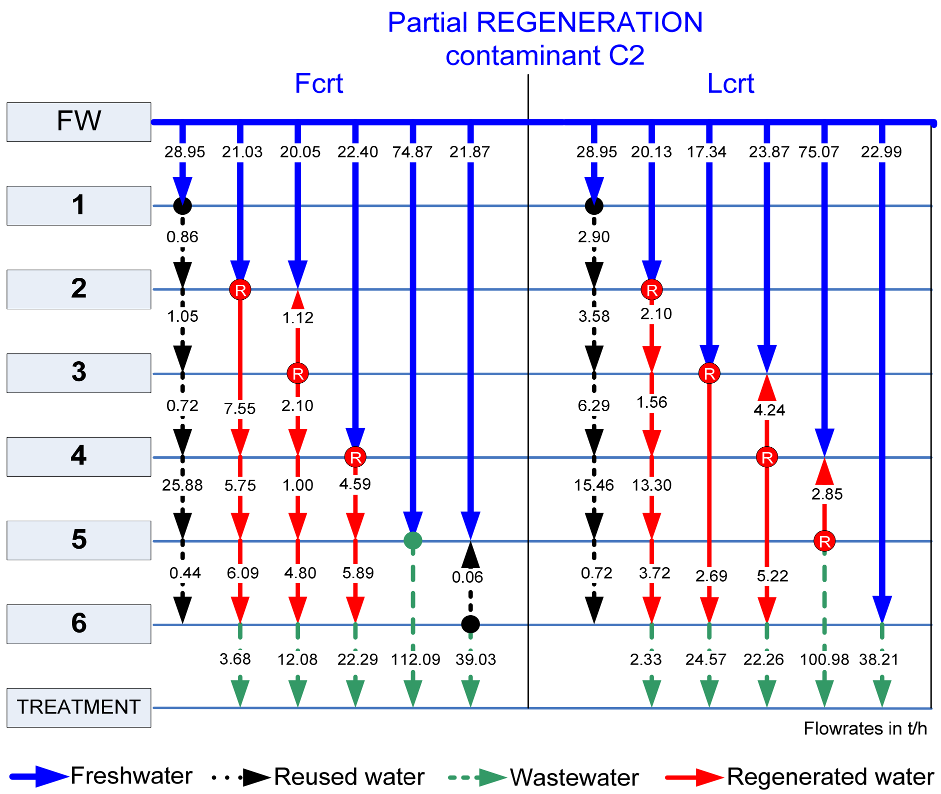


Figure 5. 14 Water network topology for Scenario A

The topology obtained for Fcrt ranking criterion is more attractive as just three water streams (effluents from U2, U3 and U4) are regenerated compared to the topology guaranteed for Lcrt ranking criterion where four streams (effluents from U2, U3, U4 and U5) are regenerated. Otherwise the ranking criteria give quite close results.

The conclusion of this scenario is that regeneration of critical contaminant does not guarantee an attractive solution for water network topology. The IRQ is 36% for Fcrt and 43.8% for Lcrt ranking criteria.

5.9.3.2. Scenario B: Partial regeneration for bottlenecking island J_2={C1&C2}

In this scenario, regeneration of bottleneck island, J_2={C1&C2} is proposed. Optimisation results are presented in Table 5.13 and water network topology is illustrated in Fig. 5.15. Supply water flowrate is reduced by 17.7% for Fcrt criterion and by 15.7% for Lcrt criterion. Same reduction is recorded for wastewater generation. Reused water is constant ~ 29 t/h compared to Scenario A, instead regenerated water flowrate increases in the total reused water from ~56% in Scenario A to ~66% in current scenario.

Table 5. 13 Supply water, reused water, regenerated water and wastewater flowrates Scenario B: regeneration for bottlenecking island

Water-using units	Fcrt				Lcrt			
	Supply water flowrate (t/h)	Reused water flowrate (t/h)	Regenerated water flowrate (t/h)	Waste water flowrate (t/h)	Supply water flowrate (t/h)	Reused water flowrate (t/h)	Regenerated water flowrate (t/h)	Waste water flowrate (t/h)
U1	28.95	0.00	0.00	0.00	28.95	0.00	0.00	0.00
U2	18.99	4.45	1.02	0.00	20.13	4.82	0.00	1.94
U3	20.07	5.40	0.00	0.00	22.45	4.60	0.00	0.00
U4	12.17	14.75	11.20	34.09	23.78	6.54	4.63	34.95
U5	72.19	2.88	23.70	98.74	70.33	8.08	21.98	96.79
U6	13.84	1.65	20.04	35.38	5.44	4.91	27.05	37.40
Total flowrate (t/h)	**168.21**	**29.13**	**55.96**	**168.21**	**171.08**	**28.95**	**53.66**	**171.08**

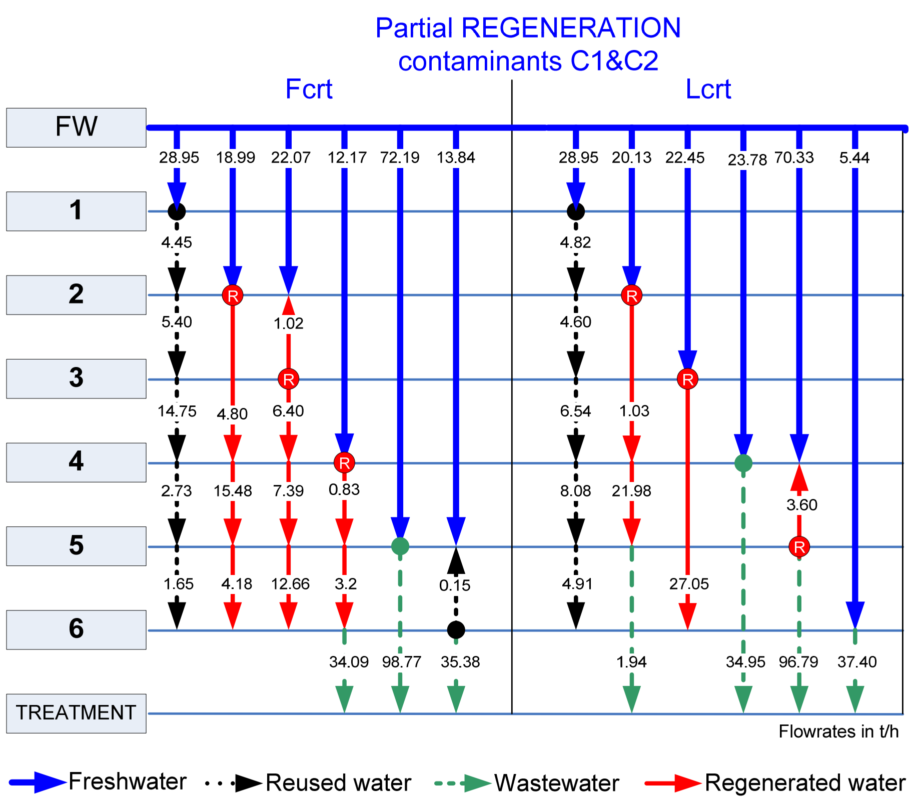


Figure 5. 15 Water network topology for Scenario B

Water network topology is simplified especially for Lcrt criterion, regarding internal circulation of reused/regenerated water, but there are four streams to wastewater treatment unit. The topology for Fcrt criterion is somewhat more complicated but there are just three wastewater streams. Total flowrates are quite similar for all types of water streams when compared ranking criteria.

Comparing to Scenario A, this topology is simplified, appearing more attractive. Units effluent streams have maximum four splits (unit U3) in Scenario B, compared to maximum five splits in Scenario A (unit U3). The potential to use regenerated water in Scenario B increases significantly (by about 30%), especially for units U5 and U6.

5.9.3.3. Scenario C: Partial regeneration of contaminants C1, C2 & C3

In this scenario I consider that the regeneration unit is able to remove three contaminants (C1, C2 & C3), which form a bottleneck island of critical contaminant.

Results of this scenario are presented in Table 5.14 and topology of water network is presented in Fig. 5.16.

Supply water flowrate did not reduced significantly compared to Scenario B (~5% in average for both ranking criteria). Reused water flowrate increased just slightly, but regenerated water flowrate increased significantly (~30%).

Table 5. 14 Supply water, reused water, regenerated water and wastewater flowrates Scenario C: regeneration of contaminants C1, C2 & C3

Water-using units	Fcrt				Lcrt			
	Supply water flowrate (t/h)	Reused water flowrate (t/h)	Regenerated water flowrate (t/h)	Waste water flowrate (t/h)	Supply water flowrate (t/h)	Reused water flowrate (t/h)	Regenerated water flowrate (t/h)	Waste water flowrate (t/h)
U1	28.95	0.00	0.00	0.00	28.95	0.00	0.00	0.00
U2	19.27	4.39	0.00	0.00	18.94	4.97	0.00	0.00
U3	21.54	6.51	0.00	15.61	12.27	7.13	10.25	29.65
U4	16.49	7.75	10.21	0.00	18.45	9.62	6.95	0.00
U5	65.94	8.22	28.08	108.25	77.53	11.95	10.75	88.71
U6	11.67	14.52	26.12	40.00	0.80	6.80	30.98	38.58
Total flowrate (t/h)	**163.86**	**41.39**	**64.41**	**163.86**	**156.94**	**40.47**	**58.93**	**156.94**

The complexity of water network topology do not changed significantly compared with topology in Scenario B. There are three water streams from units U3, U5 and U6 (only in Lcrt topology). Also water stream from unit U1 is reused in all water-using units (as in other scenarios), but only two streams are regenerated (from U2 and U4). Keeping in mind possible technological difficulties in regeneration of three contaminants compared to the regeneration of two contaminants and slight modifications in performances compared to scenario B, I can draw the conclusion that Scenario C is not very attractive.

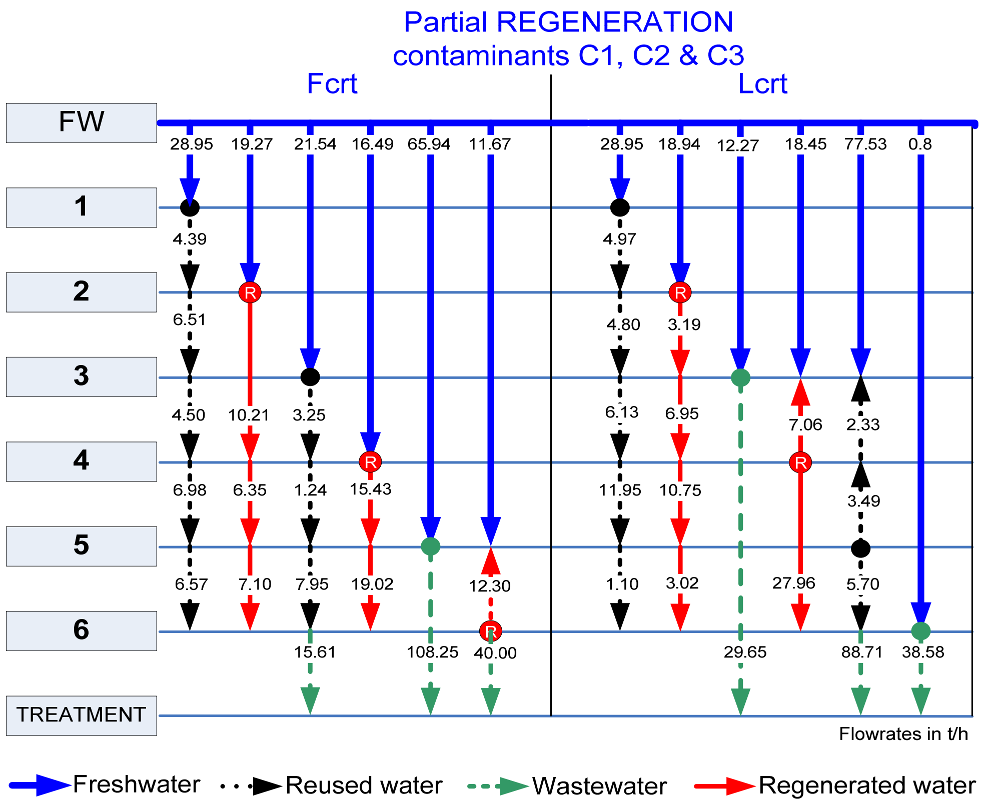


Figure 5. 16 Water network topology for partial regeneration of contaminants C1,C2 & C3

5.9.3.4. Scenario D: Total regeneration (zero discharge)

In this scenario there are no wastewater streams to treatment unit. Effluents of all water using units are regenerated to get characteristics of supply water (all contaminants vanish). As a consequence, there is no supply water (as in this case study losses are neglected) and there is no reused water. For this special scenario, effluents for the water using units have two roles: either regenerated-reused water to other units or to build the pool of water supply to some units. The results of water network optimisation are given in Table 5.15 and water network topology in Fig. 5.17. The total flowrate satisfying water network operation is produced in regeneration unit. The results for ranking criteria are quite different : 201.68 t/h for Fcrt and 283.69 t/h for Lcrt. From this amount, 94.67 t/h for Fcrt and 96.06 t/h for Lcrt (quite close) are used as supply water regenerated by all units for fcrt and just by three units for Lcrt.

Table 5. 15 Supply water, reused water, regenerated water and wastewater flowrates

Scenario D: Total regeneration (zero discharge)

Water-using units	Fcrt			Lcrt		
	Supply water /Regenerated flowrate (t/h)	Reused regenerated water flowrate (t/h)	Total regeneration unit flowrate (t/h)	Supply water /Regenerated flowrate (t/h)	Reused regenerated water flowrate (t/h)	Total regeneration unit flowrate (t/h)
U1	28.95	28.95	28.95	28.95	0.00	28.95
U2	13.74	8.05	21.79	9.34	12.45	21.79
U3	14.96	9.73	24.69	0.00	42.60	42.60
U4	8.96	22.62	31.58	0.00	30.95	30.95
U5	28.06	24.83	52.89	57.77	37.63	95.40
U6	0.00	41.78	41.78	0.00	64.00	64.00
Total flowrate (t/h)	**94.67**	**107.01**	**201.68**	**96.06**	**187.63**	**283.69**

The topology is enough complex, as I presented in Fig. 5.17. These results are enabled me that this scenario is attractive just in the extreme case of legislative restrictions, when no other technical solution can be applied.

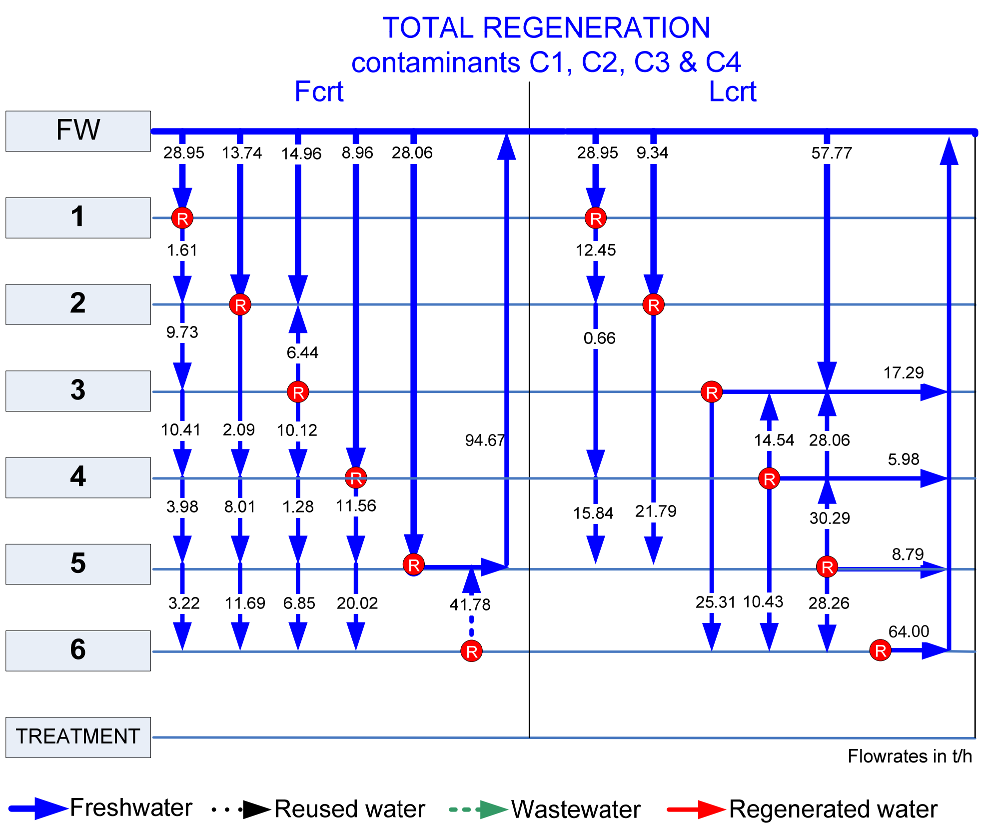


Figure 5. 17 Water network topology for case : Total regeneration

To draw a final conclusion, some relevant data from each scenario are compared in Table 5.16.

Table 5. 16 Summary of scenarios results

Scenario	Fcrt				Lcrt			
	Supply water flowrate (t/h)	Reused water flowrate (t/h)	Regenerated water flowrate (t/h)	Waste water flowrate (t/h)	Supply water flowrate (t/h)	Reused water flowrate (t/h)	Regenerated water flowrate (t/h)	Waste water flowrate (t/h)
Base case	204.27	57.95	0.00	204.27	202.87	64.10	0.00	202.87
A	189.17	29.01	38.89	189.17	188.35	28.95	35.68	185.48
B	**168.21**	**29.13**	**55.96**	**168.21**	**171.08**	**28.95**	**53.66**	**171.08**
C	123.86	41.39	110.41	123.83	156.94	40.47	58.93	156.94
D	94.67	107.01	201.68	0.00	96.06	187.63	283.69	0.00

For this analysis, the most attractive solution is those obtained in Scenario B, for regeneration of bottlenecking island of critical contaminant, because has lower internally circulated water flowrate and quite simple water network topology. Scenario D is applicable only if discharge regulations become so strict that zero discharge is compulsory.

This case study illustrates the usefulness of the methodology proposed to analyse the opportunity for contaminant regeneration. The proposed result is based just on one objective function optimisation, which underlines the specific aspects of studied topic. For specific applications, when more technical data about regeneration technology is available and cost data can be provided a broader support for decision can be considered. However the critical contaminant based methodology, as originally I introduced in this Chapter, is an important step in any generalised methodology to be applied in specific practical situations.

5.10. Water network retrofit through regeneration

In this case study I propose to retrofit an existing water network considering regeneration. Seven water-using units, one water source (only freshwater available), four contaminants and a regeneration unit are considered. Water network limiting data is presented in Tables 5.17 and 5.18. Known pipes length is given in Table 5.19. The results concerning this case study are partially published in the paper Lavric et al., 2007. The optimisation methodology is applied to retrofit water network considering minimum supply water flowrate objective function, using regeneration of some designated contaminants (as resulted from critical contaminant analysis). Water network topology is evaluated by topological index (defined in paragraph 4.4.2.1).

Table 5. 17 Limiting concentration for water-using units

Contaminant	Water-using units														Regeneration unit	
	$C^{in,max}$ (ppm)							$C^{out,max}$ (ppm)							Concentration (ppm)	
	U1	U2	U3	U4	U5	U6	U7	U1	U2	U3	U4	U5	U6	U7	Inlet	Outlet
C1	0	10	15	14	17	22	20	198	63	81	80	75	35	127	50	10
C2	0	8	12	18	8	23	19	38	49	73	78	63	95	85	40	8
C3	0	17	18	28	12	25	21	114	27	47	67	100	120	55	30	10
C4	0	21	16	15	13	20	25	32	80	102	175	110	150	72	50	13

Table 5. 18 Mass loads of contaminants for water-using units

Contaminant mass load (g/h)	Water-using units						
	U1	U2	U3	U4	U5	U6	U7
C1	750	1200	2000	1300	7100	2100	2190
C2	2100	1950	3800	2100	3200	4150	4370
C3	3970	3000	3030	2850	3750	3800	4800
C4	150	1300	600	1500	3500	2350	2750

Table 5. 19 Pipes length for water network

$\mathscr{L}_{ij}$ (m)	S1	U1	U2	U3	U4	U5	U6	U7	T
S1	-	500	600	400	200	500	400	100	-
U1	x	-	300	100	500	200	200	100	500
U2	x	x	-	300	300	500	400	300	400
U3	x	x	x	-	250	100	300	200	300
U4	x	x	x	x	-	300	300	200	400
U5	x	x	x	x	x	-	800	600	200
U6	x	x	x	x	x	x	-	150	600
U7	x	x	x	x	x	x	x	-	500
T	x	x	x	x	x	x	x	x	-

Four scenarios are considered to identify the optimal topology: Scenario A - partial regeneration of critical contaminant, Scenario B - partial regeneration of neighbour of critical contaminant (both form bottleneck island), Scenario C - partial regeneration of contaminants belonging to the bottleneck island and Scenario D - total regeneration of contaminants.

Base case: the water network is optimised considering only reusing strategy. The supply water flowrate is 48.62t/h for Fcrt and 42.54 t/h for Lcrt criterion. Water network topology is presented in Fig.5.18. All water using units receive freshwater and produce wastewater. Few units send reused water to other units. Topological index gives information about usage percentage from total pipes length: 56% for Fcrt and 52% for Lcrt criterion, due water reuse between units. Consequently, the topology is quite rigid and further improvement is expected.

From critical contaminant analysis, C2 and C3 are identified as bottleneck contaminants. Consequently, in next scenarios contaminants C2 and C3 are regenerated.

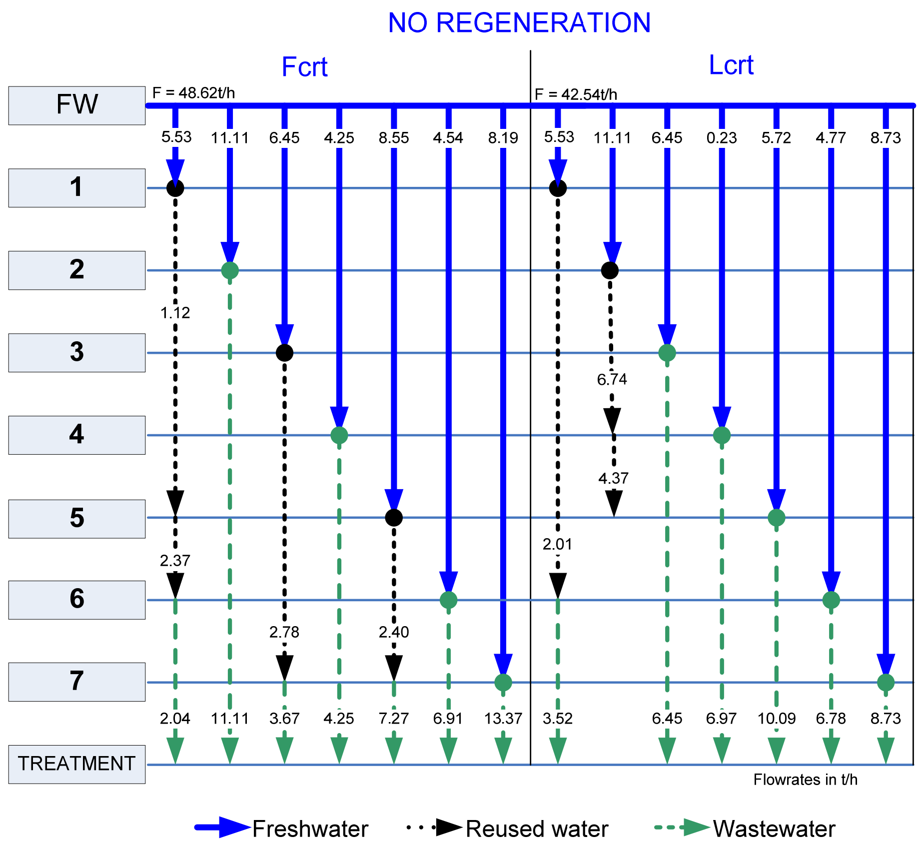


Figure 5. 18 Water network topology for base case

Scenario A : Partial regeneration of critical contaminant

In this scenario, contaminant C3 is regenerated. Supply water decreases with 8.8% for Fcrt and with 14% for Lcrt, compared to base case. Reused water is replaced with regenerated water for three water-using units, as presented in Fig.5.19. The flowrate of regenerated water is quite different for each ranking criterion (12.13 t/h -

Fcrt and 20.35 t/h - Lcrt). Effluents for three water using units are regenerated. The other units produce just wastewater.

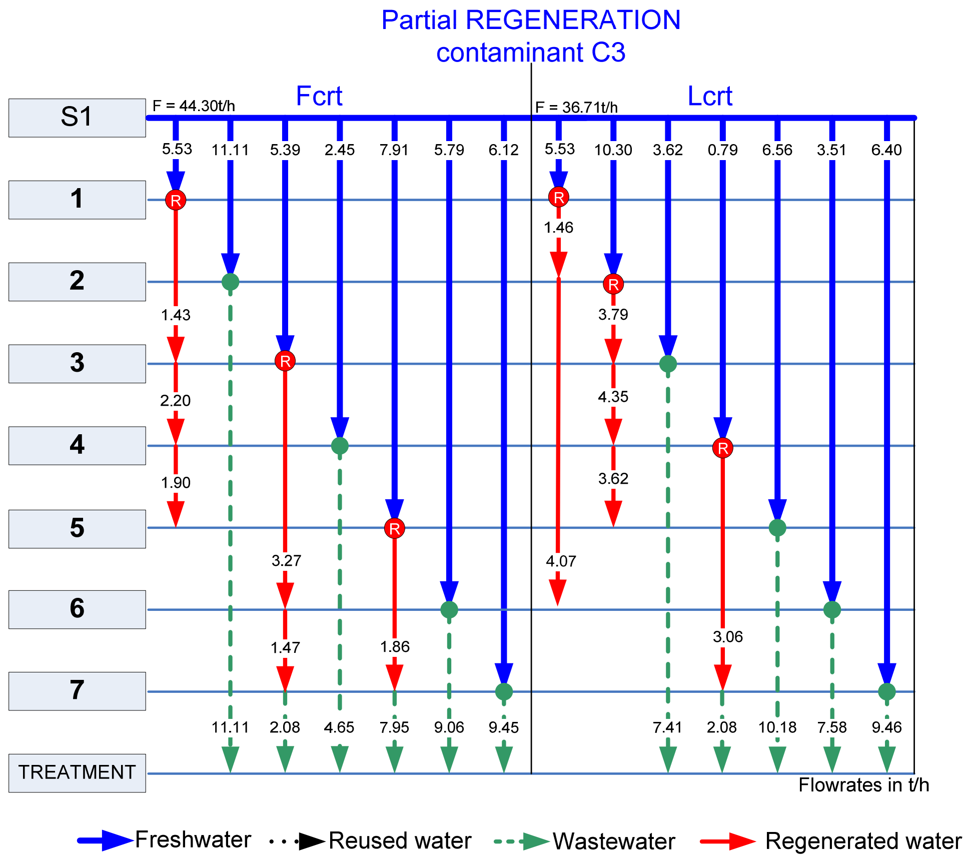


Figure 5. 19 Water network topology for Scenario A

Compared to base case the topology is slightly simplified as topological index for Scenario A is 58% for Fcrt and 53% for Lcrt. Lcrt solution provides lower supply water flowrate and lower topological index. From data related to mean component availability (Table 5.20), results in lower mean component availability for C2. Consequently, contaminant C2 becomes critical as it has lowest mean component availability (9.98 ppm for Fcrt and 9.20 ppm for Lcrt). In conclusion, regeneration of contaminant C3 is not a good solution for debottlenecking this water network.

Scenario B: Partial regeneration of neighbour of critical contaminant

In this scenario, the effect of contaminant C2 regeneration on water network debottlenecking is studied. In Table 5.20, data for base case shows that mean component availability of C2 is very closed to that of C3. Supply water flowrate is 47.97 t/h for Fcrt and 43.00 t/h for Lcrt, very close to the base case. For Fcrt criterion only 18% of effluents are regenerated (from U1, U3 and U5) and network topology (Fig. 5.20)for this scenario is not very different of base case (topological index is 56%,) same units provide wastewater of initial pipe length of water network. For Lcrt criterion, 35% of effluents are regenerated (from U1 and U2) using 58% of total pipes length. This scenario does not represent a very good solution for improving water network topology.

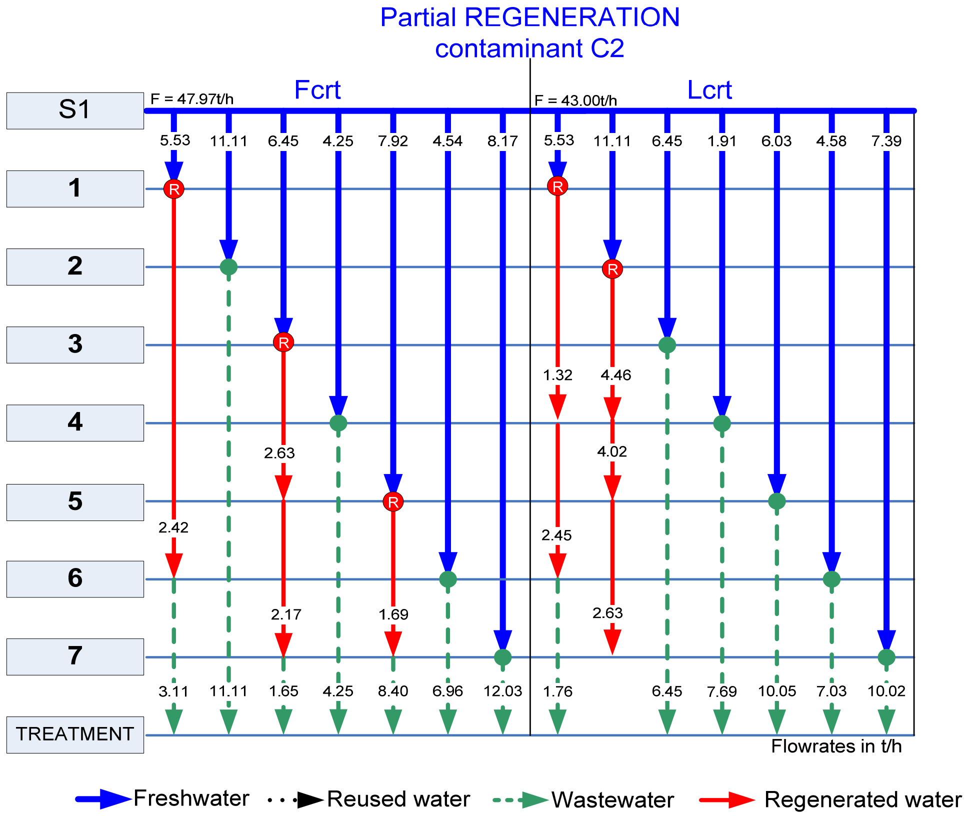


Figure 5. 20 Water network topology for Scenario B

Scenario C: Partial regeneration of bottleneck island contaminants J_3={C_2,C_3}

As I show above, from critical contaminant analysis the bottleneck island of critical contaminant C3 is J_3={C_2, C_3} because as presented in Table 5.20 their mean contaminant availability is very closed (14.13 ppm and 14.98 ppm). Consequently, in this scenario, the effect of bottleneck island regeneration on water network is analysed. Supply water network is reduced with 20-25%. Effluents of four water using units are regenerated (U1, U3, U4, U7 for Fcrt and U1, U2, U4, U6 for Lcrt). Just four units produce wastewater. Regenerated water flowrate is 19.34 for Fcrt respectively 29.15 t/h for Lcrt. As illustrated in Fig. 5.21, water network topology is simplified; the topological index is 50% for Fcrt and 53% for Lcrt. Regenerating the bottleneck island mean availability of all contaminants increases for both ranking criteria, in the range from 28.45 ppm to 42.63 ppm. Consequently, no further improvement could be expected if another contaminant is regenerated.

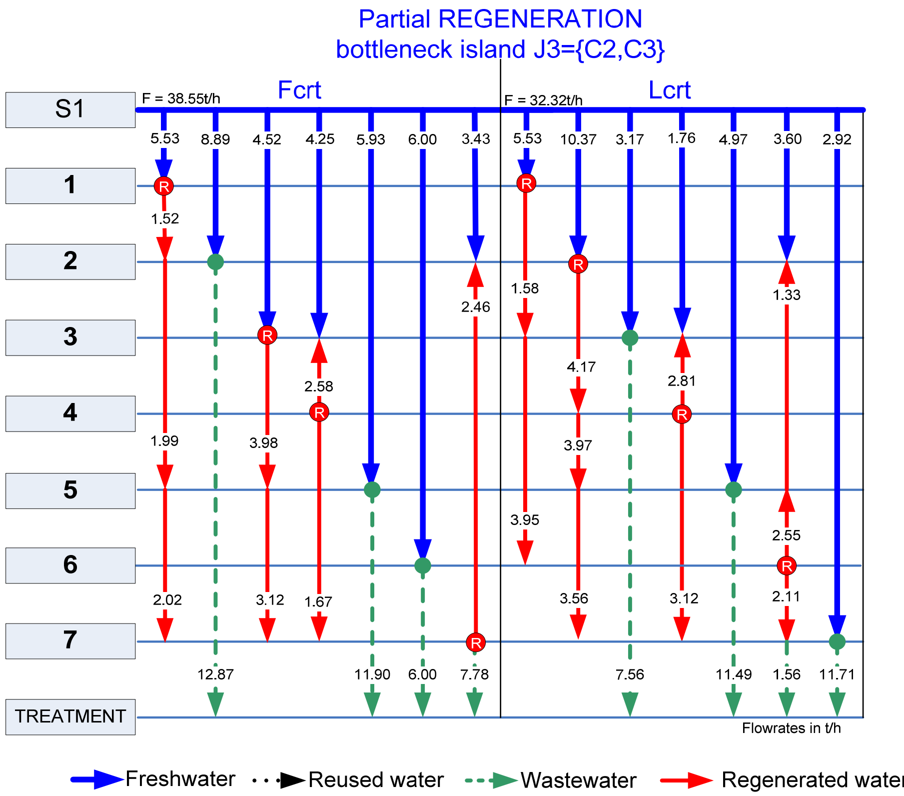


Figure 5. 21 Water network topology for Scenario C

Scenario D: Total regeneration of all contaminants

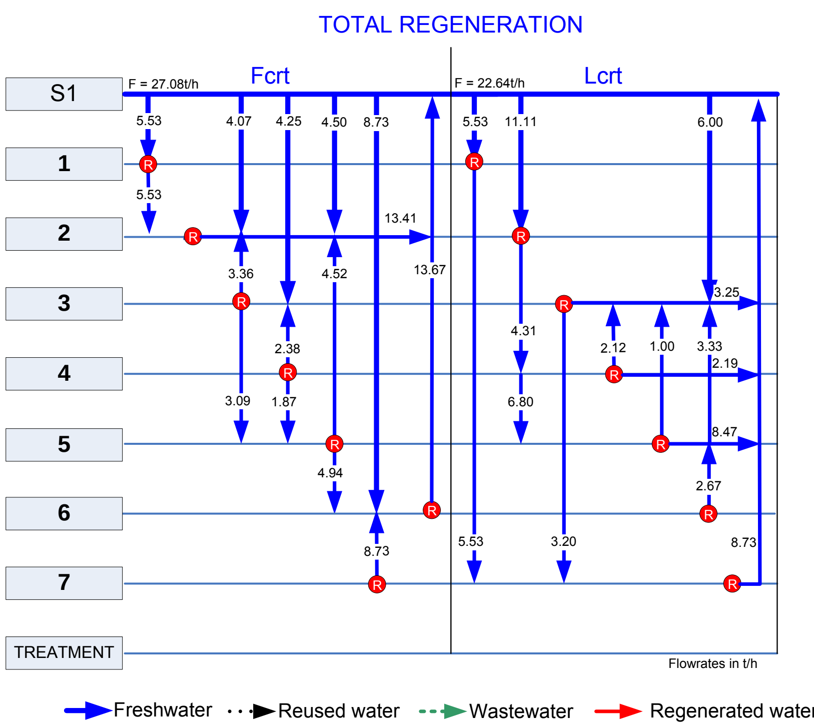


Figure 5. 22 Water network topology for Scenario D

In this scenario I analyse the situation when existing water network should be modified for zero discharge, i.e. all contaminants should be removed. The topology is presented in Fig. 5.22. Regenerated supply water flowrate is reduced with 45% compared to base case. The topological index is lower than other scenarios (45%-46%). For Lcrt criterion, the topology is simplified, as presented in Fig.5.22.

The complete results of retrofit analysis are summarised in Table 5.20.

Table 5. 20 Results: Minimum supply water flowrate and topological index

Scenario	Ranking criteria	Supply water flowrate, t/h	Topological Index %	Mean Contaminant Availability, [ppm]			
				C1	C2	C3	C4
Base case	Fcrt	48.62	56	35.61	14.75	14.73	47.27
	Lcrt	42.54	52	37.02	14.98	14.13	46.47
Scenario A	Fcrt	44.30	58	33.57	9.98	38.07	46.87
	Lcrt	36.71	53	34.15	9.20	35.15	44.11
Scenario B	Fcrt	47.97	56	32.02	31.23	13.35	42.63
	Lcrt	43.00	58	31.48	33.46	14.60	41.06
Scenario C	Fcrt	38.55	50	37.24	33.27	36.03	47.15
	Lcrt	32.32	53	35.59	28.45	29.82	47.31
Scenario D	Fcrt	27.08	46	53.43	39.60	44.90	58.66
	Lcrt	22.64	45	52.28	37.07	42.57	57.11

As discussed above, Scenario C for water network optimisation considering regeneration of bottleneck island J_3={C2, C3} and Fcrt criterion represent the most attractive option because the supply water flowrate decreased with ~20%, there is the lowest usage of total pipes length (topological index 50%) and contaminant mean availability is comparable for all four contaminants as summarised in Table 5.21.

Table 5. 21 Results: Selected solution

Scenario	Ranking criteria	Supply water flowrate, t/h	Topological Index %	Mean Contaminant Availability, [ppm]			
				C1	C2	C3	C4
Base case	Fcrt	48.62	56	35.61	14.75	14.73	47.27
	Lcrt	42.54	52	37.02	14.98	14.13	46.47
Scenario C	**Fcrt**	**38.55**	**50**	**37.24**	**31.23**	**13.35**	**47.15**
	Lcrt	32.32	53	35.59	33.46	14.60	47.31

Of course if zero discharge is imposed Scenario D is the solution for water network retrofit.

5.11. Conclusions

In this chapter I continue to extend water network optimisation methodology considering regeneration. Water regeneration as a waste minimisation part is included in reduction and prevention strategies. On this topic, I published two papers (Iancu et al., 2007, Lavric et al., 2007). New original concepts are introduced in this chapter to support the extension of methodology (mean availability, critical contaminant analysis, bottleneck island, internal/external reuse quotient and partial and total regeneration). I developed specific physical / mathematical models for regeneration. This analysis does not consider the influence of treatment technology or removing agents.

A six steps procedure to identify critical contaminant is proposed and proven on a synthetic example with six water-using units and four contaminants. Critical contaminant analysis allows deciding on regeneration strategy.

The physical model for water network is based on assimilation of water network with an oriented multicomponent graph. Based on this assumption, mathematical model for water network with regeneration, both to design a new water network and to retrofit an existing one is formulated in an original manner, in similar terms as in Chapter 3. There are only some streams which ca be regenerated if the bottleneck island contaminants concentration is greater then regeneration threshold concentration. Special notation is introduced to separate these streams for inlet streams. Independent variables are internal flowrates between water-using units X_{ij} as in other chapters. Regeneration unit model is based on limiting concentration data. Regeneration unit retains a certain mass load from the stream such as the exit specific stream has limiting exit concentration. For the new streams introduced by regeneration no additional independent variables are considered as the equations related to regeneration unit model allow the calculation. Those appear as auxiliary variables. The methodology allows also treating zero discharge problem in an original way.

In the case of retrofit of water network, a different approach is developed, compared to techniques presented in literature. Topological index is considered to keep the network as simple as possible. The performance of retrofitted network is evaluated with respect to topological index, contaminant mean availability and internal/external reuse quotient. For this problem, the initial values of flowrates, compositions, etc, are provided by the state of existing network.

The mathematical problem formulated in this chapter (either design or retrofit) is highly non linear, representing a large NLP problem. As in previous chapters, a modified variant of GA is used to find optimum solution, completing the steps for computing with calculation of regeneration mass load.

In graphical representation a specific original approach added to the model presented in previous chapters allows to integrate in water network representation of regeneration unit. It is proven that this offers a better understanding to network topology as well as it is an easier instrument for water balance.

Two case studies (both for design and retrofit of water network) are investigated to establish which type of regeneration influences most the topology (remove only one contaminant, some or all contaminants). I use above described approach to evaluate which one of the contaminants should be removed to obtain the best trade-off between decrease of supply water flowrate and the increase in network complexity. The results confirm the methodology and proof that the approach allows a better solution for water network with regeneration.

In the first case study a water network from a petrochemical site (six water using units and four contaminants) is considered. Following the methodology developed in this chapter, critical contaminant analysis is illustrated to find the bottleneck island (C2 is critical contaminant and J_2={C1,C2} is island group). Four scenarios are analysed and compared to base case to investigate the potential to minimise the supply water consumption and to improve water network topology: Scenario A – regeneration of contaminant C2, Scenario B – regeneration of bottleneck island J2, Scenario C – regeneration of three contaminants (C1,C2, C3), Scenario D - total regeneration. Supply water, reused water regenerated water and wastewater flowrates are computed and compared with base case and between scenarios to find most attractive solution when total supply water flowrate is objective function.

Regeneration of bottleneck contaminants gives promising results for water saving (bottleneck island J_2 is regenerated due to lower internally circulated water flowrate and quite simple network topology). Of course zero discharge solution is attractive for this case study but it is foreseen that investment in technology should be very important.

The second case study tackles a certain problem of retrofit to improve the total pipes length, considering regeneration. Both supply water consumption and total pipes length used for different scenarios are analysed. Based on critical contaminant analysis the bottleneck island is determined. Regeneration of critical contaminant, of the neighbour of critical contaminant, of bottleneck island and zero discharge are analysed, finding C3 as critical contaminant and J3={C2,C3} as bottleneck island. Four scenarios are proposed to identify the optimal topology (Scenario A – partial regeneration of critical contaminant, Scenario B – partial regeneration of neighbour of critical contaminant, Scenario C – partial regeneration of bottleneck island J3, Scenario D – total regeneration). The most attractive scenario for partial regeneration is bottleneck island contaminants regeneration because supply water flowrate decreases with ~20% and topological index with ~50%. Of course zero discharge scenario is selected only if this is a must. This case study is also a good illustration of the methodology developed in this chapter.

6. Final conclusions

In my Thesis I tackle process integration for water minimisation in oil processing and petrochemistry creating an original methodology including formulation of physical/ mathematical model for water network as oriented graph, solution of optimisation problem with original variant of hybrid genetic algorithm (GA) and illustrative case studies. I developed the study in three directions: optimisation with supply water flowrate objective function for multiple water sources, optimisation with economic based objective functions for same basic model and optimisation with consideration of regeneration for supply water flowrate objective function for design and retrofit. I created an original new graphical format for water network topology visualisation, facilitating also relevant water balance representation for industrial applications. In literature different approaches for water networks design/retrofit are presented but mainly two problems can be formulated.

- *Water minimisation problem* – when the analysis is concentrated on water using units transferring contaminants from process streams to water streams, involving a variety of basic processes not only mass transfer.
- *Mass exchange network approach* – when mainly mass transfer is taken into account and alternative mass transfer agents can be concurrent to water network.

In my Thesis I considered that water minimisation problem is more relevant for the application field focused (oil processing and petrochemistry). This determined me to dedicate the objective of this Thesis to develop an original methodology tackling this problem. Chosen approach belongs to the category of source reduction design/retrofit methodologies, involving identification and implementation of plant modifications based on water streams reuse and (partial) regeneration. I did not tackle recycle as less relevant from the point of view of equipartition of driving force principle. The target was to minimise supply water flowrate and/or to improve several indexes related to water network topology and/or economic aspects with a systematic approach.

In **Chapter 1** I presented an overview of the Thesis: objectives, structure and general approach.

I presented in Chapter 2 a literature survey of more than 100 publications systematically organised on following subjects:

- *Process integration concepts and applications* based either on graphical and optimisation approaches
- *Mathematical models* for problems related to water networks
- *Algorithms* for water networks optimisation.

As a way to reduce the utilities and the environmental impact, process integration is a good and state-of-art tool used in last years. Water is an important utility which must be reduced in the future. Huge amount of effluents discharged into the environment are strongly limited by legislation. Waste minimisation is one of the source reduction methodologies for environmental process design. It is used for design/retrofit of water networks by reuse, regeneration reuse or regeneration recycling of water streams to minimise the supply water flowrate and also the wastewater flowrate. Different techniques for water minimisation were developed in the last period. Some of them gave minimum flowrate of water supply before design based on graphical representation (Pinch Analysis), the others were based on mathematical programming.

Graphical techniques are based on mass load transferred between process streams and water streams, are interactive methods, based on first and second laws of thermodynamics. The advantage of these techniques is to provide valuable conceptual insights into the performance or behaviour of the system under consideration. There are some limitations when dealing with complex water networks. Graphical insights are of importance in practice because they allow the engineer to incorporate many factors that mathematical programming does not consider.

Mathematical programming techniques are based on formulation of mathematical models and solve with different optimisation algorithms (deterministic or stochastic). In many cases, these techniques were applied to obtain minimum freshwater consumption for water network or total cost or investment cost, etc. These techniques considered simultaneously the targeting and design stages. Using intensively the computer these methods can tackle more complex problems. However, much of the conceptual insight available through the Pinch Analysis based approach is lost.

Many authors proposed different graphical representations which could be used to calculate the freshwater targets: composite curve diagram (El-Halwagi & Manousiouthakis, 1989), Water Pinch Diagram (Wang & Smith, 1994a), Pinch Diagram (Dhole et al., 1996), Source - Sink diagram (El-Halwagi et al., 1996), Water surplus diagram (Hallale, 2002), Resources conservation diagram (El-Halwagi, et al., 2003), Nearest neighbors diagram (Prakash & Shenoy, 2005), Property based composite curve (Kazantzi & El-Halwagi, 2005), Quality based composite curve (Bandyopadhyay, 2006),etc. These methods were used to understand better the tools for water minimisation, but had limitations in handling multiple contaminants or in providing information about the topology of water network.

Since the graphical approach had limitations for complex systems, when multiple contaminants are involved, the mathematical programming became most popular technique for water network design.

In last two decades, increased efforts to formulate detailed mathematical models for water networks are recorded. A state of art of mathematical models formulated for water network from 1980 till today was presented in this study. For each model *the hypotheses*, *the equations*, *the constraints* and *the objective function* specific for design an optimal water network were presented.

Takama et al., 1980 were the first authors who formulated a complete model for an oil refinery considering reusing and regeneration as strategy for water minimisation. El-Halwagi & Manousiouthakis,1990 built a concentration interval diagram using limiting compositions of rich and lean streams and the equations are based on mass balance around this interval. Rossiter & Ravi, 1995 included in a model all possible recycle and reuse options for each water stream. Alga-Algaez et al.,1999 developed mathematical models for single and multiple contaminants based on concepts of El-Halwagi. For multiple contaminants, Yang et al., 2000 formulated the model based on complex superstructure and Suh & Lee, 2002 for designing water network under parameter uncertainty or with internal water mains (Feng & Seider, 2001). Later, some authors considered treatment units as a part of water network, not only the water-using units (Koppol et al.,2003, Karuppiah & Grossmann, 2006) or internal regeneration of streams (Cao et al., 2004; Wang et al., 2003). Feng &Chu, 2004 decomposed the water network into three subsystems: water utilisation system, water regeneration system and wastewater treatment system.

Depending on the nature of constraints and the types of variables involved in the model, different algorithms were required to solve the optimisation problems. Most of the optimisation problems were postulated as a superstructure which allowed a representation of all possibilities to reuse streams between water-using units, in a systematic way. The optimisation of superstructure was usually formulated as a NLP problem which involved or not discrete variables. The source of nonlinearities was contaminant material balance equations which involved bilinear terms from multiplication of water flowrate by contaminant concentration.

A review of optimisation algorithms based on superstructure was presented in literature in some papers: Branch and Bound algorithm (Al-Khayyal, 1992; Al-Khayyal & Falk, 1983; Horst & Tuy, 1987), Outer-Approximation (OA) algorithm (Horst et al., 1992), Cutting Plane algorithm (Tuy et al., 1985), Difference of Convex (DC) and Reverse Convex algorithm (Tuy, 1987), Interval algorithm (Hansen, 1980), Outer Approximation (OA) and Generalised Benders Decomposition (GBD) (Grossmann, 2002).

For water minimisation and design of water network, some authors suggested solving algorithms for superstructure-based model decomposing the NLP models (for a complex network with seven water-using units and three contaminants-Alva-Argaez et al., 2006, Bagajewicz et al., 1999) or using effective heuristic procedure (Galan & Grossmann, 1998).

The superstructure-based algorithms have also disadvantages: no guarantees to find global optimality for complex optimisation problem and need a feasible starting guess. Some of these problems can be solved using *Evolutionary algorithms* which search a population of points in parallel, not just a single point, use probabilistic transition rules and can provide a number of potential solutions to a given problem.

The most promising evolutionary algorithm is Genetic Algorithm (GA). An overview on how chromosomes are computed and how is working this algorithm was presented. GA were used successfully in different fields: optimisation of heat exchanger network (Lewin et al.,1998; Lewin, 1998), synthesis of mass exchange network without/with regeneration for single contaminant system (Lewin et al., 1998, Garrard & Fraga, 1998), irrigation system rehabilitation (Cisty, 2000), cost-optimal and least-consumption water usage and treatment networks (Tsai & Chang, 2001), water minimisation problem for single contaminant (Prakotpol & Srinophakun, 2004), pinch multi-agent genetic algorithm (PMAGA) for optimising water networks (Cao et al., 2007).

Design of an optimal water network using water minimisation as an integration tool had a large interest in the last years. In Romania, is a large potential to apply process integration tools to reduce the amount of supply water used in industrial large sites (i.e. oil refinery site or petrochemical site) as I identified in previous reports to my thesis Iancu, 2005a and Iancu, 2005b. GA algorithm was used as optimisation tools, in an original format, for an original formulation of water network model, as oriented graph.

Chapter 3 represents the core of the Thesis having following structure:

- Introduction and motivation
- Problem statement-Physical model
- Mathematical model
- Design criteria
- Optimisation algorithm
- Water network graphical representation
- Case studies to illustrate and support the methodology
- Conclusions.

Original approach for water minimisation, for physical/mathematical models, for optimisation algorithm and water network graphical representation are formulated and presented in detail. Case studies illustrate and support the methodology, allowing to obtain better results compared to other published approaches and to tackle bigger size problems, closer to industrial demands. In this chapter the objective function for optimisation problem was water supply flowrate.

In this chapter, I proposed a process integration methodology to design optimal water network with more supply water external sources for a water minimisation type problem. Original physical and mathematical models based on water network representation as oriented graph were developed. The objective function used in optimisation was water supply flowrate. Solving technique was based on GA optimisation algorithm. Main achievements and original contributions in Chapter 3 are summarised below:

a. Physical model for water network was based on oriented graph topology where water-using units are knots and water streams are arches.
    - Water-using units were considered perfectly mixed vessels. Process streams transfer to water stream a certain (given and constant) mass load for each contaminant in each unit.
    - Equipartition of driving force principle was considered for taking advantage of the oriented multicomponent graph nature of the water network to rank the unit. Two criteria were considered: ‘‘by load’’ and ‘‘by fresh water’’.
    - Supply water sources with different degrees of contamination could be taken into account. Water-using units could be grouped in clusters associated to each water source (according to their contaminant concentration constraints at the entrance). This is an original concept introduced in my paper Lavric et al., 2005.
    - Water recycling is not taken into consideration to observe the “equipartition of driving force” principle.

b. Mathematical model for water-using units was based on total and partial (for contaminants) mass balances. Associated constraints based on *Limiting Water Profile* concept in terms of input and output maximum allowable contaminants concentration were also formulation. Objective function was based on supply water flowrate. As a consequence a new NLP formulation for water network mathematical model was proposed. This approach is different of usual approaches in literature, where mathematical models are based on superstructures associated to water network. My development allowed me to solve different practical problems:
    - Numerous contaminants and large number of water using.
    - The integration of water streams was based on water reusing strategy.

c. Hybrid modified GA solving technique was used for NLP mathematical model. Internal flowrates were independent variables, allowing to calculate model dependent variables and water network topology design, observing the imposed inlet and outlet constraints for each unit.

d. I proposed a new graphical form for water network topology visualisation. The units were classified in water sources and water sinks and the streams were the links between them. Each water unit could be a **source** of reused water and/or wastewater and/or a **sink** for supply water and/or reused water. Water flowrates were also written, creating to user an easy instrument to check mass balances.

e. A literature test case (ten water-using units, three contaminants and one supply water source) was used to proof the capacity to solve better the problem with GA optimisation technique proposed. This case study was proposed in the paper Savelsky et al,. 1999. Authors' solution was classified as a local optimum, because in my approach a better solution was obtained.

f. A more complex water network case study (ten water-using units, six contaminants and four supply water sources) was solved to demonstrate the possibility to tackle problems not yet presented in literature. A problem of this dimension was not yet reported to be solved using superstructure-based algorithms. Using GA optimisation technique optimal solution and also the correspondingly water network topology for both ranking criteria were obtained. The influence of contamination level of water sources were studied in four scenarios to find the best water network supply structure.

g. A large scale case study from an oil refinery was developed to take advantage of my new methodology. Fifteen water-using units, six contaminants, four available water sources (with different levels of contamination) and a treatment unit were considered. To design the optimal water network topology with the minimum fresh water consumption, for each water-using unit there was imposed the maximum allowable pollutant input concentration and the maximum allowable pollutant output concentration. Four particular scenarios (A-one water source, B- two water sources, C-three water sources and D-four water sources) were analysed using both units ranking criteria (Lcrt and Fcrt). The influence of available water sources on topology and on optimal solution was analysed. Following results are obtained:

- The most attractive solution was simultaneously usage of two sources: freshwater (source S1) and slightly contaminated water (source S2).
- The other combinations of water sources gave only the modification of topology, neither freshwater supply savings nor involving important changes in water reuse.
- 24 % savings from Source S1 was found compares to Scenario A.

The solution technique, based on GA algorithm, developed in this chapter was able to give all information to engineer regarding water network design (minimum supply water source flowrate, the best combination of supply water sources, the most recommended topology of water network) for minimum supply water source flowrate. Graphical representation of water network topology is simple and clear with good visual properties.

I continue in Chapter 4 the work developed in Chapter 3, considering objective functions based on economic aspects. Main parts of this chapter are:

- Introduction
- Physical/mathematical model with emphasis on objective function formulation, based on pipes optimal diameter calculation, to diminish frictional losses.
- Design criteria based on total annualised cost and water network topological index, introduction of weighted objective function
- The new form of optimisation algorithm
- Case studies with relevance for oil refining industry are presented for minimisation of total annualised cost
- Case study to illustrate water network design with topological index minimisation or weighted objective function (linear combination between supply water flowrate and topological index).
- Conclusions on results for water network optimisation based on economical indexes.

In this chapter water network problem modelling and optimisation was formulated as original approach to take into account objective functions based on economic considerations. Total annualised cost objective function was calculated in original manner accounting for optimal pipes diameter. Minimum total annualised cost for pumping and fixed charges provided basis for minimum pipes diameter calculation. This approach was not yet reported in literature. The value of optimal diameter could be obtained combining principles of fluid dynamics with cost considerations. Solution of water network NLP mathematical model was performed with GA optimisation tool. An original objective function based on water network topological index was proposed. Despite the fact that it does not include explicitly economic variables, the water network cost strongly depends on total active pipes length. Another option is to formulate a weighted objective function obtained as linear combination of water supply flowrate and topological index. My analysis encourages using it when there is scarce economic data.

As illustration of new methodology for total annualised cost objective function an industrial large scale case study was solved: 15 water-using units, 6 contaminants and four water sources with different degree of contamination, as described in Iacob et al., 2004. The influence of using simultaneously more water sources was considered in four scenarios of this case study developed in Chapter 3.Total annualised cost objective function was formulated for this case study and NLP problem solved with GA. Case study results published in my paper Lavric et al., 2007a, I compared both approaches.

Scenario A: network was optimised for one water source: freshwater. Compared to the case study developed in Chapter 3 same scenario, the minimum flowrate of supply water is a little bit increased but the total annualised cost (investment and operating costs) were reduced drastically. These aspects have important influence on water network topology, total length of piping system was reduced.

In Scenarios B, C and D simultaneous use of more supply water sources was taken into account. The flowrate of freshwater (the expensive water source) was reduced but the difference was given by an increased flowrate supplied by the other source(s). For the same value of total water flowrate, total annualised cost was lower for the scenarios of this case study, compared with results obtained in Chapter 3. Significant differences in water network topology are also to notice. Consequently pipes length reduced when cost based objective function was used for optimisation, compared to supply water flowrate objective function. This can be explained by search mechanism to find optimum. When using water supply flowrate as objective function, search process stops after finding minimum supply water flowrate. No attempts were made to reduce the pipes length. When using an economic based objective function, finding the minimum supply water throughput flow was accomplished in a first step, afterwards the search for better combinations of internal streams continued to find water network topology simplification as much as possible. Operating cost and investment cost were also compared. From data analysis I noticed that the maximum degree of freedom exists only for non-contaminated supply water. Remarkably, when using combination of water sources the water throughput flowrate was the same for both objective functions. I noticed that reused water flowrate reduces in the case of cost based objective function. Comparing results, the most attractive solution depended on optimisation criterion.

- *For supply water flowrate objective function*, water network most attractive solution with more water sources was given by Scenario B (733.4 t/h), when sources S1 and S2 were used for Fcrt ranking criterion. However, for this case the total annualised cost was **1,911,676 $/year**.
- *For minimum total cost annualised objective function*, the optimal solution was using Scenario C (740.7 t/h), total annualised cost was **1,320,472 $/year**, when three sources (S1, S2 and S3) were used and water network was ranked by Fcrt. Some results of this study were also published in my paper Lavric et al., 2005.

A variation of operating cost, investment cost and total annualised cost was presented for different scenarios and objective functions. Operating cost decreased when cheaper water sources were used. Water flowrate increased if the contamination of water source increased (comparing Scenarios B, C and D). Investment cost increased when more water sources are considered (eg scenario A vs scenario B). This means that there was a trade off between operating cost and investment cost given by minimum of total annualised cost. The most attractive solution in my study was given in Scenario C involving also a simpler topology. While total annualised cost was **1,320,472 $/year**, the water network used **740.7 t/h** (338.4 t/h from S1, 395.0 t/h from S2 and 7.3 t/h from S3) instead of 1,198.8 t/h for the base case, that means supply water flowrate saving of **38.8%.** As final result for both case studies developed in Chapter 3 and Chapter 4 respectively and different scenarios the proposed water network flowsheet was presented. Piping system was modified compared to base case and total piping length was proposed **23,420 m.**

In the case of scarce economic data I proposed in this chapter an implicit cost based objective function, topological index, because active pipes length was implicitly related to some components of cost based objective function. But this last one was related as well to supply water flowrate. As a consequence, I proposed another original objective function a weighted one as a linear combination between water supply flowrate and topological index, of factor ω. In the case study presented, I obtained interesting results reported as well in my paper Iancu et al., 2007. For topological index objective function quite close total pipes length to cost based objective function was calculated, but in some scenarios quite different supply water flowrate was reported. If weighted objective function was considered (ω=0.5), mutual influence of components on the objective function combined in synergy. Consequently, Scenario C gave most attractive results compared to other scenarios for all objective functions evaluated when supply water flowrate and total pipes length were considered.

In Chapter 5 I followed a similar scheme with previous chapter to develop the methodology for contaminant(s) regeneration. This chapter had following content:

- Introduction on relevance of regeneration for water networks optimisation
- New concepts to formulate and illustrate the methodology
- Water minimisation problem statement
- An original approach to retrofit strategy
- Detailed mathematical models for water-using unit with regeneration and for regeneration unit
- Design criteria for methodology formulation
- Solving strategy and optimisation algorithm
- Original contribution to water network graphical representation for regeneration

- Methodology illustration for two case studies using data from petrochemical plants for design with regeneration respectively for retrofit
- Conclusions

In this chapter I continued to extend water network optimisation methodology considering regeneration. Water regeneration as a waste minimisation part was included in reduction and prevention strategies. On this topic I published two papers Iancu et al., 2007 and Lavric et al.,2007. New original concepts were introduced in this chapter to support the extension of methodology (mean availability, critical contaminant analysis, bottleneck island, internal/external reuse quotient and partial and total regeneration). I developed specific physical / mathematical models for regeneration.

The physical model for water network was based on assimilation of water network with an oriented graph. There were only some streams which ca be regenerated, if the bottleneck island contaminants concentration was greater then regeneration threshold concentration. Independent variables are internal flowrates between water-using units X_{ij} as in other chapters. Regeneration unit was modelled in an original manner based on limiting concentration data. A stream was considered to need regeneration if selected contaminants concentration was over the threshold value. Regeneration unit retained a certain mass load from the stream such as the unit exit the specific stream had limiting exit concentration. For the new streams introduced by regeneration no additional independent variables were considered as the equations related to regeneration unit model allowed the calculation. Those appear as auxiliary variables. Based on this assumption, mathematical model for water network with regeneration, both to design a new water network and to retrofit an existing one is formulated in an original manner, in similar terms as in Chapter 3. The methodology allowed also treating zero discharge problems in an original way.

In the case of retrofit of water network, a different approach was developed, compared to techniques presented in literature. Topological index was considered to keep the network as simple as possible. The performance of retrofitted network was evaluated with respect to topological index, contaminant mean availability and internal/external reuse quotient. For this problem, the initial values of flowrates, compositions, etc, were provided by the state of existing network.

The problem formulated in this chapter (either design or retrofit) was highly non linear, representing a large NLP problem. As in previous chapters, a modified variant of GA was used to find optimum solution, completing the steps for computing with calculation of the regeneration mass load.

In graphical representation a specific original approach added to the model presented in previous chapters allowing regeneration unit integration in water network graphical representation. It was proven that this offered a better understanding to network topology as well as it was an easier instrument for water balance.

Two case studies (both for design and retrofit of water network) were investigated to establish which type of regeneration influences most the topology (remove only one contaminant, some or all contaminants). I applied above described approach to evaluate which one of the contaminants should be removed to obtain the best trade-off between decrease of the supply water flowrate and the increase in network complexity. The results confirmed the methodology and proved that the approach allowed a better solution for water network with regeneration.

In the first case study a water network from a petrochemical site (six water using units and four contaminants) was considered. Following the methodology developed in this chapter, critical contaminant analysis was illustrated to find the bottleneck island (C2 is critical contaminant and J_2={C1,C2} was island group). Four scenarios were analysed and compared to base case to investigate the potential to minimise the supply water consumption and to improve water network topology: Scenario A – regeneration of contaminant C2, Scenario B – regeneration of bottleneck island J2, Scenario C – regeneration of three contaminants (C1,C2, C3), Scenario D - total regeneration. Supply water, reused water regenerated water and wastewater flowrates were computed and compared with base case and between scenarios to find most attractive solution for total supply water flowrate objective function.

Regeneration of bottleneck contaminants gave promising results for water saving (bottlenecking island J_2 was regenerated due to lower internally circulated water flowrate and quite simple network topology).

The second case study tackled a certain problem of retrofit to improve the total pipes length, considering regeneration. Both supply water consumption and total pipes length used for different scenarios are analysed. Based on critical contaminant analysis the bottleneck island was determined. Regeneration of critical contaminant, of the neighbour of critical contaminant, of bottleneck island and zero discharge were analysed, finding C3 as critical contaminant and J3={C2,C3} as bottleneck island. Four scenarios are proposed to identify the optimal topology (Scenario A – partial regeneration of critical contaminant, Scenario B – partial regeneration of neighbour of critical contaminant, Scenario C – partial regeneration of bottleneck island J3, Scenario D – total regeneration). The most attractive scenario for partial regeneration was bottleneck island contaminants regeneration because supply water flowrate decreased with ~20% and topological index with ~50%. Of course zero discharge scenario can be selected only if this is a must. This case study was also a good illustration of the methodology developed in this chapter.

Concluding remark of the research on my research work reported in this Thesis are formulated below. I studied process integration for water minimisation to create a new methodology specifically applicable in oil processing industry and petrochemistry based on process optimisation. My Thesis was structured in five chapters, two annexes, notations and literature references. The literature survey of more than 100 papers and books allowed me to formulate the directions of original research to achieve state of art results. I was focused on process integration applications as graphical and optimisation approaches formulation of mathematical models related to water networks, algorithms for solving specifically formulated models. In the last years, my work was reported in 15 papers, communications to international conferences (as PRES or ESCAPE) and scientific reports.

In Chapter 3 I developed and illustrated the methodology for water networks optimisation based on original representation of water network as oriented graph ranked after two criteria. Mathematical model (included mass balance equations and additional restrictions related to limiting concentration conditions) was subjected to supply water flowrate as objective function. Constant mass load for each contaminant in each water-using unit was considered. A formulation as a NLP problem resulted in. For solution an original form of a hybrid GA was used as a tool implemented in a software application. Illustration and confirmation of methodology was made in some case studies: one already presented in the literature (to show that better solution was obtained in my approach) and two industrial based case studies of bugger complexity as yet reported in literature. The analysis in case studies was systematically grouped in scenarios. The last two case studies continued to be analysed with same or different scenarios in next chapters for extension of methodology.

In Chapter 4 original objective functions based on economical consideration were developed. Introducing the optimal diameter calculated in classical manner in the formulation of a total annualised cost objective function I obtained an original form. Using the other components of the physical /mathematical model developed in Chapter 3, an extended formulation of the methodology resulted in. For the case of scarce economic data, two objective functions based on effective water network pipe length (formalised in topological index) were formulated. The first objective function was topological index, who represent implicitly economic aspects as total annualised cost depends strongly on this variable. The second objective function was obtained weighting two remarkable variables included in total annualised cost: supply water flowrate and topological index. These two objective functions allowed me to extend again the water network optimisation methodology.

In Chapter 5 regeneration opportunity for water streams inside water network was accounted for formulating an original physical model. The mathematical model developed in previous chapters was extended considering water streams connecting regeneration unit to water streams. In formulation of NLP problem, water supply flowrate objective function was formulated. Also, an original formulation of a retrofit problem was introduced. The new extension of methodology was illustrated and supported in two industrial type case studies.

As a general conclusion, my work tackled water minimisation problem to optimise water network from oil processing and petrochemistry, based on a systematic and original approach not yet reported by other authors but published by me in 15 publications.

-Optimisation problem was based on original physical model for water network as oriented graph to observe equipartition of driving force principle.

-Mathematical model included mass balances and restrictions related to Water Limiting Profile approach (known mass load of contaminants in water-using units and limiting entrance exit concentrations).

-Different functions were analysed and some of original form proposed; water supply flowrate, total annualised cost, topological index, weighted objective function between water supply flowrate and topological index.

-Optimisation algorithm was based on original formulation and implementation in software (not resulted in my Thesis) of GA.

-The new methodology was illustrated and proven both for already reported in literature case study (better results were obtained) and for complex industrial case studies specific to oil processing and petrochemistry) whose dimension was not yet reported in literature (fifteen water-using units, six contaminants four water supply sources, a treatment unit with/without regeneration unit).

Future work

In future I intend to extend the methodology for economic considerations objective functions to regeneration-reuse problem. I intend to improve the other aspects which can be considered during water network synthesis. Special attention I intend to give to calculation of optimal outlet concentration of contaminants for regeneration unit in correlation with different treatment technologies. Regarding optimisation algorithms I foresee to search for last moment developments in this field, trying to improve the methodology continuously.

I am interested to develop numerous case studies with industrial relevance for petrochemistry, chemical industry and other process industries with integrated large sites.

LIST OF NOTATIONS

A	constant in friction factor dependency on Re in Eq.4.3, [dimensionless]
A'	factor in Eq. 4.5
c_k	contaminant k
$\mathscr{C}$	set of total annualised pipe cost per unit length optimised with respect to pipe diameter $\mathscr{D}_{ij}$
$\mathscr{C}_{ij}$	unit length total annualised cost for the pipe linking the units u_i and u_j, [\$/m/year]
$[\mathscr{C}]_{pumping}$	annualised pumping costs, [\$/year]
$[\mathscr{C}]_{pipe}$	annualised fixed charges for piping system, [\$/year]
C	set of contaminants
C_{ki}	concentration of contaminant k in water stream from unit u_i, [ppm]
C^{in}	set of current inlet concentration per contaminant and unit, [ppm]
C_{ki}^{in}	concentration of contaminant k in water stream entering to unit u_i, [ppm]
ΔC_{ki}^{in}	contaminant k difference of concentration at unit u_i entrance, [ppm]
$C^{in,max}$	set of inlet limiting contaminant concentration for water network, [ppm]
C_k^r	concentration of contaminant k at exit of regeneration unit, [ppm]
C_{kr}^{in}	concentration of contaminant k at the entrance in regeneration unit, [ppm]
$C_r^{in,min}$	limiting concentration set at regeneration unit entrance, [ppm]
$\Delta C_{ki}\big\rvert_{mean}$	average concentration difference for each contaminant k for water-using unit u_i, [ppm]
$\overline{\Delta C_k}$	mean availability of contaminant k, [ppm]
$C_{ki}^{in,max}$	limiting concentration of contaminant k in water stream entering in unit u_i, [ppm]
C^{out}	set of current outlet concentration per contaminant and unit, [ppm]
C_{ki}^{out}	contaminant k concentration in effluent from water-using unit u_i, [ppm]
ΔC_{ki}^{out}	difference of contaminant k concentration at the exit of unit u_i, [ppm]
$C^{out,max}$	set of outlet limiting concentration per contaminant and unit, [ppm]

$C_{ki}^{out,max}$	limiting concentration of contaminant k in effluent of water-using unit u_i, [ppm]
$C_{ki}^{p,max}$	concentration of contaminant k at the entrance of u_i when it is possible that at least one contaminant (p) reaches the inlet limiting concentration, [ppm]
$C_{ki}^{q,max}$	concentration of contaminant k at the exit of u_i when it is possible that at least one contaminant (q) reaches the outlet limiting concentration, [ppm]
C_{kh}	concentration of contaminant k coming from regeneration unit, [ppm]
C_{kj}	concentration of contaminant k in water stream from unit u_j, [ppm]
$C_{kr}^{out,max}$	limiting concentration of contaminant k at exit of regeneration unit, [ppm]
$C_{r}^{out,max}$	limiting concentration set at exit of regeneration unit, [ppm]
C^{s}	set of contaminant concentration for each water supply source, [ppm]
C_{k}^{s}	concentration of contaminant k in source S, [ppm]
C_{total}	water network total annualised cost, [$/year]
$\mathscr{D}$	set of pipes optimal diameter for entire water network, [m]
$\mathscr{D}_{ij}$	optimum economic diameter of the pipe linking the units u_i and u_j, [m]
D_r	the reference diameter, [m]
E	efficiency of the motor and pumps, [dimensionless]
f	ratio of the total cost for fittings and the installation to the purchase cost for the new pipe, [dimensionless]
Fcrt	ranking criterion by freshwater consumption
F_{i}^{max}	maxim admissible supply water flowrate for unit u_i, [t/h]
F^{s}	set of water supply flowrate for each u_i, [t/h]
F_{i}^{s}	supply water flowrate for unit u_i, [t/h]
$F_{i,in}^{s,min}$	minimum supply water flowrate at the entrance of unit u_i, [t/h]
$F_{ik}^{s,min}\Big\|_{in}$	minimum supply water flowrate for contaminant k at the entrance of unit u_i, [t/h]
$F_{i,out}^{s,min}$	minimum supply water flowrate at the exit of unit u_i, [t/h]
$F_{ik}^{s,min}\Big\|_{out}$	minimum supply water flowrate for contaminant k at the exit of unit u_i, [t/h]
G_F	annualised fixed charges including maintenance, expressed as a fraction of initial cost for the completely installed pipe, [dimensionless]

H_y hours of operation per year, [h]

J the frictional loss due to fittings and bends expressed as equivalent fractional loss in a straight pipe, [dimensionless]

J_K set of contaminants forming bottleneck island of contaminant k

K number of contaminants

ℓ_{ij} length of pipe between unit u_i and u_j, [m]

$\mathscr{L}$ set of pipes length between sources and water-using units, between water-using units and between water-using units and treatment unit, [m]

L set of water losses flowrate, [t/h]

L_i water loss stream from unit u_i and flowrate, [t/h]

Lcrt ranking criterion by mass load

m_{ki} mass load of contaminant k in unit u_i, [g/h]

Δm_{rij}^{k} mass load of contaminant k removed by regeneration unit in the effluent stream of unit u_i targeted to unit u_j, [g/h]

M set of mass load of all contaminants and all units, [g/h]

n coefficient for steel pipes depending on reference diameter D_r, Eq. 4.9

N number of water-using units

NS number of water sources

q contaminant reaching the outlet limiting concentration for accepted inlet flowrate

q_{ij} volumetric flow rate of stream between unit u_i and u_j, [m^3/h]

p contaminant reached the inlet limiting concentration for accepted inlet flowrate

Δp_{ij} pressure drop on unit length for pipe between units u_i and u_j, [Pa/m]

Re Reynolds number, [dimensionless]

s_j supply water source j

S set of supply water sources

T price per unit length of pipe, [$/m]

u_i generic water-using unit

u_h water-using unit placed before unit u_i

U^s set of water-using units associated in cluster of water source S

U set of water-using units

X chromosomes of internal flowrates, [t/h]

X_{ij}	internal water stream from unit u_i to unit $u_{j,}$ i<j and flowrate, [t/h]
$X_{ir(j)}$	reused water stream satisfying the contamination condition for regeneration and flowrate, [t/h]
$X_{(i)rj}$	effluent stream from unit u_i targeted to unit u_j, going to regeneration unit and flowrate, [t/h]
X_{hi}	elements of water flowrate matrix from unit u_h to the unit u_i, h<i, [t/h]
$X_{(h)ri}$	stream targeted from unit u_h leaving regeneration unit directed to unit u_j and flowrate, [t/h]
W	set of wastewater flowrates, [t/h]
W_i	wastewater stream from unit u_i and flowrate, [t/h]
ρ	fluid density, [kg/m^3]
χ	Fanning friction factor , [dimensionless]
μ	fluid viscosity, [Pa.s]
ε	electric energy cost, [$/kWh]
γ	constant in friction factor dependency on Reynolds number in Eq.4.3, [dimensionless]
χ_{hi}	flowrate of stream coming from unit u_h or from regeneration unit, [t/h]
ς_{hi}	contaminant concentration of stream coming from unit u_h or from regeneration unit, [ppm]
χ_{ij}	flowrate of u_i effluent stream going to u_j or to regeneration unit, [t/h]
τ	topological index, defined in paragraph 4.4.2.1
$\mathcal{J}$	weighted objective function defined in Eq. 4.20

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ANNEX 1

ALGORITHM TABLE TO CALCULATE DEPENDENT VARIABLES FOR SUPPLY WATER FLOWRATE OPTIMISATION

Consider an ordered water network (after Fcrt or Lcrt ordering criteria) with the following *parameters*:

N number of water using units

K number of contaminants

NS number of water sources

$M = \{m_{ki} \mid i = 1,2,...,N,\ k=1,2,...,K\}$ set of mass load per unit u_i and contaminant k

$L = \{L_i \mid i = 1,2,...,N\}$ set of water losses for each unit

$C^s = \{C_k^s \mid k = 1,2,...,K,\ s = 1,2,...,NS\}$ set of contaminants concentration for each water supply source

$C^{in,max} = \{C_{ki}^{in,max} \mid k = 1,2,...,K,\ i = 1,2,...,N\}$ set of inlet limiting concentration per contaminant and unit

$C^{out,max} = \{C_{ki}^{out,max} \mid k = 1,2,...,K,\ i = 1,2,...,N\}$ set of outlet limiting concentration per contaminant and unit.

The *dependent variables* for the water network optimisation problem are:

$F^s = \{F_i^s \mid i = 1,2,...,N\}$ water supply flowrate for each unit u_i

$W = \{W_i \mid i = 1,2,...,N\}$ wastewater flowrate from each unit u_i

$C^{in} = \{C_{ki}^{in} \mid i = 1,2,...,N\ ;\ k = 1,2,...,K\}$ concentration of contaminant k at the entrance of u_i when at least least one contaminant reached the inlet or outlet limiting concentration

$C^{out} = \{C_{ki} \mid i = 1,2,...,N\ ;\ k = 1,2,...,K\}$ concentration of contaminant k at the exit of u_i when at least one contaminant reached the outlet limiting concentration.

The algorithm table has the following steps:

a) Calculate the dependent variables for the first water-using unit u_1 :

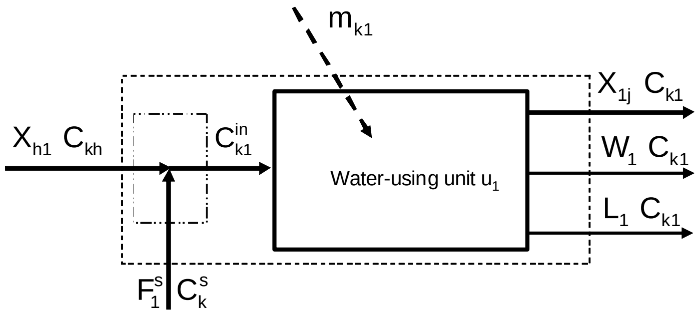


Figure A1.1 Schematic model of water-using unit u_1

F_1^s Minimum freshwater flowrate:

Because inlet limiting concentration is zero, there are no streams from other units. Freshwater is only the available water source. This variable is calculated with Eqs.(A1.1):

$$F_{1k}^{s,min}\Big|_{out} = \frac{m_{k1}}{C_{k1}^{out,max} - C_k^s} \qquad k=1,2,...,K$$
$$F_1^s = \max_{k=1}^{K}(F_{1k}^{s,min}\Big|_{out}) = F_1^{s,min} \tag{A1.1}$$

W_1 wastewater flowrate:

$$W_1 = F_1^s\text{-}L_1\text{-}\sum_{j=2}^{N} X_{1j} \tag{A1.2}$$

C_{k1}^{in} inlet concentration of each contaminant at entrance of water-unit 1:

$$C_{k1}^{in}=C_k^s \tag{A1.3}$$

C_{k1} outlet concentration of each contaminant k at exit of water-unit u_1 (the values for X_{ij} are generated by GA algorithm):

$$C_{k1}=\frac{F_1^s + m_{k1}}{W_1 + L_1 + \sum_{j=2}^{N} X_{1j}} \tag{A1.4}$$

b) Calculate the dependent variables for water-using units u_i (i=2,…,N-1) (Fig.(A1.2)):

F_1^s Minimum freshwater flowrate:

The flowrate from water supply source is calculated based on maximum allowable concentrations at inlet and outlet:

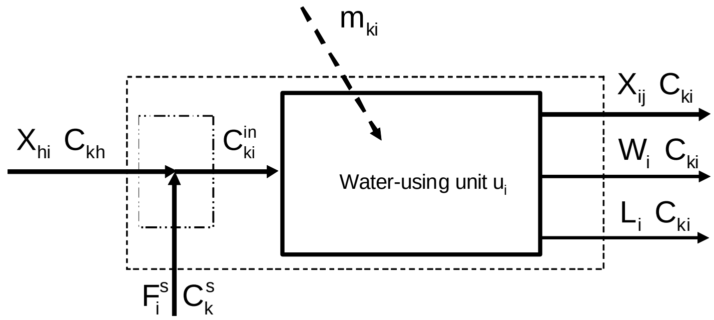


Figure A1.2 Schematic model of water-using unit, u_i

$$F^{s,min}_{ik}\Big|_{in} = \frac{\sum_{h=1}^{i-1} X_{hi}(C_{ki} - C^{in,max}_{ki})}{C^{in,max}_{ki} - C^s_k} \qquad k=1,2,...,K \tag{A1.5}$$

A maximum flowrate is calculated assigning the component p for which this condition is fulfilled:

$$F^{s,min}_{i}\Big|_{in} = \max_{k=1}^{K}(F^{s,min}_{ik}\Big|_{in}) = F^{s,min}_{i,p} \tag{A1.6}$$

Similar calculations are performed for the minimum outlet water supply flowrate:

$$F^{s,min}_{ik}\Big|_{out} = \frac{\sum_{h=1}^{i-1} X_{hi}(C_{ki} - C^{out,max}_{ki}) + m_{ki}}{C^{out,max}_{ki} - C^s_k} \qquad k=1,2,...,K \tag{A1.7}$$

Then, the maximum value for these flowrates is calculated assigning the component q for which this condition is fulfilled:

$$F^{s,min}_{i}\Big|_{out} = \max_{k=1}^{K}(F^{s,min}_{ik}\Big|_{out}) = F^{s,min}_{i} \tag{A1.8}$$

The accepted value for supply water flowrate is:

$$F^{s,min}_{i}\Big|_{out} = \max_{k=1}^{K}(F^{s,min}_{ik}\Big|_{out}) = F^{s,min}_{i,q} \tag{A1.9}$$

The accepted value for supply water flowrate from source s is:

$$F^{s}_{i} = \max(F^{s,min}_{i}\Big|_{in}, F^{s,min}_{i}\Big|_{out}) \qquad i=2,...,N-1 \tag{A1.10}$$

W_i wastewater flowrate:

$$W_i = F^s_i - L_i - \sum_{j=i+1}^{N} X_{ij} + \sum_{h=1}^{i-1} X_{hi} \qquad i=2,...,N-1 \tag{A1.11}$$

C^{in}_{ki} inlet concentration of each contaminant at entrance of water-unit u_i:

$$C_{ki}^{in}=\frac{F_i^s C_k^s+\sum_{h=1}^{i-1} X_{hi} C_{kh}}{W_i+L_i+\sum_{j=i+1}^{N} X_{ij}} \quad k=1,...K \quad \text{(from partial mass balance)} \tag{A1.12}$$

C_{ki} outlet concentration of each contaminant at exit of water-using unit u_i (the values for X_{ij} are generated by GA algorithm):

$$C_{ki}=\frac{F_i^s C_k^s+\sum_{h=1}^{i-1} X_{hi} C_{kh}+m_{ki}}{W_i+L_i+\sum_{j=i+1}^{N} X_{ij}} \quad k=1,...K \quad \text{(from partial mass balance)} \tag{A1.13}$$

c) Calculate the dependent variables for the N^{th} water-using unit: (Fig.(A1.3)):

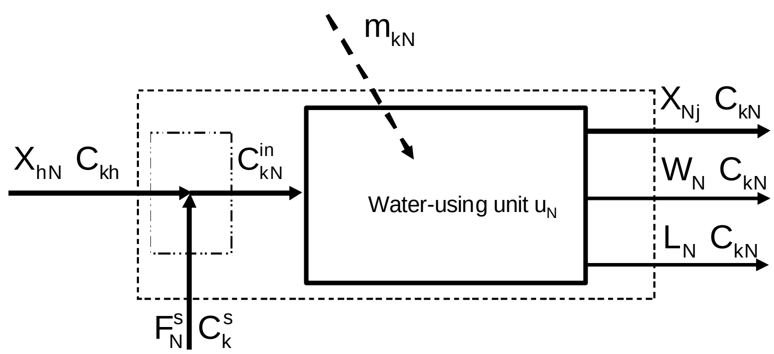


Figure A1.3 Schematic model of water-using unit, u_N

F_N^s Minimum freshwater flowrate: is calculated with the same eqs. (A1.5)-(A1.10) as at step b).

W_N wastewater flowrate:

$$W_N = F_N^s - L_N + \sum_{h=1}^{i-1} X_{hN} \tag{A1.14}$$

C_{ki}^{in} inlet concentration of each contaminant at entrance of water-unit u_N :

$$C_{kN}^{in}=\frac{F_N^s C_k^s+\sum_{h=1}^{N-1} X_{hN} C_{kh}}{W_N+L_N} \quad k=1,...K \quad \text{(from partial mass balance)} \tag{A1.15}$$

C_{kN} outlet concentration of each contaminant at exit of water-using unit u_N (the values for X_{hN} are generated by GA algorithm):

$$C_{kN}=\frac{F_N^s C_k^s+\sum_{h=1}^{N-1} X_{hN} C_{kh}+m_{kN}}{W_N+L_N} \qquad k=1,...K \quad \text{(from partial mass balance)} \qquad (A1.16)$$

It is important to stress that the calculation is cascaded due to the oriented graph nature of the water network.

d) Finally, the value of objective function is computed for the selected chromosome X

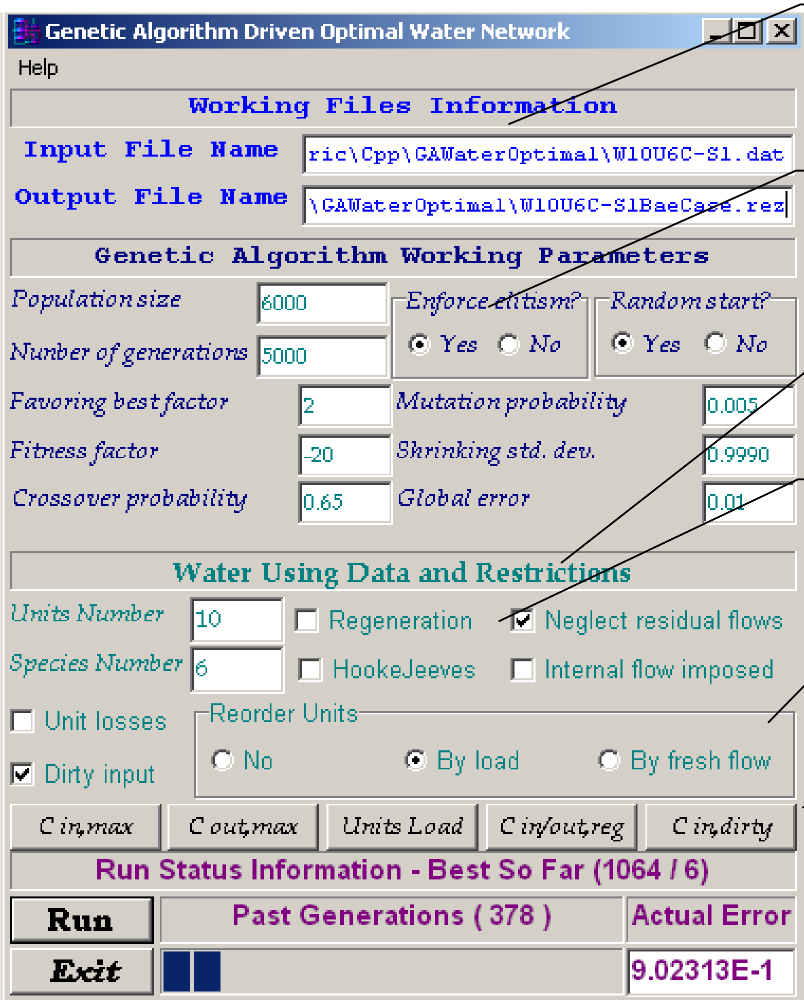
$$fo\big|_X=\sum_{s=1}^{NS}\sum_{i=1}^{N} F_i^s \qquad (A1.15)$$

e) The fitness can be evaluated for selected chromosome

f) Then the control is transferred to the GA algorithm routine.

ANNEX 2

GA INTERFACE (Lavric, et al. 2004a)



Input data file for a network of 10 units and 6 contaminants. Fresh water from Source-1, contaminated

When active, propagate the best individual thru generations; after cross-over, randomly generate individuals from a shrinking vicinity of the best individual

When active, neglect internal flows under a specified value (1 t/h, customary)

When active, reorder units in the network descending, according to the maximum contaminant load per unit

When active, reorder units in the network descending, according to the maximum fresh water needed per unit

Inspect/change input data buttons: maximum input/output unit concentrations, contaminants load per unit, regeneration unit input/output concentrations, contaminants load in fresh water