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HYBRID APPROACH IN TOTAL SITE WATER NETWORKS

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Abstract. *The advantages of using an optimization approach with superstructure in the synthesis of water networks in industrial plants are well known, among which we can mention: (1) capacity to assess a large number of structural and operational alternatives, simultaneously, (2) possibility of automation to a higher level the synthesis procedure and (3) ability to deal efficiently with many issues, such as process streams constraints, etc. However, this approach does not eliminate inherent nonlinearities and the transparence and visualization of the synthesis procedure is almost completely lost. This paper proposes a systematic way to link the methodology of the Water Sources Diagram (WSD) with a mathematical programming procedure for the maximization of water reuse in total site industrial plants. The results obtained show that the hybrid approach is extremely useful for the general understanding of the problem and for the determination of a better result.*

Keywords: *Hybrid Approach, Water Sources Diagram, Water Networks.*

1. INTRODUCTION

With the development and expansion of the computer's processing power, it has become possible, especially over the last decade, to develop software that were previously unfeasible in view of the computational effort required to perform the calculations. Tasks which were performed only on clusters, started also, running on ordinary desktops (Stephanopoulos & Reklaitis, 2011).

As a result, both mathematical programming methods and graphical and heuristic based on algorithms, could be inserted in the industrial environment through the implementation of effective computational tools, with respect to the use, cost of implementation and the associated economic return (Ravnjak *et al*. 2004). However, the search for the global optimum and more efficient and robust techniques have somewhat slowed the development of applications with practical use in industry. An example of this can be noticed by the fact that the amount of software for the integration of water networks is much smaller in comparison to the available computer packages for the integration of heat exchangers networks (Klemeš, 2013). This can be explained by a historical ramification between different methodologies that aim at the constant search for better and better results.

From the mid-1990s to the present day we have seen a predominance in the use of techniques based on Water Pinch methodology for the integration of water networks in industry. One explanation for this is the smaller capital investment needed (Hamaguchi & Park, 2009) and the fact that the type of techniques based on mathematical programming is considered as a "black box" because it provides the engineer with few perspectives on how the water reuse network is constructed (Yoo *et al*. 2006). Despite the greater use of water-based Pinch methods, mathematical programming approaches have shown better results when the process presents multiple contaminants (Mehrdadi *et al*. 2009). On the other hand, graphical and algorithmic-heuristic methods tend to facilitate the understanding and decision making of process engineers (Karthick *et al*. 2010). Despite the divergences between these approaches, there seems to be a consensus that a computerized analysis guided by in-depth knowledge of the process can provide a broader spectrum of solutions and better insights about a potential reconfiguration of the water network (Jacob *et al*. 2002).

Thinking about the practicality and applicability of algorithmic-heuristic methods without neglecting the robustness and precision of mathematical programming strategies, the approach presented herein shows that combine both methods may be the way to get reliable results through a practical and understandable for both industry and academia. This paper propose the use of WSD method (Gomes *et al*. 2013) with a mathematical programming model to minimize the use of freshwater between units of the same industry or among different sites of an industrial hub. The procedure was automated by the implementation in a software package written in VBA/EXCEL which interfaces with GAMS optimization packages.

2. THE TOTAL SITE WSD APPROACH

The Water Sources Diagram is probably one of the most promising algorithmic-heuristic procedures for the synthesis and optimization of water consumption in industrial processes. It meets the criteria of simplicity, industrial applicability, efficiency and economy, being one of the main tools in the management of industrial waters (E. E. da S. Calixto, 2011). The field of application of WSD is vast. It has been successfully employed in regeneration processes (Karthick et al., 2010), integration between water and thermal networks (Moreira e Silva, 2012), in the generation of wastewater treatment networks (Hungaro, 2005), Oil refineries (Ulson de Souza *et al*. 2009), in batch processes (Immich *et al*. 2007), in the pulp and paper industry (Francisco *et al*. 2014) and in the textile industry (Ulson de Souza *et al*. 2010).

Even providing good results in all these types of application, WSD algorithm has some issues when dealing with problems which have multiple contaminants in their process streams. In this case, WSD is unable to deal with multiples contaminants simultaneously, forcing the choice of one of them (the most restrictive one in terms of concentration), usually called the reference contaminant, to perform de calculations. For this reason, in some cases, the final network present violations in the maximum inlet and outlet concentrations of some contaminants of one or more operations. To eliminate this violation(s), a last step is required in the WSD procedure. It is carried out by increasing the freshwater consumption or by redirecting the outlet split stream that is upstream of the operation where the violation is observed. The other concept is related to the identification of the reference operation, i.e, the head operation which requires the cleaner water from an external water source and distributes freshwater for the rest of operations in the process.

In this context, over the years some efforts have been made to circumvent and avoid most WSD algorithm issues. One of them is the one proposed by (Calixto *et al*. 2015) which is related with the decomposition of the macro problem in small ones called "blocks". The WSD is applied to each block and then combinatorial analysis is performed to generate all the flowsheet possibilities and the operations which may belong to a given block. Some of these flowsheets will eventually present violations and other won't. The one that has no violation and present the minimum freshwater consumption is chosen flowsheet.

The idea of block decomposition may be applied to a set of operations of the same plant, different plants of the same site or even different sites of the same industrial hub (e.g, water reuse between a petrochemical and a refinery industry). A is shown in Figure 1.

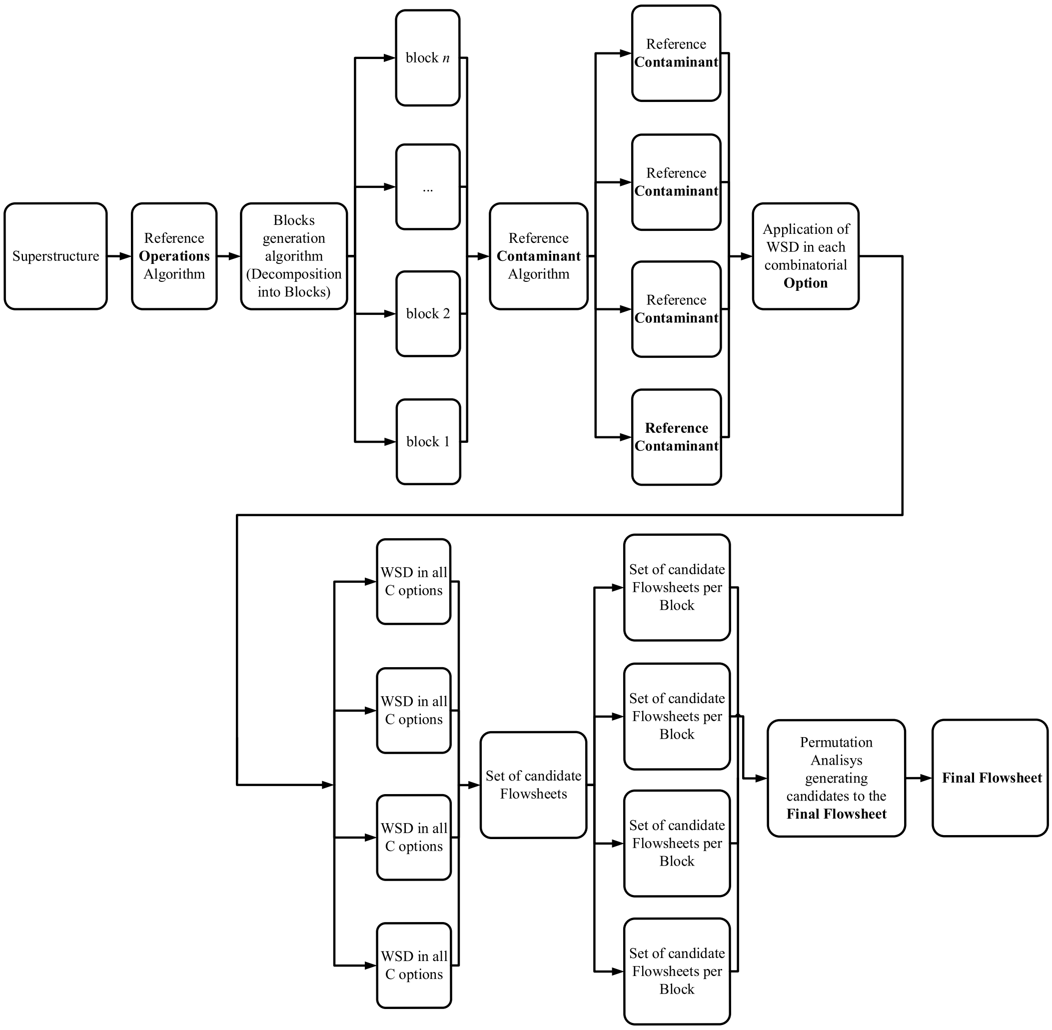

Figure 1 - Decomposition Algorithm Flowsheet. Adapted from Calixto *et al*. (2015).

For a given set of operations, units or even industry sites, the problem is decomposed based on a mathematical combination to generate all the flowsheets:

$$C_k^n = CC = \frac{n!}{k!\,(n-k)!} \quad (1)$$

Where,

$$k = n_b - 1$$
$$n = N_{op} - N_b \tag{2}$$

Where: N_{op} is the total number of operations and N_b is the number of blocks used to decompose the master problem. The generated flowsheets are arranged in terms of the lower freshwater consumption to become the candidate flowsheets and compose the final network. To identify all possible combinations of operations we can have inside each block a binomial coefficient is used $\binom{n+k-1}{n}$ (Feller, 1950). There is only one reference operation for each decomposed block. Therefore, as the reference operations are fixed in the block we nee to know the combinations of the other operations that are not reference. It is represented by the following binomial coefficient:

$$N_{opt} = \binom{N_{op} + N_b - N_b - 1}{N_{op} - N_b} = \binom{N_{op} - 1}{N_{op} - N_b} = \frac{(N_{op} - 1)!}{(N_{op} - N_b)!\left[(N_{op} - 1) - (N_{op} - N_b)\right]!} \tag{3}$$

The relation between the number of blocks and the number of operations has an impact in the computational effort, which can lead to a combinatorial explosion. It is represented by following equation:

$$N_{CC}^{total} = \sum_{j=1}^{N_{opt}} \sum_{i=1}^{N_b} CC_{i,j} = \sum_{j=1}^{N_{opt}} \sum_{i=1}^{N_b} \frac{(N_{op} - N_b)!}{\left(n_{b_{i,j}} - 1\right)!\left[(N_{op} - N_b) - \left(n_{b_{i,j}} - 1\right)\right]!} \tag{4}$$

where *i* represents the blocks going from 1 to N_b and *j* the options going from 1 to N_{opt}. It is worth noting that the number of blocks must not exceed the number of operations in a process $N_b \leq N_{op}$.

3. MATHEMATICAL MODEL OF WATER NETWORKS SYSTEMS

3.1. Water Balance through the water-using units

The nonlinear model used to describe the problem was initially proposed by Faria & Bagajewicz (2010) and it was later adapted in the work of Calixto (2016). It is represented by the following set of equations:

$$\sum_{w} FWU_{w,u} + \sum_{u^* \neq u} FUU_{u^*,u} + \sum_{r} FRU_{r,u} = \sum_{s} FUS_{u,s} + \sum_{u^* \neq u} FUU_{u,u^*} + \sum_{r} FUR_{u,r} \; \forall u \tag{5}$$

where $FWU_{w,u}$ is the freshwater flow rate from an external water source *w* and that is sent to a unit *u*, $FUU_{u^*,u}$ is the flow rate between units *u** and *u*, FUU_{u,u^*} is the flow rate between units *u* and *u**, $FRU_{r,u}$ is the flow rate from a regeneration process *r* to a unit *u*, $FUS_{u,s}$ is the flow rate from a unit *u* to a sink *s* and $FUR_{u,r}$ is the flow rate from a unit *u* to a regeneration process r.

3.2. Water balance through the regeneration units

The water mass balance for the regeneration units are as follows:

$$\sum_{w} FWR_{w,r} + \sum_{u} FUR_{u,r} + \sum_{r^* \neq r} FRR_{r^*,r} = \sum_{u} FRU_{r,u} + \sum_{r^* \neq r} FRR_{r,r^*} + \sum_{s} FRS_{r,s} \; \forall r \tag{6}$$

where $FWR_{w,r}$ is the freshwater flow rate from an external source *w* that is sent to a regeneration process *r*, $FRR_{r^*,r}$ is the flow rate from the regeneration process r^* to a regeneration process *r* and $FRS_{r,s}$ is the flow rate from a regeneration process *r* to a sink *s*.

3.3. Contaminant balance through the water-using units

The contaminant mass balance in the water-using operations is represented by the following equations:

$$\sum_{w}\left(CW_{w,c} FWU_{w,u}\right) + \sum_{u^* \neq u}\left(FUU_{u^*,u,c} C_{u^*,c}^{out}\right) + \sum_{r}\left(FRU_{r,u,c} CR_{r,c}^{out}\right) + \Delta M_{u,c} = \sum_{u^* \neq u}\left(FUU_{u,u^*,c} C_{u,c}^{out}\right) + \sum_{s}\left(FUS_{u,s,c} C_{u,c}^{out}\right) + \sum_{r}\left(FUR_{u,r,c} C_{u,c}^{out}\right) \; \forall u, c \tag{7}$$

where $CW_{w,c}$ concentration of contaminant *c* in the external water source *w*, $\Delta M_{u,c}$ is the mass load of contaminant *c* from unit *u*, $C_{u,c}^{out}$ is the concentration of contaminant *c* at the outlet of unit *u* and $CR_{r,c}^{out}$ is the concentration of contaminant *c* not treated at the outlet of the regeneration unit *r*.

3.4. Maximum inlet concentrations at the water-using units

The following equation represents the limiting concentrations at the water-using units.

$$\sum_{w}\left(CW_{w,c} FWU_{w,u}\right) + \sum_{u^* \neq u}\left(FUU_{u^*,u,c} C_{u^*,c}^{out}\right) + \sum_{r}\left(FRU_{r,u,c} CR_{r,c}^{out}\right) \leq C_{u,c}^{in,max} \times \left(\sum_{w} FWU_{w,u} + \sum_{u^* \neq u} FUU_{u^*,u} + \sum_{r} FRU_{r,u}\right) \forall u, c \tag{8}$$

where: $C_{u,c}^{in,max}$ is the maximum allowed concentration of contaminant *c* at the inlet of unit *u*.

3.5. Maximum outlet concentrations at the water-using units

The maximum outlet concentration at the water-using units is guaranteed by the following expression:

$$C_{u^*,c}^{out} \le C_{u,c}^{out,max} \ \forall u, c \tag{9}$$

where $C_{u,c}^{out,max}$ is the maximum allowed concentration of contaminant *c* at the outlet of unit *u*.

3.6. Flow rate through the regeneration process

The following equation represents de capacity of the regeneration process:

$$FR_r = \sum_w FWR_{w,r} + \sum_u FUR_{u,r} + \sum_{r^* \ne r} FRR_{r^*,r} \ \forall r \tag{10}$$

where FR_r is the flow rate of the regeneration process *r*.

3.7. Contaminant balance at the regeneration process

The contaminant mass balance at the regeneration is represented by the following equations:

$$FR_{r,c} CR_{r,c}^{in} = \sum_w \left(FWR_{w,r} CW_{w,c}\right) + \sum_u \left(FUR_{u,r} C_{u,c}^{out}\right) + \sum_{r^* \ne r} \left(FRR_{r^*,r} CR_{r^*,c}^{out}\right) \ \forall r, c \tag{11}$$

$$CR_{r,c}^{out} = CR_{r,c}^{in}\left(1 - XCR_{r,c}\right) + CRF_{r,c}^{out} XCR_{r,c} \tag{12}$$

where $CR_{r,c}^{in}$ is the concentration of contaminant *c* at the inlet of a regeneration process *r*, $CRF_{r,c}^{out}$ is the outlet concentration of contaminant *c* at the regeneration process *r* e $XCR_{r,c}$ is the binary parameter which indicates if contaminant *c* is treated by regeneration process *r*. It is considered that $CRF_{r,c}^{out}$(the concentration of the treated contaminant) is known and constant.

3.8. Maximum concentration at the inlet of the regeneration processes

The limiting inlet concentration at a regeneration process is represented by the following equation:

$$CR_{r,c}^{in} \le CR_{r,c}^{in,max} \ \forall r, c \tag{13}$$

3.9. Maximum allowed discharge concentration

All kinds of sinks impose the discharges limits. The following equation represents this constraint.

$$\sum_u \left(FUS_{u,s,c} C_{u,c}^{out}\right) + \sum_r \left(FRS_{r,s,c} CR_{r,c}^{out}\right) \le C_{s,c}^{discharge,max} \left(\sum_u FUS_{u,s} + \sum_r FRS_{r,s}\right) \forall s, c \tag{14}$$

where $C_{s,c}^{discharge,max}$ is the maximum allowed discharge in the sink s.

3.10. Objective Function

The objective functions consider the minimization of clean water consumption and of the total annual cost.

Minimum freshwater consumption

$$Min \sum_{w} \left(\sum_{u} FWU_{w,u} + \sum_{r} FWR_{w,r} \right) \tag{31}$$

Minimum total annual cost

$$Min \left[OP \left(\sum_{w} \alpha_w \left(\sum_{u} FWU_{w,u} + \sum_{r} FWR_{w,r} \right) + \sum_{r} OPN_r FR_r \right) - af\ FCI \right] \tag{32}$$

where OPN_r are the operation cost of the regeneration processes, OP is the hours of operation per year. The last term of the equation is the annualized capital cost, where FCI is the fixed capital cost and af is any factor for the annualization of the capital cost (it is usually 1/N, where N is the number of years of deprecation). The fixed capital of investment is calculated using the sum of the sum of the piping costs and the new regeneration units' costs as follows:

$$\begin{aligned} FCI = {} & \sum_{u} \left(\sum_{w} YWU_{w,u} CCWU_{w,u} + \sum_{r} YUR_{u,r} CCUR_{u,r} + \sum_{u^* \neq u} YUU_{u,u^*} CCUU_{u,u^*} + \sum_{s} YUS_{u,s} CCUS_{u,s} \right) \\ & + \sum_{r} \left(\sum_{w} YWR_{w,r} CCWR_{w,r} + \sum_{r^* \neq r} YRR_{r,r^*} CCRR_{r,r^*} + \sum_{u} YRU_{r,u} CCRU_{r,u} + \sum_{s} YRS_{r,s} CCRS_{r,s} + CCR_r (FR_r)^{0,7} \right) \end{aligned} \tag{33}$$

that uses a set of capital costs parameters to assign cost to the connections $CCWU_{w,u}$, $CCWR_{w,r}$, $CCUU_{u,u^*}$, $CCUS_{u,s}$, $CCUR_{u,r}$, $CCRU_{r,u}$, $CCRR_{r,r^*}$ and $CCRS_{r,s}$ and also to the regeneration process, CCR_r.

4. CASE STUDY

To evaluate the both decomposition and mathematical programming approaches we used a case study proposed by Leewongtanawit & Kim (2008). The process contains ten units and four contaminants with two external water sources making available 0 ppm and 10 ppm. After applying the decomposition procedure, the resulting flowsheet is shown in Figure 2. The problem was decomposed in three blocks and the final flowsheet is a recomposition of the best alternatives of operation distributed for each one. A total amount of 614,18 t/h of freshwater was obtained.

To analyze the robustness of the mathematical programming model the equations presented herein were implemented in the same case study. GAMS/BARON optimization package was used. Figure 3 shows the resulting flowsheet.

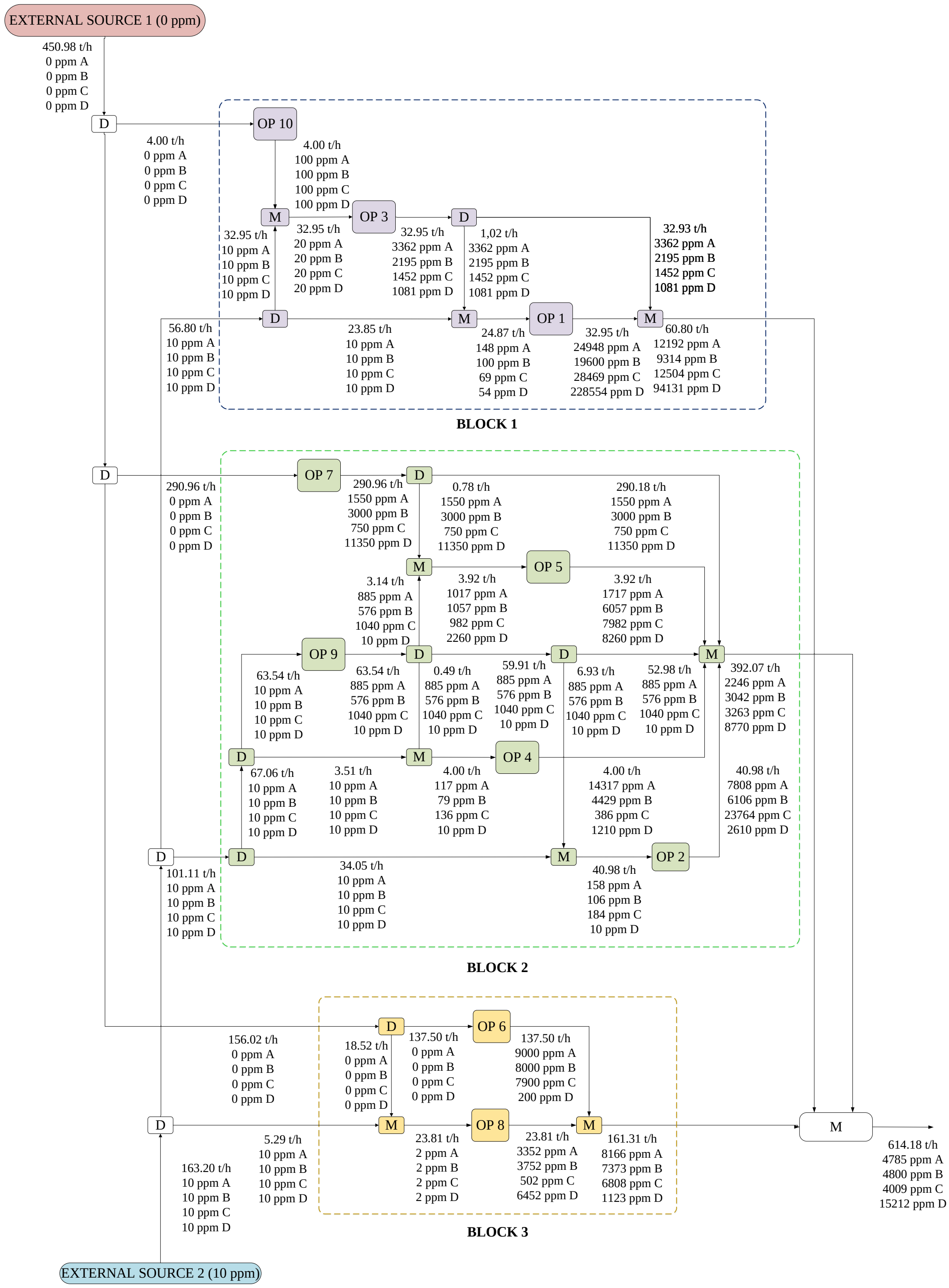

Figure 2 - Final Flowsheet generated using the decomposition approach.

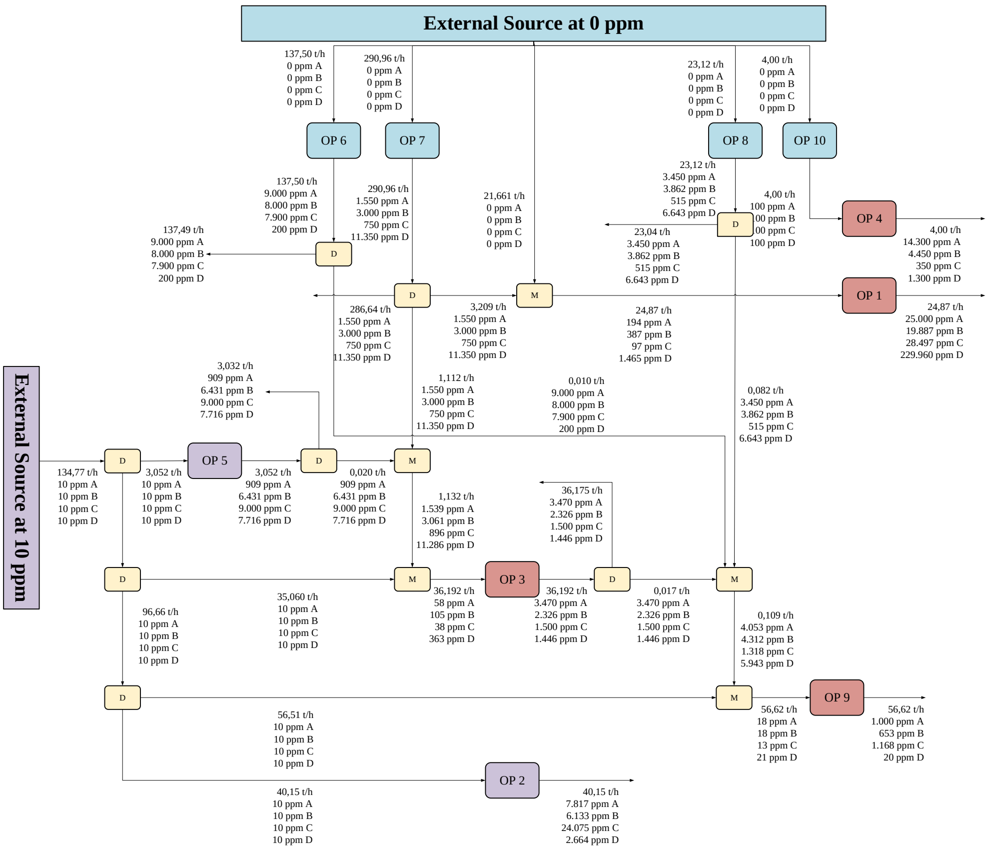

Figure 3 -Flowsheet for the water network generated by the optimization procedure.

A total flow rate of 612,56 t/h was obtained. A difference of 15,15 % is observed when we compare with the decomposition procedure.

5. CONCLUSIONS

This paper shows two robust procedures to get a minimum freshwater consumption for a water allocation problem. WSD procedure was successfully applied in the decomposition approach resulting in a consumption closer to that from mathematical programming. Both methodologies may be linked using the result from the decomposition approach as a initial guess for the optimization model. One of the disadvantages of the decomposition procedure is the fact that it is very time consuming if it is done "by hand". For future work, we propose an automation of the procedure and a complete integration with the mathematical model.

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