# A ROBUST METHOD TO OBTAIN OPTIMAL AND SUB-OPTIMAL DESIGN AND RETROFIT SOLUTIONS OF WATER UTILIZATION SYSTEMS WITH MULTIPLE CONTAMINANTS IN PROCESS PLANTS

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**Abstract**
*In this paper, a simple new approach for the grassroots and retrofit design of water utilization systems with multiple contaminants is presented. This approach uses a combination of mathematical programming and necessary conditions of optimality to automatically generate the optimal solution featuring minimum capital and operating costs. This paper presents the only existing method to solve this problem that can guarantee global optimality.*

## Introduction

Water is one of the most highly used commodities in industry. Its scarcity, rising energy costs and stricter environmental regulations on industrial effluents has created in the last years different view on water usage. The water allocation problem in its restricted form consists of finding the minimum amount of fresh water that each water-using process needs, together with the maximum amount of water effluent from these processes that can be reused in other processes. Many innovative solutions to this problem have been published. Many of these procedures rely on simplifying assumptions, built expertise condensed in guidelines that are many times contradictory and cannot be implemented automatically. Others require the use of full non-linear optimization models, which in many cases require the use of good initial points that may not be available. The water allocation problem in its more general form consists of obtaining the optimal freshwater allocation and wastewater flow between processes, such that an economical objective is met. *In this paper, the economical objective is total annualized cost.*

We omit a literature review, which can be found in Bagajewicz *et al*. (2000) who developed a set of water allocation rules and a tree-searching algorithm that can identify globally optimal solutions featuring minimum freshwater consumption. In this work, we extend the method developed by Bagajewicz *et al*. (2000) to take into account capital and operating cost considerations. In addition, a model for retrofit allocation is presented.

## Problem Statement

*Given a set of water-using/water-disposing processes, it is desired to determine a network of interconnections of water streams among the processes so that the overall annualized cost is minimized while the processes receive water of adequate quality.* Limits on inlet and an outlet concentration of each pollutant are imposed a-priori on every process and a fixed load of contaminants is used. These inlet and outlet concentrations limits account for corrosion, fouling and maximum solubility, etc.

The paper is organized as follows. The tree-searching algorithm developed by Bagajewicz *et al.* (2000) is first presented. Next, the modifications introduced in this work to perform grassroots design and retrofit are discussed. Following a refinery example is described and solved.

## Tree Searching Algorithm

The multicomponent necessary conditions were presented by Savelski and Bagajewicz (2000). They are:

- *Maximum Outlet Concentrations*: If a solution of the WAP problem is optimal, then all freshwater-using processes reach their maximum possible outlet concentration for at least one component.
- *Key Component Concentration Monotonicity*: If a solution is optimal, then at every process, the outlet concentration of a key component is not lower than the concentration of the combined wastewater stream coming from all the precursors. The key component of a

process is obtained as follows: The minimum freshwater flowrate needed to pick up the load of each component in the process is calculated. The key component is the one corresponding to the largest of these flowrates.

Thus, the WAP problem for a multiple contaminants system can be formulated using the following NLP problem:

$$Min\left( c_W \sum_j F_j^w + Capital\ \ Cost\ + Pumping\ \ Cost \right)$$

*s.t.*
*Material and Component Balances*
*Maximum Concentration Constraints*

Capital cost includes the annualized cost of piping and pumps to be installed. To solve this problem a constructive approach was developed (Bagajewicz *et al*., 2000). This approach consists of using maximum reuse flows from a given set of potential precursors to a particular process. This maximum reuse rule consists of minimizing the freshwater consumption of a process, assuming wastewater from a set of precursors is available. Next, the notion of maximum reuse structure was introduced. Such a structure is constructed by assuming a sequence of processes and water/wastewater allocation taking place in such a way that a) each process has only as precursors the previous elements of the sequence, b) the maximum reuse rule applies for each member of the sequence.

Bagajewicz *et al*. (2000) proved that when the sequence is fixed, the maximum reuse structure is a global optimal solution. The design procedure is therefore based on developing a tree structure of processes. Each branch of this tree is a maximum reuse structure. This strategy allows the identification of optimal and sub-optimal solutions. We now show how this method is reformulated so that cost is used as the objective function:

- Consider head processes first and do not include them as new branch nodes.
- Develop one branch of the tree to include all the processes using the maximum reuse rule every time a node is considered. This constitutes the current upper bound.
- Whenever the accumulated cost on any node is larger that the current upper bound, do not develop the sub-tree developed by this node any further.
- If a branch is fully developed to include all processes, update the current upper bound.

This procedure guarantees global optimality for the case where all the wastewater users are terminal processes. The proof of this assertion was given by Bagajewicz *et al*. (2000) when the total freshwater intake was the objective function. *We argue that this is also true for the case of cost.* Note that the branch-pruning criterion based on key component monotonicity used when the objective function is freshwater minimization is no longer employed. The reason for this is that a branch violating monotonicity can have low capital costs and therefore qualify for being part of the optimum.

**Optimality**

We first note that the tree contains all possible sequences. By using the above procedure, we are building maximum reuse structures as in the freshwater minimization case, but we are screening them for cost. Consider any such sequence. Since the freshwater consumption for this sequence is already the minimum possible, we can only increase it. As the freshwater is increased, the flowrates increase and the diameters of the piping are likely to increase. Therefore, the outcome of increasing freshwater flowrate is also an increase capital and pumping cost. Nevertheless, one can think that the possibility exists that certain piping connections can be eliminated if the freshwater input to a process is increased, leading to an overall lower cost. Given the high cost of water treatment (which is proportional to the flowrate), this is at simple glance unlikely. As we shall see from the results, giving further consideration to this is a moot point.

The proposed search allows exploring different design alternatives, capability that other methodologies fail to provide. Some of these alternative networks may have larger cost than the optimal case but they may still present an interesting option if the interconnections among processes are somehow limited. To capture sub-optimal solutions, one needs to establish a bound on the freshwater penalty that one is willing to pay. Thus the pruning criteria on freshwater consumption can be redefined to only stop the exploration of the tree if the current node cumulative freshwater consumption is larger than the current upper-bound plus the penalty.

**Example**

Table 1 shows the process limiting data for a system that contains typical refinery water using processes. Table 2 provides economical data, Table 3 presents the distances between processes and Table 4 shows the amount of water consumption corresponding to a solution where no reuse is performed. Piping diameters were obtained using a fixed water velocity in the pipes. The optimal solution is shown in Figure 1. Table 5 shows some sub-optimal solutions.

**Table 1.** Process Limiting Data

| ***Process*** | ***Contaminant*** | $C_{in}^{max}$ ***(ppm)*** | $C_{out}^{max}$ ***(ppm)*** | ***Load (kg/hr)*** | ***Pressure (psig)*** |
|---|---|---|---|---|---|
| **(1)** Caustic Treating | Salts | 300 | 500 | 0.18 | 30 |
| | Organics | 50 | 500 | 1.20 | |
| | $H_2S$ | 5000 | 11000 | 0.75 | |
| | Ammonia | 1500 | 3000 | 0.10 | |
| **(2)** Distillation | Salts | 10 | 200 | 3.61 | 10 |
| | Organics | 1 | 4000 | 100 | |
| | $H_2S$ | 0 | 500 | 0.25 | |
| | Ammonia | 0 | 1000 | 0.80 | |
| **(3)** Amine Sweetening | Salts | 10 | 1000 | 0.60 | 30 |
| | Organics | 1 | 3500 | 30.0 | |
| | $H_2S$ | 0 | 2000 | 1.50 | |
| | Ammonia | 0 | 3500 | 1.00 | |
| **(4)** Sweetening (Merox I) | Salts | 100 | 400 | 2.00 | 30 |
| | Organics | 200 | 6000 | 60.0 | |
| | $H_2S$ | 50 | 2000 | 0.80 | |
| | Ammonia | 1000 | 3500 | 1.00 | |
| **(5)** Sweetening (Merox II) | Salts | 100 | 350 | 3.00 | 30 |
| | Organics | 200 | 6000 | 75.0 | |
| | $H_2S$ | 50 | 1800 | 1.90 | |
| | Ammonia | 1000 | 3500 | 2.10 | |
| **(6)** Hydrotreating | Salts | 85 | 350 | 3.80 | 30 |
| | Organics | 200 | 1800 | 45.0 | |
| | $H_2S$ | 300 | 6500 | 1.10 | |
| | Ammonia | 200 | 1000 | 2.00 | |
| **(7)** Desalter I | Salts | 1000 | 9500 | 120 | 200 |
| | Organics | 1000 | 6500 | 480 | |
| | $H_2S$ | 150 | 450 | 1.50 | |
| | Ammonia | 200 | 400 | 0.00 | |
| **(8)** Desalter II | Salts | 800 | 9500 | 140 | 200 |
| | Organics | 1200 | 6500 | 220 | |
| | $H_2S$ | 150 | 450 | 1.20 | |
| | Ammonia | 200 | 400 | 0.00 | |
| Freshwater | | 0 | | | 30 |

**Table 2.** Economic Data

| | |
|---|---|
| Water Cost (Includes freshwater cost end-of-pipe treatment) ($/ton): | 1.5 |
| Pipe Cost Factor ($/in-ft): | 75 |
| APR (%): | 5 |
| Payout Periods (years): | 10 |
| Operation Days per Year: | 350 |
| Water Reasonable Velocity (ft/s): | 7 |
| Pump Efficiency (%): | 85 |
| Motor Efficiency (%): | 95 |
| Electricity Cost ($/kW-h): | 0.066 |
| Centrifugal Pump Cost ($/hp): | 2,000 |

**Table 3.** Distance (d) Between Processes

| ***From*** | ***To*** | ***d (feet)*** |
|---|---|---|
| Caustic Treating | Distillation | 1200 |
| | Amine Sweetening | 600 |
| | Sweetening (Merox I) | 900 |
| | Sweetening (Merox II) | 1200 |
| | Hydrotreating | 600 |
| | Desalter I | 900 |
| | Desalter II | 1200 |
| Distillation | Amine Sweetening | 900 |
| | Sweetening (Merox I) | 900 |
| | Sweetening (Merox II) | 1200 |
| | Hydrotreating | 1200 |
| | Desalter I | 900 |
| | Desalter II | 600 |
| Amine Sweetening | Sweetening (Merox I) | 1200 |
| | Sweetening (Merox II) | 1500 |
| | Hydrotreating | 300 |
| | Desalter I | 600 |
| | Desalter II | 300 |
| Sweetening (Merox I) | Sweetening (Merox II) | 300 |
| | Hydrotreating | 1500 |
| | Desalter I | 1800 |
| | Desalter II | 1500 |
| Sweetening (Merox II) | Hydrotreating | 1800 |
| | Desalter I | 2100 |
| | Desalter II | 1800 |
| Hydrotreating | Desalter I | 300 |
| | Desalter II | 600 |
| Desalter I | Desalter II | 300 |
| Freshwater Header | Caustic Treating | 1200 |
| | Distillation | 1500 |
| | Amine Sweetening | 900 |
| | Sweetening (Merox I) | 2100 |
| | Sweetening (Merox II) | 2400 |
| | Hydrotreating | 600 |
| | Desalter I | 300 |
| | Desalter II | 600 |

**Table 4.** Results (No Water Reuse)

| ***Process*** | ***Freshwater (ton/h)*** | ***Piping Diameter (in)*** |
|---|---|---|
| Caustic Treatment | 2.4 | 1 |
| Distillation | 25 | 3 |
| Amine Sweetening | 8.57 | 2 |
| Sweetening (Merox I) | 10.0 | 2 |
| Sweetening (Merox II) | 12.5 | 2 |
| Hydrotreating | 25 | 3 |
| Desalter I | 73.85 | 6 |
| Desalter II | 33.85 | 3 |
| *Total (ton/h)* | 191.17 | |
| *Total Cost ($/year)* | 2,651,800 | |

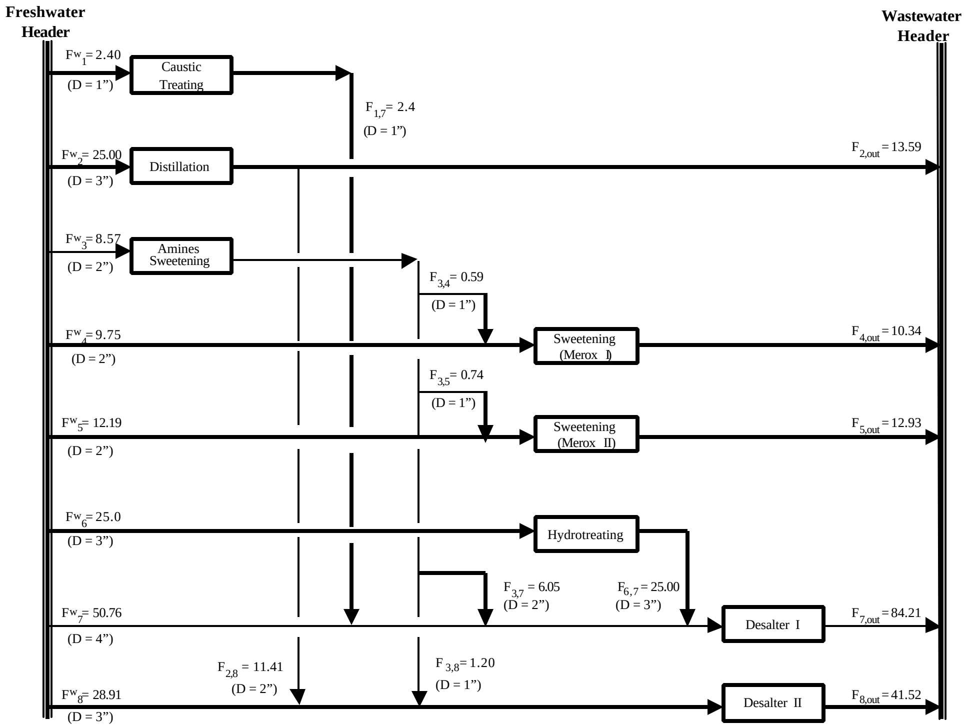


**Figure 1.** Scheme with Water Reuse - Optimal Solution Network

**Table 5.** Scheme with Water Reuse - Sub-optimal Solutions

| *Process* | *Freshwater* $F^w$ *(ton/h)* | *Piping Diameter (in)* | *Reuse Water* $F_{i,j}$ *(ton/h)* | *Piping Diameter (in)* |
|---|---|---|---|---|
| **Sub-Optimal Solution #1** | | | | |
| **(1)** Caustic Treatment | 2.40 | 1.0 | - | - |
| **(2)** Distillation | 25.00 | 3.0 | - | - |
| **(3)** Amine Sweetening | 8.57 | 2.0 | - | - |
| **(4)** Sweetening (Merox I) | 8.39 | 2.0 | $F_{2,4} = 0.31$  $F_{1,4} = 1.65$ | 1.0 ; 1.0 |
| **(5)** Sweetening (Merox II) | 12.28 | 2.0 | $F_{2,5} = 0.65$ | 1.0 |
| **(6)** Hydrotreating | 24.46 | 3.0 | $F_{1,6} = 0.75$ | 1.0 |
| **(7)** Desalter I | 52.72 | 4.0 | $F_{3,7} = 6.28$  $F_{6,7} = 25.21$ | 2.0 ; 3.0 |
| **(8)** Desalter II | 28.77 | 3.0 | $F_{2,8} = 10.45$  $F_{3,8} = 2.29$ | 2.0 ; 1.0 |
| **Sub-Optimal Solution #2** | | | | |
| **(1)** Caustic Treatment | 2.40 | 1.0 | - | - |
| **(2)** Distillation | 25.00 | 3.0 | - | - |
| **(3)** Amine Sweetening | 8.57 | 2.0 | - | - |
| **(4)** Sweetening (Merox I) | 9.76 | 2.0 | $F_{3,4} = 0.59$ | 1.0 |
| **(5)** Sweetening (Merox II) | 12.19 | 2.0 | $F_{3,5} = 0.74$ | 1.0 |
| **(6)** Hydrotreating | 25.00 | 3.0 | - | - |
| **(7)** Desalter I | 51.52 | 4.0 | $F_{2,7} = 5.29$  $F_{6,7} = 25.00$  $F_{1,7} = 2.40$ | 2.0 ; 3.0; 1.0 |
| **(8)** Desalter II | 28.15 | 3.0 | $F_{2,8} = 6.12$  $F_{3,8} = 7.24$ | 2.0 ;2.0 |

**Table 6.** Economic Comparison. Grassroots Design

| | | *Solutions with Water Reuse* | | | | |
|---|---|---|---|---|---|---|
| | *Without Water reuse* | *Optimal Solution* | *Sub-Opt. Solution # 1* | *Sub-Opt. Solution # 2* | *Sub-Opt. Solution #3* | *Sub-Opt. Solution #4* |
| *Freshwater Flow (ton/hr)* | 191.17 | 162.59 | 162.59 | 162.59 | 162.89 | 163.25 |
| *Freshwater & End-of-Pipe Treatment Cost* | $ 2,408,700 | $ 2,048,600 | $ 2,048,600 | $ 2,048,600 | $ 2,052,400 | $ 2,057,000 |
| *Piping and Pumping Cost* | $ 243,100 | $ 337,600 | $ 342,500 | $ 342,600 | $ 339,100 | $ 336,600 |
| *Total Cost* | $ 2,651,800 | $ 2,385,900 | $ 2,391,100 | 2,391,200 | $ 2,391,500 | $ 2,393,600 |
| *Freshwater Flow Savings (%)* | - | 15.0% | 15.0 % | 15.0 % | 14.8 % | 14.6 % |
| *Economic Savings (%)* | - | 10.0 % | 9.8 % | 9.8 % | 9.8 % | 9.7 % |

One important conclusion to make is that for real systems, this problem can exhibit several sub-optimal alternative solutions that are very close in cost to the optimal one. A comparison between the grass-roots design and the scheme without reuse water is given in Table 6.

**Retrofit Case**

The retrofit problem consists of the same constraints and a slightly modified objective function. In this objective function, it is considered to a) putting new piping where there is none, and b) adding a pipe and/or a pump where there is one. The existing installation for the example being studied is detailed in Table 7. Figure 2 shows the optimal solution. The piping costs are reduced tenfold with comparison to the grassroots solution. The general results of the first four sub-optimal solutions, which feature the same water consumption (162.59 ton/hr), are given in Table 8. The optimal solution whose cost is $2,048,600 differs from the first sub-optimal solution in only $1,100 (0.05%), which can be considered negligible. This difference comes from piping costs.

**Conclusions**

This paper introduced a tree searching methodology with efficient branch cutting criteria to solve globally the multicomponent water allocation problem with a cost objective function. The methodology is also capable of providing alternative sub optimal solutions. The results show that this problem can exhibit several solutions that are very close to each other and which from a practical point of view should be sorted out using some additional criteria.

**Table 7.** Existing Piping (diameter) and Pumping (power)

| ***From*** | ***To*** | ***d (in)*** | ***hp*** |
|---|---|---|---|
| *Desalter I* | Caustic Treating | 2 | 5 |
| | Distillation | 2 | 5 |
| | Amine Sweetening | 2 | 5 |
| | Sweetening (Merox I) | 2 | 5 |
| | Sweetening (Merox II) | 2 | 5 |
| | Hydrotreating | 2 | 5 |
| | Desalter II | 2 | 5 |
| *Desalter II* | Caustic Treating | 2 | 5 |
| | Distillation | 2 | 5 |
| | Amine Sweetening | 2 | 5 |
| | Sweetening (Merox I) | 2 | 5 |
| | Sweetening (Merox II) | 2 | 5 |
| | Hydrotreating | 2 | 5 |
| *Freshwater Header* | Caustic Treating | 2 | 5 |
| | Distillation | 2 | 10 |
| | Amine Sweetening | 3 | 5 |
| | Sweetening (Merox I) | 3 | 5 |
| | Sweetening (Merox II) | 3 | 5 |
| | Hydrotreating | 3 | 5 |
| | Desalter I | 6 | 45 |
| | Desalter II | 4 | 20 |

**Table 8.** Economic Comparison. Retrofit Design

| | | *Retrofit Solutions* | | | | |
|---|---|---|---|---|---|---|
| | *Grass-roots Design* | *Optimal Solution* | *Sub-Opt. Solution # 1* | *Sub-Opt. Solution # 2* | *Sub-Opt. Solution #3* | *Sub-Opt. Solution #4* |
| *Freshwater Flow (ton/hr)* | 162.59 | 162.59 | 162.59 | 162.59 | 162.59 | 162.59 |
| *Freshwater & End-of-Pipe Treatment Cost* | $ 2,048,600 | $ 2,048,600 | $ 2,048,600 | $ 2,048,600 | $ 2,048,600 | $ 2,048,600 |
| *Piping and Pumping Cost* | $ 337,600 | $ 59,500 | $ 60,600 | $ 67,300 | $ 67,600 | $ 68,400 |
| *Total Cost* | $ 2,385,900 | $ 2,108,100 | $ 2,109,200 | $ 2,115,900 | $ 2,116,200 | $ 2,117,000 |

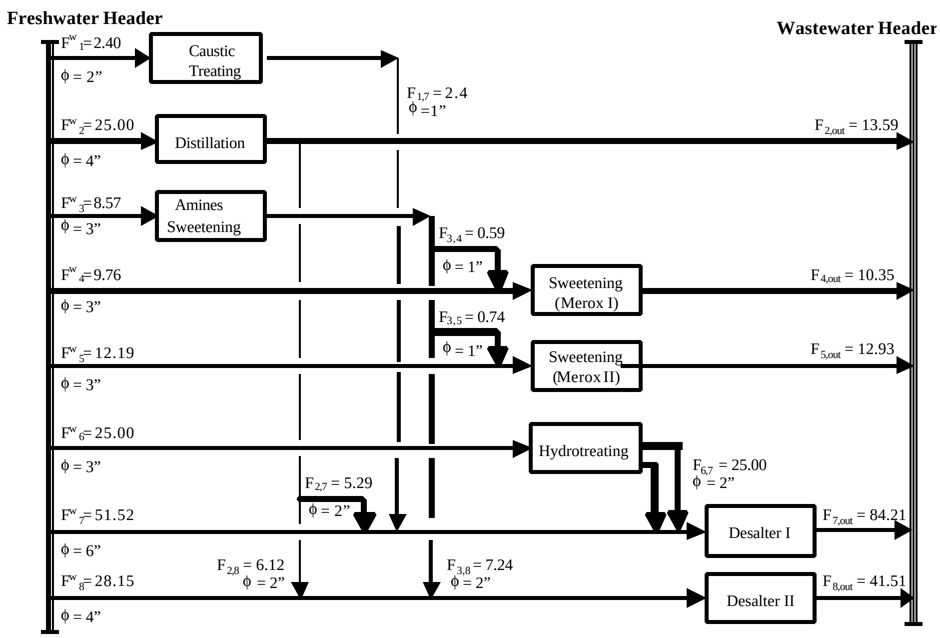


**Figure 2.** Retrofit Optimal Solution

## Notation

$F$ water flowrate, ton/h

c cost factor

Subscripts

*i*: process *i*

*j:* process j

Superscripts

*w*: fresh water

## References


- Bagajewicz, M., M. Rivas and M. Savelski. *A New Approach to the Design of Water Utilization Systems with Multiple Contaminants in Process Plant.* 1999 Annual AIChE Meeting. Submitted to Computers and Chemical Engineering (2000).
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(Unpublished references are available at: http://www.ou.edu/class/che-design/water-papers**)**