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Extension of the water sources diagram method to systems with simultaneous fixed flowrate and fixed load processes

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ABSTRACT

In this article, the water source diagram (WSD) (Gomes et al., 2007) is extended to the design of water networks involving both fixed flowrate and fixed contaminant load, as well as water loss/gain operations. The algorithm targets minimum external water consumption while simultaneously synthesizing the corresponding water system structure. In addition, it is shown that the WSD can be applied to water allocation problems (WAP) based only on water sources and sinks, maintaining its good performance. To illustrate the methodology, case studies handling hybrid water system are presented, including a zero wastewater discharge discussion and data from a Brazilian pulp mill.

NomenclatureΔm_{ji} contaminant mass load transferred in operation *j* in interval *i*C_{fj} outlet concentration in *j* operationC_{ij} inlet concentration in *j* operationC_{fi} concentration upper limit in interval *i*C_{ii} concentration lower limit in the interval *i*ETS effluent treatment systemEW external waterf_j flowrate in *j* operation$f_{ava}^{ew,j}$ flowrate available in the source from *j* original operation$f_{f,j}$ outlet flowrate from *j* original operation$f_{i,j}$ inlet flowrate from *j* original operation*m* contaminant mass loadN_{op} number of operationsN_{int} number of concentration intervals in the WSD*J* operation*i* concentration interval

1. Introduction

Chemical and petrochemical plants use a large quantity of water. Water scarcity, restricting environmental laws, as well as rising costs of energy and effluent treatment suggests adopting strategies of water management. In this context, reuse, recycle, regeneration with recycle, and regeneration with reuse of water have been extensively studied aiming at reducing water consumption.

Several procedures have been proposed to design the water allocation problems (WAPs). In general, these procedures can be divided into three majors groups: conceptual engineering (i.e. pinch analysis, water pinch), algorithmic, and mathematical optimization-based procedures. Comprehensive descriptions of these procedures can be found in Bagajewicz (2000), El-Halwagi (2012, 2006), Foo (2012, 2009), Jeżowski (2010) and Klemeš (2012). These methodologies are part of process integration, an area of process system engineering. In particular, these methodologies are aimed at systematically reducing impacts on the environment through the reduction of the consumption of resources or harmful emissions (Klemeš et al., 2013).

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Water using operations in chemical processes can be divided into two groups: (1) quality controlled and (2) quantity controlled (Dhole et al., 1995; Polley and Polley, 2000; Hallale, 2002; Manan et al., 2004). Quality-controlled operations are represented by fixed load (FL) operations and the main feature is that the water using units are modeled as mass transfer process with a fixed amount of contaminant that is transferred from a process stream to water (e.g. extraction, absorption and scrubbing). The inlet and outlet stream flowrates are typically equal and hence in this kind of operations there are no water losses or gains.

Quantity-controlled operations are represented by fixed flow (FF) operations where the focus is the flowrate through the operation (e.g. cooling towers, boilers, chemical reaction with water as reagent or product), and these water using units are usually not modeled as mass transfer process

The principal characteristic for the FF operations is that water loss or gain may takes place in the operation. This kind of problems also can be characterized as water source and sinks that consumes or generates a fix quantity of water. The inlet stream are bounded by permissible upper values of concentration while the outlet stream must leave the operation at the given maximum value of concentration and are thus independent on the inlet concentrations (Fan et al., 2012; Teles et al., 2009). Aiming fresh water consumption minimization, Prakash and Shenoy (2005) stated that the outlet stream should leave the operation at the given maximum value of concentration, while the inlet stream must have the maximum specified value, in both types of problems (FL or FF).

As reported by Foo (2009) a growing emphasis to synthesize water network with FF problem was lately observed. However, as described above, a limited number of works to design systems with FF using a conceptual approach have been reported in the literature. We now focus on reviewing the work on water systems with fixed flowrate (FF) operations: originally, Wang and Smith (1995) suggested the use of splitting and local recycling of water to meet the flowrate constraints in FF problems with multiple sources of water of varying quality. To account for water loss/gain the authors neglecting changes in water flowrate and then accounted the changes in the freshwater line. Next, Dhole et al. (1995) presented a targeting methodology for WAPs with FF operations based on a graphical approach. In their graphical representation of the problem, every inlet stream is treated as a demand and every outlet stream as a source. They also suggested that stream mixing and bypassing could be proposed to reduce the fresh water consumption. Polley and Polley (2000) noted a problem in Dhole et al. (1995) method: an incorrect stream mixing option could change the composite curve and lead to an apparent target higher than the true minimum fresh water consumption. In addition, Hallale (2002) also showed that the targeting procedure of Dhole et al. (1995) does not give correct targets because it relies on one chosen mixing option and therefore they could be wrong. In the same article, Hallale (2002) suggested a graphical procedure to find the absolute targets in water systems with FF operations based on a water surplus diagram (a diagram equivalent to the source and sink composite curve). However, the plotting procedure of the water surplus diagram is iterative and turns this task in a tedious and cumbersome work of trial-and-error steps. In addition, it has limitations when generating accurate targets because of its graphical nature. In addition, the methodology cannot handle multiple water supply sources. To overcome and eliminate the iterative steps of water surplus diagram, El-Halwagi et al. (2003) proposed a rigorous targeting approach applied to FF and FL problems based on source and sink composite curves. A numerical version of source and sink composite curves was developed by Almutlaq et al. (2005), called algebraic targeting approach. This approach uses the load interval diagram (LID) (Almutlaq and El-Halwagi, 2007). Another work based on LID was published by Aly et al. (2005) who presented a systematic procedure for water minimization based on two steps. In the first step, the water target is obtained using the load problem table (LPT), which is an adapted form from the LID. The second step, the design step, uses the pinch location and some guidelines to generate the water network through a special strategy of mixing the water sources in order to satisfy the respective water demands. This approach needs the construction of a table where the cascade analysis is performed, first finding the infeasible target and lately the true target. For the network design step, it is required to make the correct link between the source and demands in each concentration interval. This approach is time consuming because it involves a trial-and-error solution to link the sources and demands.

Simultaneously, Manan et al. (2004) proposed the water cascade analysis (WCA) technique, a numerical targeting tool that can be applied to obtain the minimum freshwater and wastewater targets for both FL and FF problems with single contaminant. This procedure is a numerical version of the water surplus diagram (Hallale, 2002), but without the iterative step; it also requires the construction of two diagrams, the water cascade and the pure water surplus cascade diagrams. These two diagrams are integrated by the interval water balance table. Foo (2007) extended the WCA to handle FF problems with multiple water supply sources. The proposed extension is based on the addition of three new steps to locate the minimum consumption of pure and impure fresh water sources. Finally, Foo et al. (2006) illustrated a process involving a zero liquid discharge network in a paper mill using the WCA. Parand et al. (2013a) proposed some adjustments in WCA to allow the correct identification of infeasible targets, which are the major iterative issues of the method.

Prakash and Shenoy (2005) developed the near neighbor algorithm (NNA). This algorithm is based in the use of the nearest source streams available in the neighborhood to satisfy a specific water demand in terms of concentration. In others words, the method creates a mix source that is just above and a source that is just below the specific demand to meet the demand value for FF problems. To be applied in FL problems it is necessary to first convert it into a FF problem in terms of sources and demands. This method cannot be used in problems with multiple water supply sources and with regeneration processes. In addition, it uses a graphical approach, the material recovery pinch diagram (MRPD), to determine the minimum freshwater consumption. An extension of NNA, the enhanced NNA (Shenoy, 2012), increased the applicability of the algorithm to FL problem giving priority to local-recycle matches. Later, Agrawal and Shenoy (2006) analyzed the capability of the NNA to target the minimum freshwater consumption in FF problems for a single contaminant. They extended the composite curve concept to create the composite table algorithm (CTA) to determine the minimum fresh water consumption, which is a hybrid graphical and numerical targeting technique. Parand et al. (2013a) demonstrated the applicability of the CTA for various water network synthesis problems (e.g. FL, mixed FL and FF, multiple pinch, and threshold problems) considering reuse/recycle schemes. Nevertheless, in integrated water

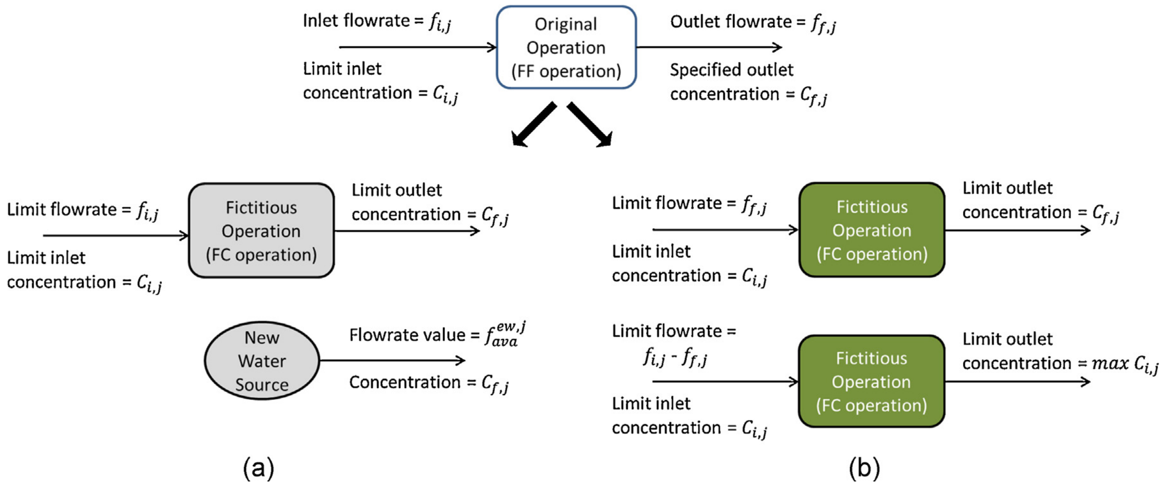

Fig. 1 – Conversion of FF operation into equivalents units. (a) Operation with water gain and (b) Operation with water loss.

Table 1 – Operational data for the illustrating example.

Operation number	C_{in} (mg L^{-1})	C_{out} (mg L^{-1})	Flowrate (t/h)	Water loss (t/h)
FF1	20	50	50	*
FF2	50	100	100	*
FF3	100	150	80	10
FF4	200	250	70	10
FL1	0	100	20	*
FL2	50	100	100	*
FL3	50	800	40	*
FL4	400	800	10	*

Source: Prakash and Shenoy (2005).

Table 2 – Rearranged operational data – illustrating example.

Operation number	C_{in} (mg L^{-1})	C_{out} (mg L^{-1})	Flowrate (t/h)
FL1	0	100	20
FF1	20	50	50
FF2	50	100	100
FL2	50	100	100
FL3	50	800	40
FF3	100	150	70
FF3′	100	800	10
FF4	200	250	60
FF4′	200	800	10
FL4	400	800	10

networks, the graphical analysis of the limiting composite curves (LCC) can be very complicated. In turn, Deng and Feng (2011) extended the method proposing the improved problem table (IPT), to target conventional and property-based water networks with multiple resources. This extension needs additional calculation to consider more than one external water source, which turns the proposed new approach somewhat complicated and/or cumbersome.

Bandyopadhyay (2006) presented a hybrid approach based on numerical and graphical techniques, which is a generalized form of the early concept of source composite curve (Bandyopadhyay et al., 2006) to reduce the waste production for a sort of applications (water management, hydrogen management and material reuse/recycle). The numerical technique is based on similar assumptions than those of the WCA, but involves only a single cascading instead of a double one. Nevertheless, in this method the cascading is made from the highest to the lowest concentrations whereas in the WCA it is in the reverse direction. The graph obtained was named source composite curve and it is plotted using the numerical result obtained first. With this plot, it is possible to predict the outlet wastewater flowrate and concentration. The source composite curve has the drawbacks of the graphical methods, with their curves being tedious and time consuming to be drawn.

Alwi and Manan (2007) presented a new procedure and a set of new heuristics, which improve the source and sink composite curves (El-Halwagi et al., 2003), in order to establish the minimum flowrate targets involving multiple water sources of utilities in FF and FL problems. Parand et al. (2013b) showed that these heuristics were not appropriate to be used above the infeasible pinch point.

Liu et al. (2007) presented a technique called modified concentration interval analysis (MCIA), which uses an equivalent process (called fictitious operation) to represent water loss and/or generation.

Alwi and Manan (2008) created a new graphical approach, called network allocation diagram (NAD), for simultaneous targeting and designing the water system for both FF and FL problems. The methodology is divided into four steps: (1) targeting; (2) allocation of sources to demands using heuristic rules; (3) design of the network using NAD, and (4) network evolution. This approach has the same drawbacks of the graphical approaches.

Foo (2009) presented a deep and ample review for WAP involving FF process for single impurity network relying on conceptual based approach. The author provides some comparisons between techniques developed for FL problems. The review covers targeting techniques for water reuse/recycle,

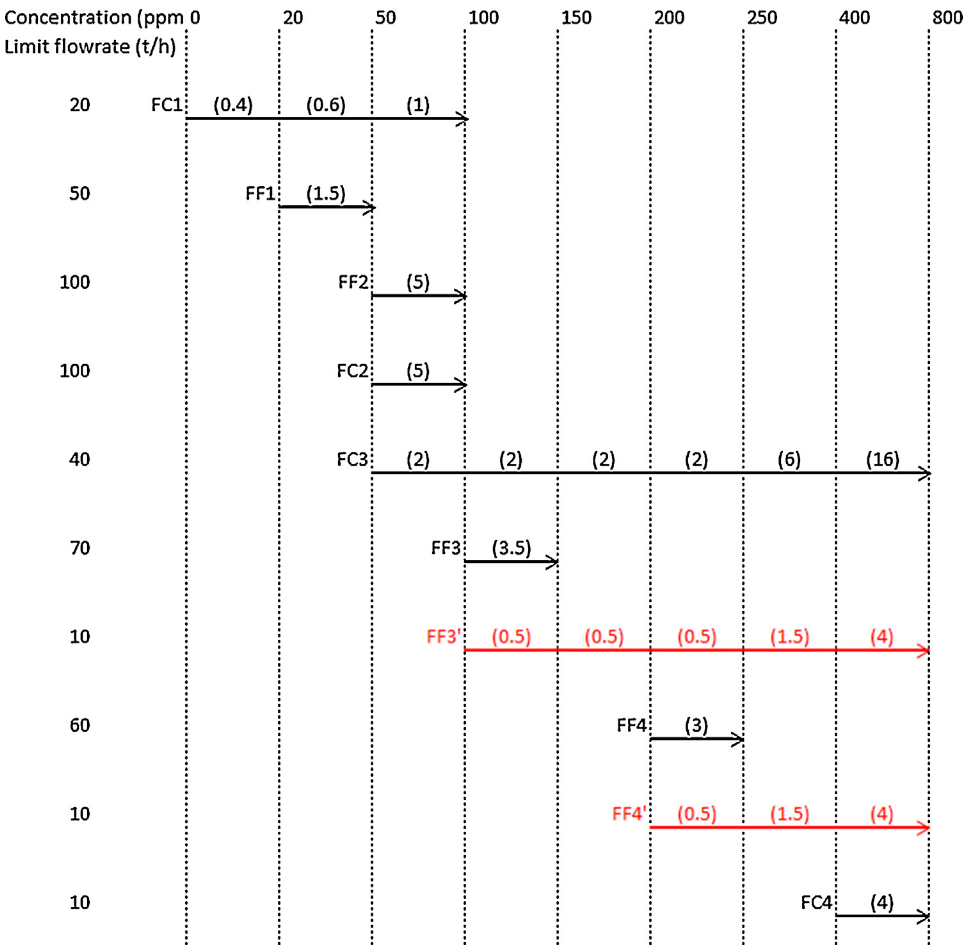

Fig. 2 – Initial WSD for the data of Table 2 – illustrating example.

regeneration, and wastewater treatment, along with the network design methods.

Deng et al. (2011) presented a new graphical approach to design the system and calculate the minimum fresh water consumption simultaneously. This approach is an extension of the limiting composite curve of Wang and Smith (1994), and can be applied in both types of problems (FF and FL). In problems that require uniform flowrate, the authors use local recycle to fulfill the flowrate constraint, and in problems with water loss/gain, the modified limiting water profile is used to find the specific value of minimum freshwater flowrate.

Fan et al. (2012) made an extension of the Liu et al. (2009) proposal, redefining the concept of concentration potential to consider recycling in fixed flowrate operations and to design the water system for both FF and FL cases. They divide the WAP into two groups of operations, fixed load and fixed flowrate operations. Initially, a design satisfying the needs of all fixed contaminant load operations is obtained followed by the addition of fixed flowrate operations to the design. They show that the results are close to the results obtained by mathematical programming. However, the procedure for hand calculations is somewhat long and tedious, needing a considerable effort to define which operation will be performed first and what stream will be used. When the calculation focused in a certain operation is completed, the initial procedure must be repeated before choosing another operation and stream to be performed.

Foo (2013) developed a generalized guideline for process changes for the synthesis of water network with FF operations. The author extended the plus–minus principle from heat exchanger network synthesis for targeting.

There are several authors who have studied processes with FF and/or FL operations including regeneration and targeting the minimum freshwater consumption (Bandyopadhyay et al., 2006; Ng et al., 2007a,b,c, 2008; Zhao et al., 2013; Parand et al., 2014). We do not review these efforts extensively because in this article, we do not study regeneration.

Furthermore, operational conditioning may fluctuate over time, leading to variations in actual mass load and/or water flowrate in the network operations. These fluctuations can lead to process disruptions affecting the operation effluents, which may become unacceptable for reuse in other operations, where they were previously acceptable. This feature makes the problem more complex. The presence of uncertainties in the water system analysis often makes it difficult to ensure feasible operation. More information about uncertainty in water systems can be found in, for example, Linninger et al. (2000), Koppol and Bagajewicz (2003), Karuppiah and Grossmann (2008), Feng et al. (2011) and Khor et al. (2014), using the mathematical programming approach, and Tan et al. (2007) and Zhang et al. (2009), adopting pinch analysis. Despite of the importance of this analysis, it will not be addressed in the present paper, because our scope, before analyzing the uncertainty effects, is to show how the WSD method can be extended to all kinds of water operations.

The majority of the methodologies previously described are focused on water consumption targets and therefore an additional approach to obtain the water system structure is needed. In the literature, there are some well-established

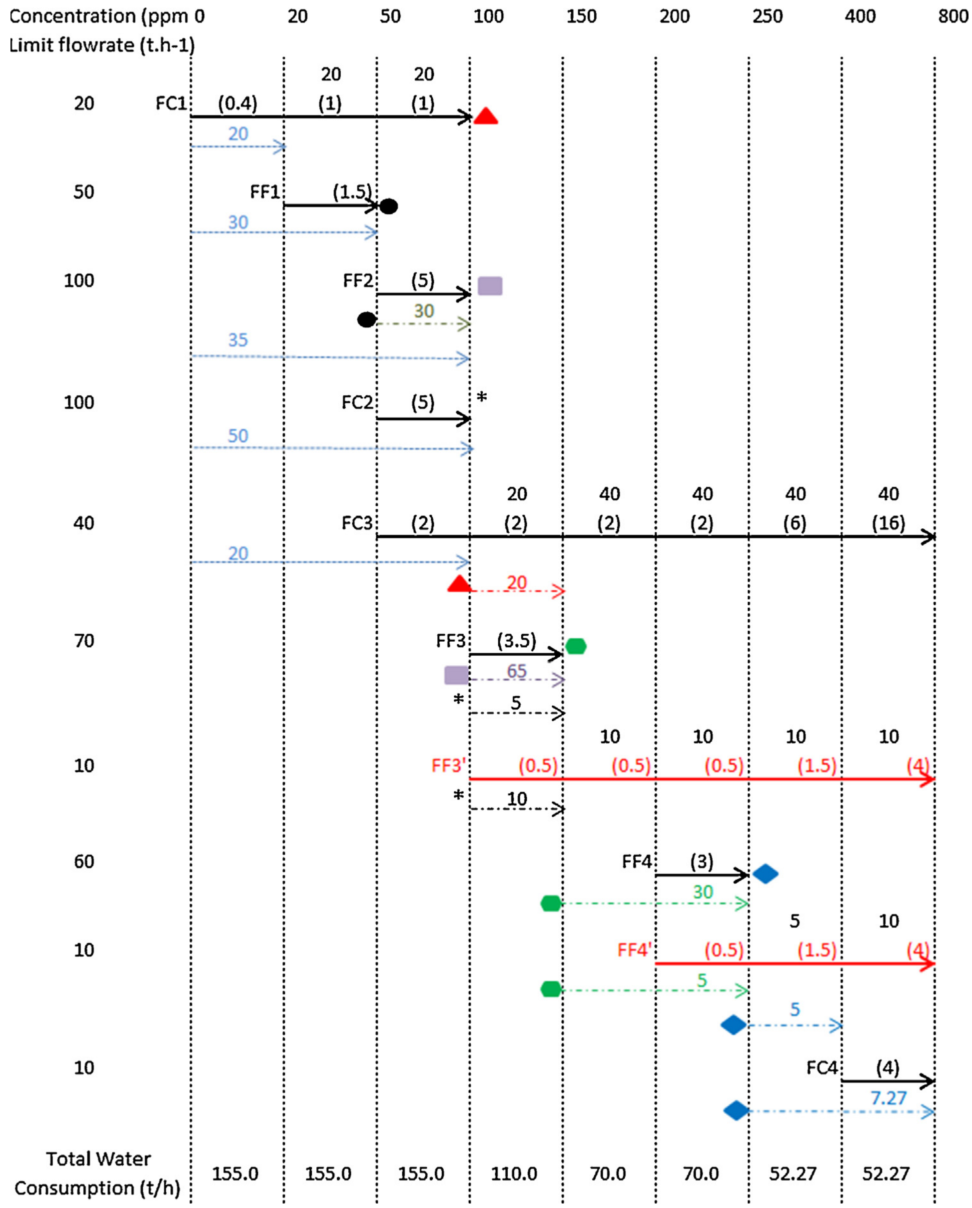

Fig. 3 – WSD for the illustrating example. (For interpretation of the references to color in text, the reader is referred to the web version of the article.)

design techniques for FL problems, e.g. water sources diagram (Gomes et al., 2007), water main method (Smith, 2005) and water grid diagram (Wang and Smith, 1994), and for FF problems, the source-sink mapping diagrams (El-Halwagi, 2006), NNA (Prakash and Shenoy, 2005) or heuristics rules (Aly et al., 2005). Among these set of methods, the WSD (Gomes et al., 2007) obtains both targets and system structure simultaneously in a direct simple manner for FL problems. It has similarities to an earlier method proposed by Gómez et al. (2001) and it has been extended to the case of multiple contaminants by Gomes et al. (2013) and to the analysis of hydrogen systems in petroleum refineries (Borges et al., 2012). It was also used in water systems with differentiated regeneration (Guelli Ulson de Souza et al., 2011). However, all the aforementioned applications/extensions of the WSD involve only the formulation of WAPs with fixed contaminant load (FL) operations.

In the present article, a simple procedure (an extension of the WSD) to determine the minimum fresh water consumption and simultaneously the system structure in water systems with FF and/or FL operations is presented; single or multiple water sources are also considered. The proposed extension does not resort to iterative procedures and cumbersome calculations when dealing with FF operations. It does not use recycles and can consider alternative network structures. It can also be used in processes including water loss/gain operations, and regeneration processes can be considered.

The extension proposed here can also be used in WAPs adopting the source/sink formulation. This type of representation is used in many methods described in the literature especially for FF problem, with water losses and/or gain. In a unit, an inlet stream may be treated as a demand (or sink) and an outlet stream may be considered as a source to other water using units (Dhole et al., 1995; Polley and Polley, 2000; Hallale, 2002; El-Halwagi et al., 2003; Prakash and Shenoy, 2005; Foo, 2009; Shenoy, 2011). Moreover, as the WSD procedure can generate different water system structures, its results can be easily adapted to industry constrains. In addition to

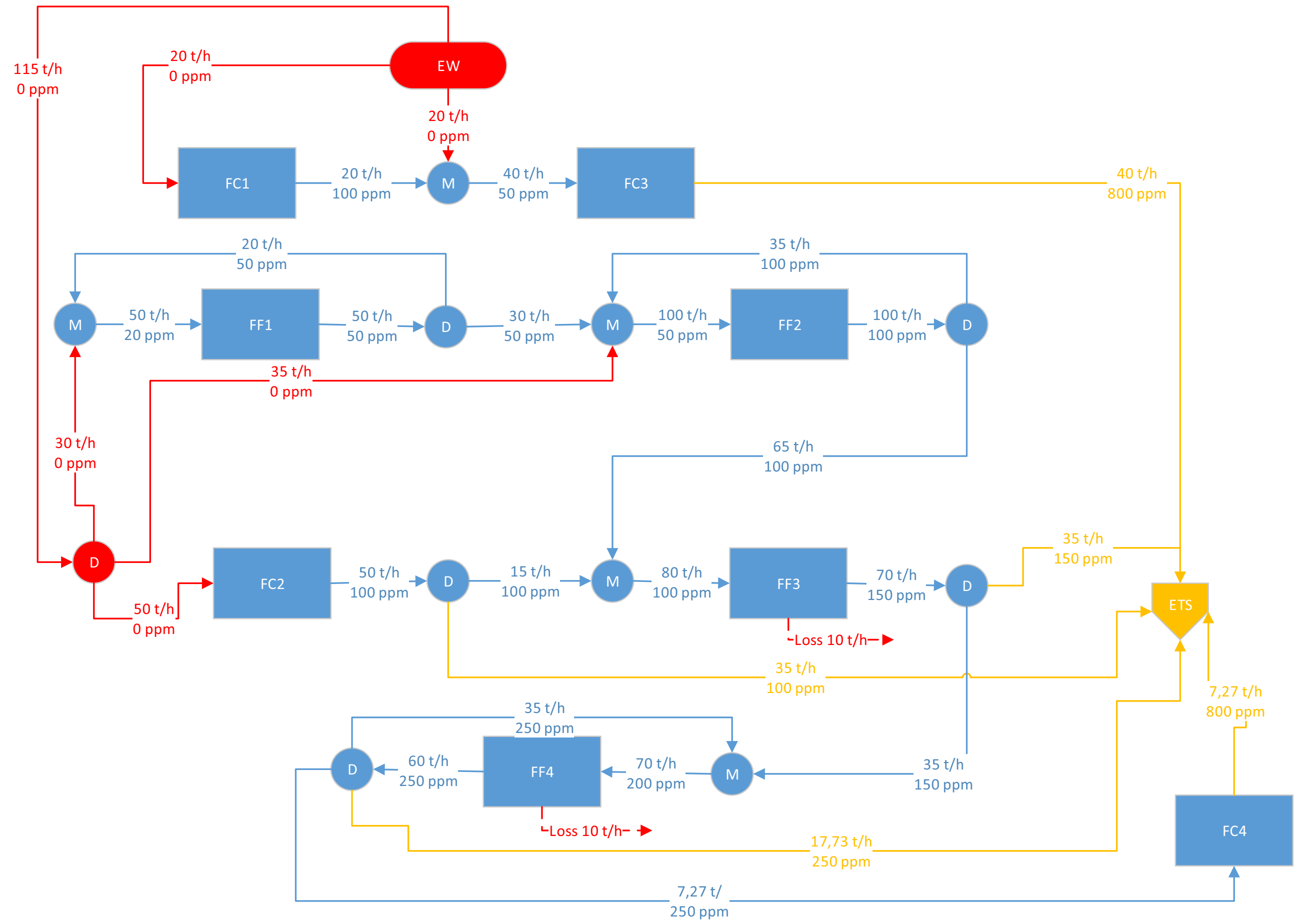

Fig. 4 – Water system structure for illustrating example.

the aforementioned two types of operations, one can use an alternative representation of sources and sinks. Indeed, an operation may also be divided in two parts (Dhole et al., 1995; Polley and Polley, 2000; Hallale, 2002; Prakash and Shenoy, 2005; Almutlaq et al., 2005; Bandyopadhyay, 2006; Alwi and Manan, 2007; Shenoy, 2011): (1) its inlet can be treated as a "sink" or a "demand", and (2) its outlet can be treated as a "source" to others operations. In this context, "sink" can be defined as a stream that goes into an operation with a specific water quality requirement and "source" is a stream going out an operation carrying the contaminant in a specific concentration. These definitions allow process having multiple inlet and/or outlet streams to be easily modeled in WAPs.

The article is organized as follows: first, the use of equivalent operations in considering FF operations is discussed. Following, the extension of the WSD procedure initially proposed by Gomes et al. (2007) to include FF operations problems is presented. Finally, five case studies from the literature are used to highlight the performance of the proposed extended WSD algorithm: the first Case Study involves a process for the production of a chemical specialty in which all operations are of the FF type, two of them presenting water loss and one involving water gain. The second Case Study is an alumina plant, with water loss in all operations. The third Case Study also involves an alumina plant, but now with a regeneration operation (centralized treatment) to achieve zero water discharge (ZWD). The fourth Case Study shows the use of the WSD procedure in WAP formulations using the definition of water sources and sinks, only. The fifth Case Study involves a retrofit of a real Brazilian pulp mill.

2. Equivalent operations in FF operations

Because the WSD procedure was developed for FL operations, we will use the concept of fictitious units (Liu et al., 2007; Zheng et al., 2006), to take into account FF operations.

When there is water generation in an operation, the original operation is represented by two equivalent operations each with constant flowrate equal to the inlet flowrate of the original operation, with the corresponding inlet and outlet concentrations, and a new water source (see Fig. 1a). The flowrate of is new water source ($f_{ava}^{ew,j}$) is:

$$f_{ava}^{ew,j} = f_{f,j} - f_{i,j} \tag{1}$$

where $f_{f,j}$ and $f_{i,j}$ are the outlet and inlet flowrates in the original operation, respectively. The concentration of this new water source is equal to the outlet concentration in the original unit.

For the case of water losses, we also propose to divide FF operations into two equivalent operations. The first has a constant flowrate equal to the value at the exit of the operation being modeled, and its inlet and outlet concentrations have values equal to the corresponding values in that operation (see Fig. 1b). The second equivalent operation has the flowrate equal to the water loss in the original operation, its inlet concentration is the same of the original one, and the outlet concentration has the maximum value of the water using system. This outlet concentration ensures that the corresponding stream will not be reused in another operation of the process. These FF operations with water loss are treated in an analogous form by Liu et al. (2007) and Zheng et al. (2006); the

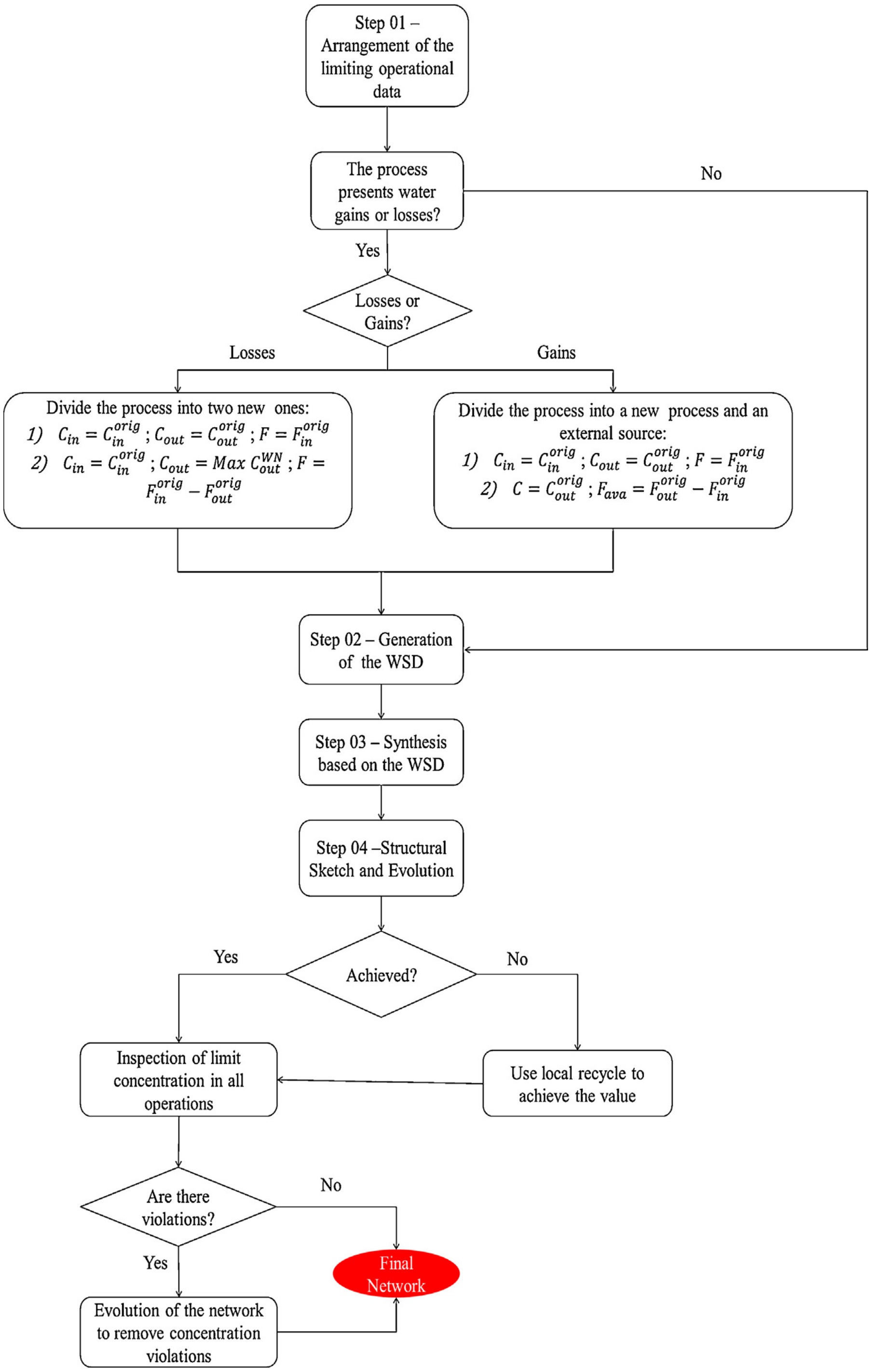

Fig. 5 – Extended WSD algorithm.

operations with water generation are described in a different way.

From the above illustrations, it is clear that limiting water data for both FL and FF problems are exchangeable. Hence, the WSD can be used to locate the minimum water flowrate and generate the water network, so long as the water limiting data is converted correctly.

3. Extended WSD algorithm for a single contaminant

We now present the extended WSD algorithm for single contaminant processes (Gomes et al., 2013, 2007). It consists of four steps:

1. Introduction of equivalent operations and/or new external water sources.
2. Generation of the WSD including all equivalent operations.
3. Application of the WSD algorithm as originally proposed for FL operations.
4. Use of an evolutionary step after the use of the original WSD algorithm. In this evolutionary step it is evaluated whether all the FF operation specifications are met or whether there is some violation in the concentration values. If violations are found, then the solution is evolved into a feasible one.

We now illustrate the steps in more detail using an example.

Table 3 – Limiting operational data for Case Study 1.

Operation number	C_{in} (mg L^{-1})	C_{out} (mg L^{-1})	Flowrate (t/h)	Water loss (t/h)	Water gain (t/h)	Operation (type)
1	100	1000	80	60	*	Reactor (FF)
2	200	700	50	*	*	Cyclone (FL)
3	0	100	10	*	30	Filtration (FF)
4	0	10	10	*	*	Steam system (FL)
5	10	100	15	10	*	Cooling system (FF)

Source: Wang and Smith (1995).

Table 4 – Rearranged limiting operational data – Case Study 1.

Operation number	C_{in} (mg L^{-1})	C_{out} (mg L^{-1})	Flowrate (t/h)	Operation
4	0	10	10	Steam system
3	0	100	10	Filtration
5	10	100	5	Cooling system
5′	10	1000	10	Cooling system
1	100	1000	20	Reactor
1′	100	1000	60	Reactor
2	200	700	50	Cyclone
External water sources		C_{in} (mg L^{-1})		Available (t/h)
FW		0		*
F1 (filtration)		100		30

Step 1 – Arrangement of the limiting operational data: Consider the limiting operational data are shown in Table 1 and an available source of external clear water (0 ppm).

The system has two operations with water loss identified by FF3 and FF4. Hence, each of them is divided into two equivalent operations represented in Table 2 by FF3, FF3′, FF4 and FF4′. The operations FF3′ and FF4′ represent the water loss in the respective original operation. The new operations (FF3′ and FF4′) have the inlet concentration equal to the inlet concentration of the respective original one and the outlet concentration equal to the maximum concentration in the whole process. As defined above, the outlet concentrations are equal to the maximum process outlet concentration to avoid the reuse of the respective outlet streams in another operation.

Step 2 – Generation of the WSD: Following the WSD method the process operations are arranged in order of increasing inlet concentration, enabling the verification of reuse possibilities among the operations. If more than one operation has the same inlet concentration, the relative position is then defined by the outlet concentration, organized from the lowest to the highest values. If more than one operation have the same inlet and outlet concentrations, these operations should be allocated in the diagram from the lowest to the highest flowrate value.

Table 2 shows the rearranged limiting operational data for the example process. The WSD procedure is based on these data and the operations will be inserted in the WSD following its relative position in this table.

Next, the concentration intervals are defined by the inlet and outlet concentrations of all operations and by the concentrations of the available external water sources. In the grid (Fig. 2), each operation is represented by arrows, from its respective inlet to outlet concentrations. The operations are inserted following the order defined in Table 2 and their respective limiting flowrates, f_j, are presented in a column on the left side of the diagram (see Fig. 2). The amount of mass

Table 5 – Comparison between WSD and other procedures – Case Study 01.

References	External water consumption (t/h)	Approach
Extended WSD	90.64	Algorithmic
Deng et al. (2011)	90.65	Graphical (PGA)
Jeżowski et al. (2003)	90.69	Mathematical programming
Mann and Liu (1999)	90.64	Graphical
Sorin and Bédard (1999)	90.70	Algorithmic
Wang and Smith (1995)	90.70	Graphical

transferred in each operation, in each interval, is calculated using the following expression.

$$\Delta m_{ji} = f_j * (C_{fi} - C_{ii}) \quad (2)$$

where Δm_{ji} is the amount of contaminant transferred in operation j in interval i; f_j is the flowrate through the operation j; C_{fi} is the concentration upper limit in interval i, C_{ii} is the corresponding concentration lower limit in interval i; and $j = 1, \ldots, N_{op}$, and $i = 1, \ldots, N_{int}$; here N_{op} is the number of operations in Table 2 and N_{int} is the number of concentration intervals in the WSD. All Δm_{ji} values are written in the WSD in parenthesis over the respective operation arrow. Finally, the equivalent operations representing the water loss and the mass transfer values in parenthesis are added. We do not claim that the addition of these equivalent operations and the changes made to the original data leads to a feasible solutions after applying the WSD algorithm. Rather, as we illustrate later, it provides a good starting point to obtain a good solution.

Step 3 – Synthesis based on the WSD: In this step the synthesis of the water system structure is applied using the three rules described in Gomes et al. (2007). Using these rules, it is possible to calculate the respective external minimum water

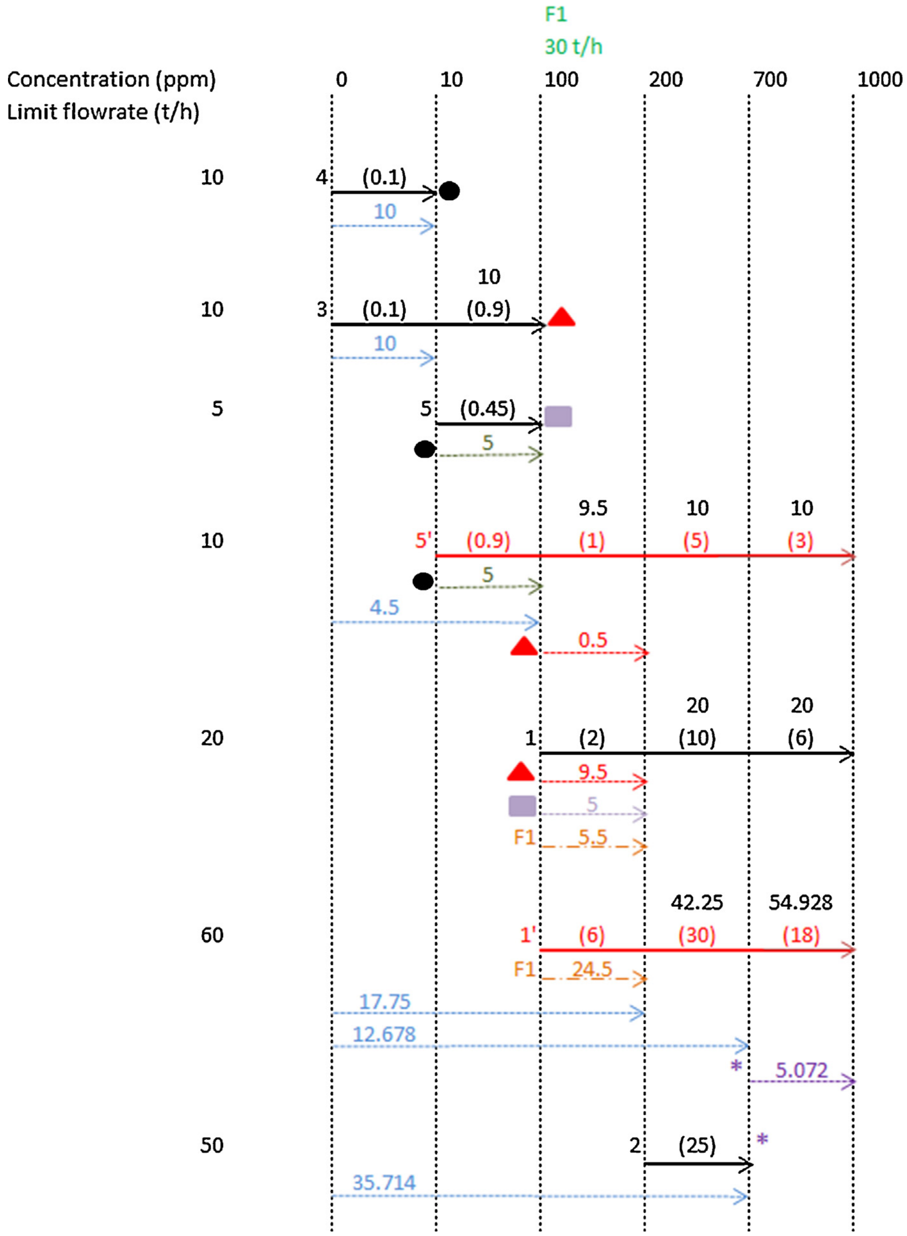

Fig. 6 – WSD – Case Study 1. (For interpretation of the references to color in text, the reader is referred to the web version of the article.)

flowrate consumption in each interval. In some intervals it is possible to choose more than one internal source and depending on the source used, different water systems structures can be obtained. Note that this WSD feature enables the simultaneous analysis of different system structures. This feature can be better observed when analyzing the third interval of this illustrative example.

In the third concentration interval, 20 t/h at 50 ppm (from operation FC1), 30 t/h at 50 ppm (from operation FF1) and the external water source at 0 ppm are available. Processes FC1, FF2, FC2 and FC3 are present in this interval. These processes need, $f_{FC1} = 20$ t/h, $f_{FF2} = 100$ t/h, $f_{FC2} = 100$ t/h, $f_{FC3} = 40$ t/h, respectively, at 50 ppm. According to WSD rules, the internal source coming from operation FC1 is used in the same operation, achieving its needs. For the remaining operations (FF2, FC2 and FC3) it is available the internal source from operation FF1 (30 t/h at 50 ppm) and the external water source (0 ppm). The rules dictate the use of internal water sources before the external, and hence there is one source for three possible uses. In real systems this choice can be oriented by process restrictions, such as distance between operations, impossibility of use of some effluent in a specific operation, and so on. How there is no information about process restrictions, the option is free, that is, the internal source available can be used in either of the three operations.

The algorithm for maximum reuse indicates a flowrate consumption analysis in each concentration interval, from the lower concentrations to the higher ones

The result of applying the WSD procedure is shown in Fig. 3.

The symbols in Fig. 3 indicate the respective wastewater reuse from one operation to another. For example, the red triangles indicate that the wastewater from operation FC1 is reused in operation FC3, and the green hexagons the reuse of the effluent from operation FF3 into operations FF4 and FF4′.

At the lower part of the WSD shown in Fig. 3, there is a row showing the total water consumption in the respective concentration interval. The interval where the first flowrate decrease is observed (100 ppm) is the pinch of the process (Gomes et al., 2007). Moreover, it is interesting to note that a coincidence between the pinch concentration and the higher

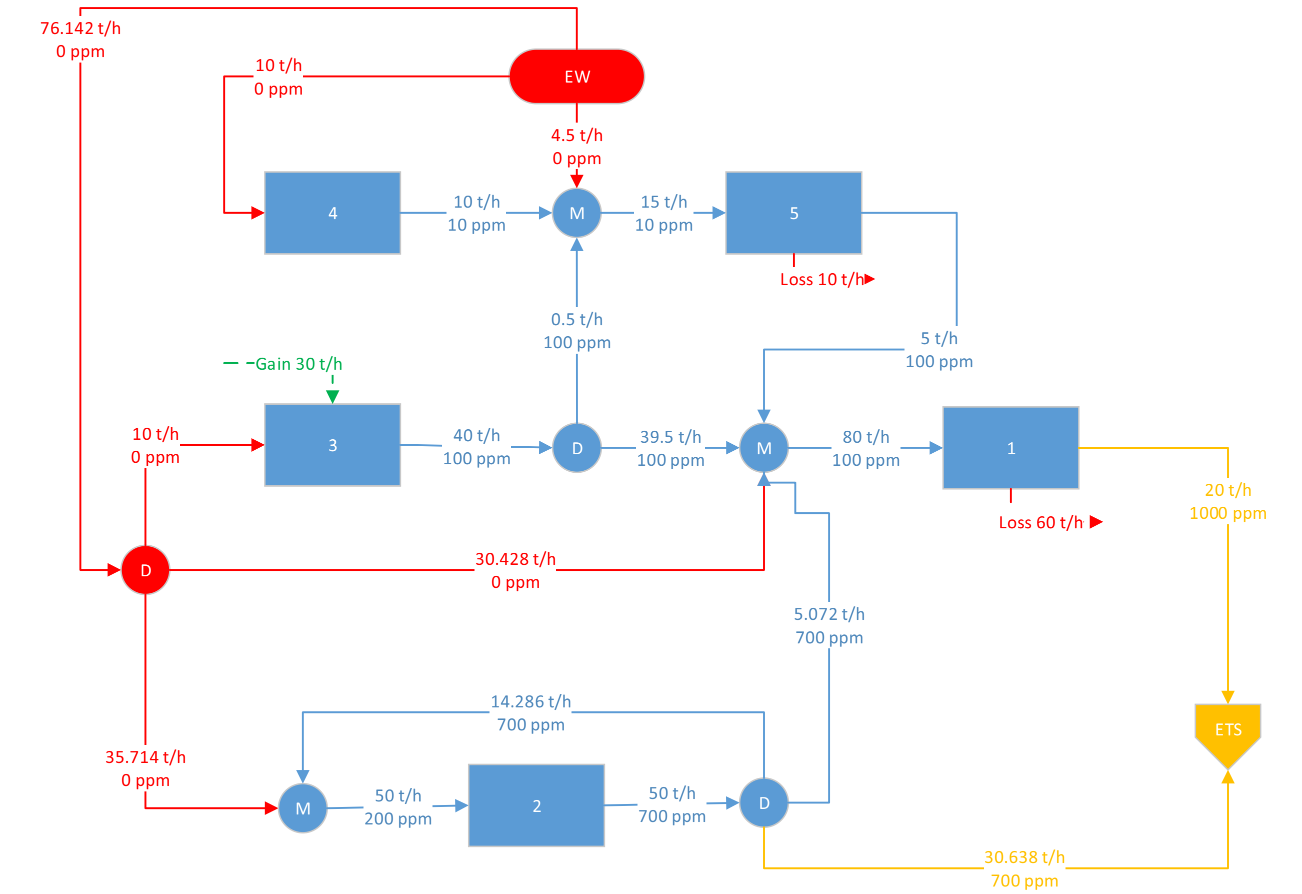

Fig. 7 – Case Study 1. Water system structure for maximum reuse.

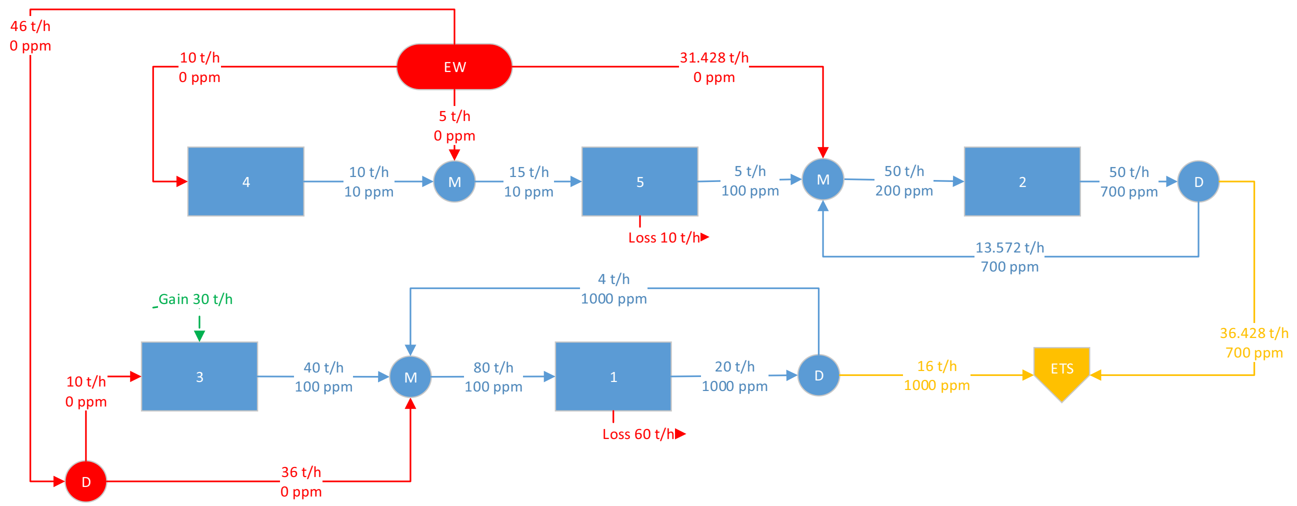

Fig. 8 – WSD result with reuse constrains – Case Study 1.

concentration of the last interval where external water is used in the WSD.

Step 4 – Structural sketch and evolution: The resulting WSD, shows that operations FF1, FF2 and FF4 do not achieve their respective water flow requirements. In one contaminant processes, the WSD algorithm does not lead to concentration violations, but flowrate violations can occur in FF or FL with some flowrate constraint. These flowrate violations are removed by using local recycles as proposed by Wang and Smith (1995), which use this idea to achieve the constraint imposed by FF operations. After the insertion of these recycles, mass balances are used to calculate the new inlet and outlet concentrations in the operations where the recycle are used and downstream of them. All remaining violations can then be eliminated by tuning the external water consumption or by redirecting the exits of some splits, which are upstream of the operation where the violation is observed.

For FL processes another possible opportunity to decrease the water consumption in the evolution step shows up, when some operation receives freshwater. This happens because these processes may present a lower freshwater consumption. This operation can be treated as an independent operation and its freshwater consumption is then recalculated independently, and its outlet stream reuse is considered. After that, if some other violation remains, the elimination procedure is repeated until all of them are removed. An inspection procedure can also be used and depends on the experience of the engineer.

Fig. 4 shows the sketch of the system structure corresponding to the WSD of Fig. 3 with the local recycles and recalculated concentrations. All remaining violations can now be eliminated by tuning the external water consumption or by redirecting the exits of some splits, which are upstream of the operation where the violation is observed. In our example, the operations FF1, FF2 and FF4 present local recycles of 20 t/h (200 ppm), 35 t/h (100 ppm) and 35 t/h (250 ppm), respectively. In the present example, the local recycles allow achieving the flowrate requirement without violating the maximum inlet concentrations and therefore there is no need for the other adjustments.

The total consumption of external water (FW) at 0 ppm is 155 t/h and the total water discharge is 135 t/h, with a pinch at 100 ppm. If all the discharges are mixed, the concentration is 377.8 ppm. Prakash and Shenoy (2005) found the same values for external water used, wastewater generated, pinch concentration and concentration of centralized discharge. However, the structure in Fig. 4 is different of the one obtained by Prakash and Shenoy (2005), indicating that the system has multiple solutions, which stem from all the alternative choices one can make using the WSD algorithm.

Summary of the proposed algorithm: The extended WSD algorithm for single contaminant processes involving fixed contaminant load and/or fixed flowrate operations (hybrid processes) is summarized in Fig. 5.

4. Case studies

Case Study 1: This case study is taken form Wang and Smith (1995) and is a process for the production of a chemical specialty; it involves both FL operations (cyclone and steam system) and FF operations (reactor, filtration and cooling system). There are water losses and water gains (cooling system and reactor). Other authors (Deng et al., 2011; Jeżowski et al., 2003; Mann and Liu, 1999; Sorin and Bédard, 1999) used this example to show the performance of their methodologies. Its original limiting data are presented in Table 3. External water available is pure (0 ppm). Table 4 shows the rearranged data after adding the equivalent operations.

Fig. 6 shows the result of applying the WSD algorithm. Note that on concentration equal to 100 ppm there is the availability of a source (F1), which has the same priority of internal sources and with the flowrate equal to 30 t/h. This source is used in operations 1 and 1′. The equivalent operations, which represent water losses and the source linked to the water gain, are in red and the mass transfer values (in kg/h) are shown in parenthesis. The corresponding minimum external water consumption is 90.642 t/h (0 ppm) and the pinch concentration is 700 ppm. Fig. 7 presents the resulting water system structure.

Appling now step 4, a comparison of the concentrations and flowrates in Fig. 6 with the respective limits in Table 4 shows that there is only a violation on the cyclone, which should be treated as a FL operation with a flowrate constrains. Note that the efficiency of a cyclone is directly linked to its flowrate. Therefore, an internal recycle is inserted around the cyclone to satisfy the flowrate constraint. With no violations, the water system of Fig. 7 is the final.

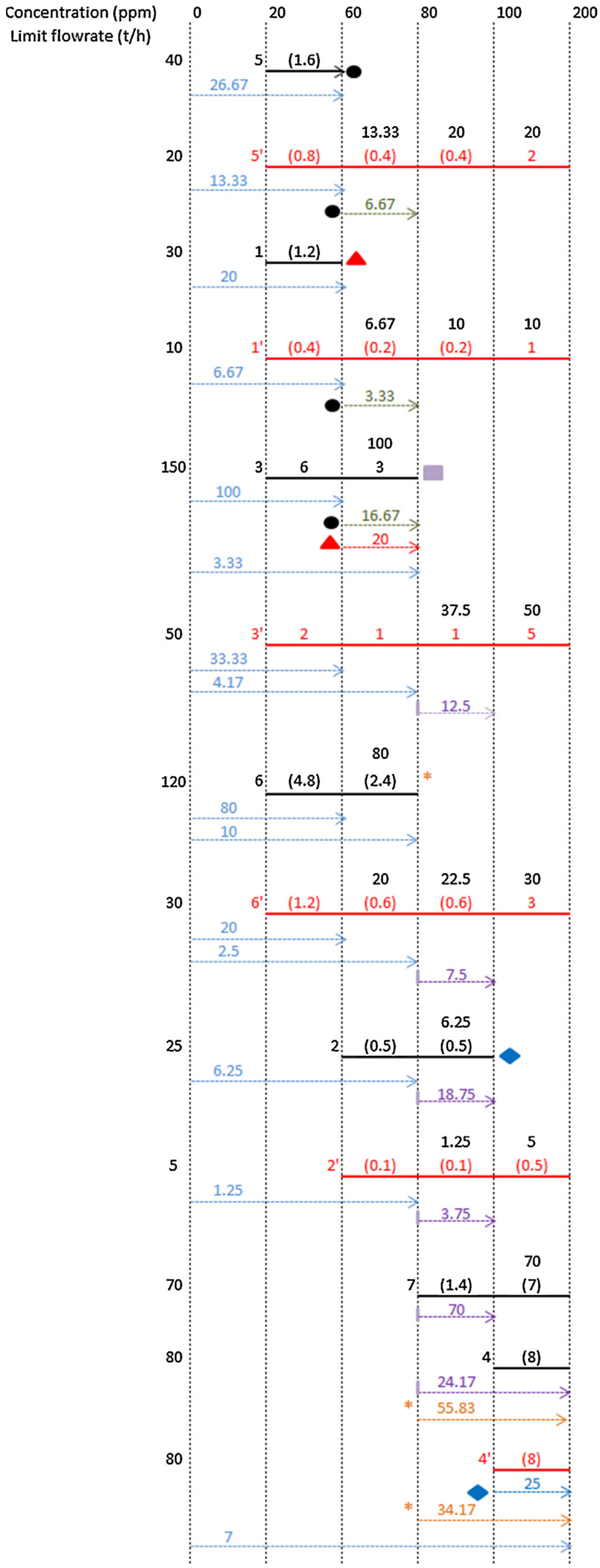

Fig. 9 – Final WSD – Case Study 2.

Table 5 compares the results of the WSD algorithm with other works, which are quite similar, showing the effectiveness of the WSD algorithm.

Analyzing the water systems obtained by the other authors (Sorin and Bédard, 1999; Mann and Liu, 1999; Jeżowski et al.,

Table 6 – Limiting operational data – Case Study 02.

Process number	C_{in} ($mg\,L^{-1}$)	C_{out} ($mg\,L^{-1}$)	Flowrate (t/h)	Water loss (t/h)	Original process
1	20	60	40	10	Cooling for raw material pump
2	60	100	30	5	Purge for outlet of lime burner
3	20	80	200	50	Cooling for sintering equipment
4	100	200	160	80	Red mud washing
5	20	60	60	20	Cooling for vacuum pump
6	20	80	150	30	Cooling for calcination equipment
7	80	200	70	70	Recirculating water system

Source: Deng and Feng (2009).

Table 7 – Rearranged limiting operational data – Case Study 02.

Process number	C_{in} ($mg\,L^{-1}$)	C_{out} ($mg\,L^{-1}$)	Flowrate (t/h)	Original process
5	20	60	40	Cooling for vacuum pump
5′	20	200	20	Cooling for vacuum pump
1	20	60	30	Cooling for raw material pump
1′	20	200	10	Cooling for raw material pump
3	20	80	150	Cooling for sintering equipment
3′	20	200	50	Cooling for sintering equipment
6	20	80	120	Cooling for calcination equipment
6′	20	200	30	Cooling for calcination equipment
2	60	100	25	Purge for outlet of lime burner
2′	60	200	5	Purge for outlet of lime burner
7	80	200	70	Recirculating water system
4	100	200	80	Red mud washing
4′	100	200	80	Red mud washing

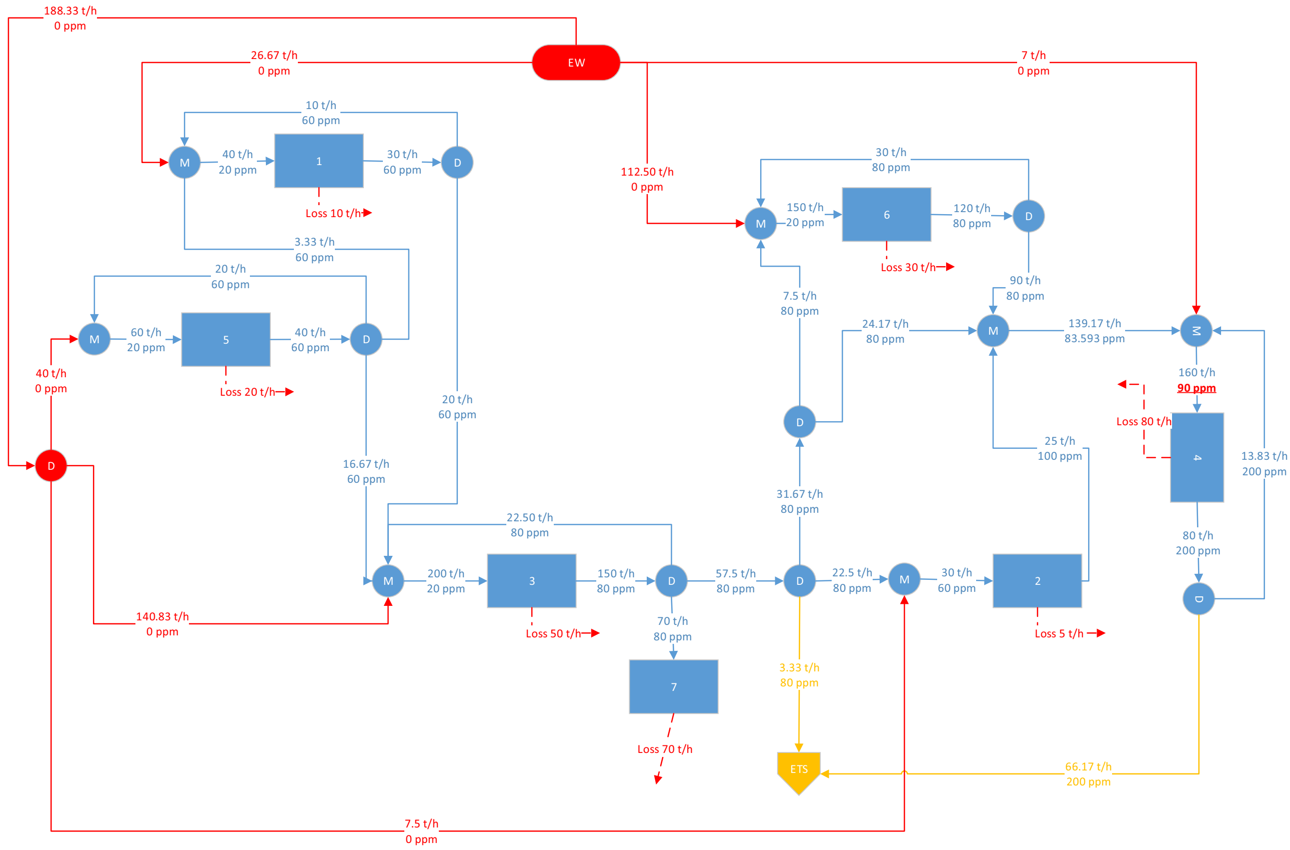

Fig. 10 – Case Study 2. Water system structure for maximum reuse.

2003; Deng et al., 2011), some differences could be noted: (1) the local recycle stream in the cyclone has the same flowrate in the systems proposed by Mann and Liu (1999) and Wang and Smith (1995), and values little higher in the systems of Deng et al. (2011) and Jeżowski et al. (2003); (2) the streams that are used in the reactor come from different operations.

According with Deng et al. (2011) is not advisable to directly reuse the cooling system blow down in the reactor, because it may be contaminated with treatment chemicals and the reactor would be sensitive to such contamination. The direct reuse is present in the structures of Mann and Liu (1999) and Wang and Smith (1995), and also in the structure obtained with the

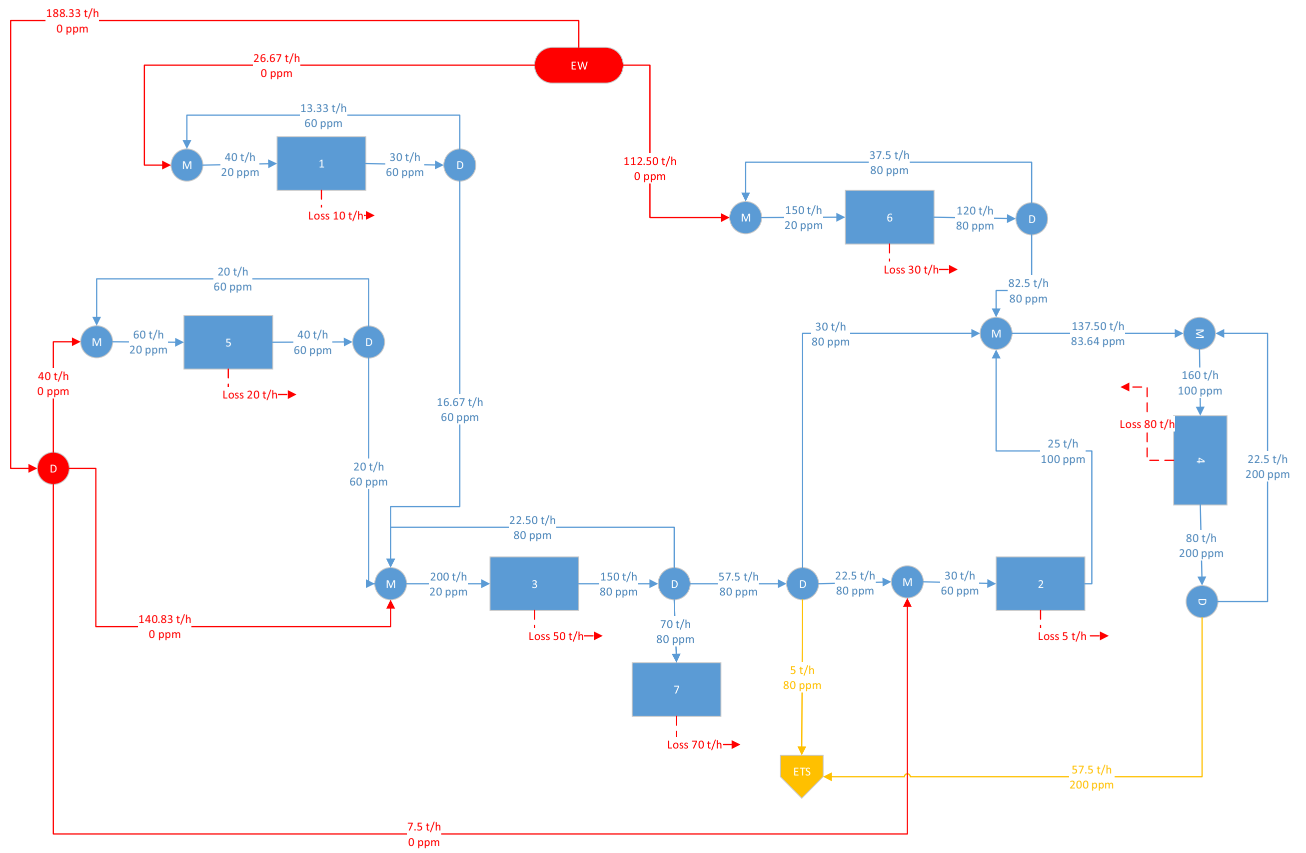

Fig. 11 – Case Study 2. Water system structure for maximum reuse.

Table 8 – Limiting operational data – Case Study 4.

Sinks SK j	C_j (mg L^{-1})	Flowrate F_j (t/h)	Sources SR$_i$	C_i (mg L^{-1})	Flowrate F_i (t/h)
1	0	120	1	100	120
2	50	80	2	140	80
3	50	80	3	180	140
4	140	140	4	230	80
5	170	80	5	250	195
6	240	195			

Source: Sorin and Bédard (1999).

WSD algorithm (Fig. 7). However, it is important to note here that a structure with no direct reuse or even with indirect reuse of this blow down in the reactor can be easily obtained with the WSD algorithm by taking into account along the algorithm the corresponding constrain. We show that in Fig. 8, where the WSD final structure has no indirect reuse and also it does not have streams with flowrates lower than 1 t/h (other possible constrain). The penalty introduced by these constrains is the increase of 1.79 t/h in the consumption of external water. This value is less than the penalty of 5 t/h cited by Deng et al. (2011). Nevertheless, the final structure proposed by Deng et al. (2011) maintains the original external water consumption but has the indirect reused of the blow down in the reactor (through the cyclone).

Case Study 2: The second case study is an industrial case represented by the water system of an alumina plant (Deng and Feng, 2009), which is a large water consumer, represented by seven water using operation, all presenting water loss. It is a hybrid water system with both FL and FF processes, related to cooling operations and washing operations, respectively. According to Deng and Feng (2009), the alumina plant consumes 710 t/h of freshwater, discharges 445 t/h of wastewater and loses 265 t/h of water along the process. The process is described with FF operations, as P1 (cooling for raw material pump), P3 (cooling for sintering equipment), P5 (cooling for vacuum pump), P6 (cooling for calcination equipment) and P7 (recirculation water-system); and FC operations as P2 (purge for outlet of lime burner) and P4 (red mud washing). Its operational data are presented in Table 6, with the corresponding water losses, inlet and outlet concentrations. External pure water at 0 ppm is available. Table 7 shows the addition of equivalent operations. Based on the operational limiting data on Table 7, steps 2 and 3 are performed to obtain the WSD shown in Fig. 9, with the corresponding water network in Fig. 10. It is important to note that the water used in operation 7 cannot be used in another operation, because all the water that enters in this operation is lost. Note also that the pinch point is located at 80 ppm.

There is no violation in the water system of Fig. 10, but the inlet concentration of operation 4 (underlined) is lower than the respective limit in Table 7. When this fact is present in operations which receive external water, an opportunity of external water consumption reduction is present. Alternatively, the constraint violation can be eliminated by increasing the flowrate of the local recycle in operation 1 without increasing the external water consumption, because they have the same concentration. A similar analysis is also possible in operation 6. Fig. 11 shows the final result, where the stream linking operations 5 and 3 to 1 and 6, respectively, are eliminated by recalculating the recycles. It has the external water consumption of 327.5 t/h and an effluent discharge (after mixing) equal to 62.5 t/h at 190.4 ppm, representing a reduction of 53.87% and 85.95% of external water consumption and effluent discharge, respectively. The external water consumption here calculated is equal to the one found by Deng and Feng (2009) applying CTA to obtain the minimum fresh water target and NNA to obtain the water network design for direct reuse. The same result was reported using the unified targeting algorithm (UTA) (Shenoy, 2011), however the network was not generated, only the water targets. These targets were obtained through the construction of UTA table and two limiting composite curves to determine the water and wastewater targets. Here is clear advantage of the applicability of WSD as a simple and easy method to obtain, simultaneously, the targets and the possible networks.

Case Study 3: This case study adds the availability of a regeneration process operating as a centralized treatment to the data of Case 2. This process configuration is used by Deng and Feng (2009) and Shenoy (2012) in the analysis of systems that can potentially render zero water discharge (ZWD). Here this configuration is used to present an initial discussion of how the presence of regeneration processes can be introduced in the WSD algorithm.

According to Wang and Smith (1994), regeneration processes are classified as those with fixed removal ratio or those with fixed outlet concentration. In the former, the outlet concentration is not specified and is a function of the inlet condition of the regeneration process. The fixed outlet concentration regeneration processes are treated as an external source in the WSD algorithm used only after the total use of the actually external source is minimized.

The analysis here presented is restricted to centralized regeneration processes with fixed outlet concentration. In this case, lower outlet concentrations are linked with lower regeneration flowrates, and commonly higher flowrates and lower outlet concentrations imply in higher regenerations costs.

Like Deng and Feng (2009) and Shenoy (2012), the outlet concentration of the regeneration process is here assumed to be 20 ppm, equal to the minimum value required for the operations with nonzero inlet concentration. This value is chosen, because when considering the water system with ZWD the post-regeneration concentration cannot be higher than the minimum limiting inlet concentration of all the operations (Deng et al., 2008).

Comparing with the procedure used in Case Study 02, on step 2, an additional external water source at 20 ppm must be added in the WSD to take into account the regenerated water. Starting step 3, from data of Table 6 and with a global mass balance a necessity of 265 t/h of fresh external water flowrate is obtained. Then, the rules are used and the WSD of Fig. 12 is obtained and the respective water network in Fig. 13. Note that the total mass balance calculated early guarantees that all wastewater streams from operations are treated in the regeneration process.

Comparing this result with the Deng and Feng (2009) and Shenoy (2012), the effluent sent to the regenerator (83.33 t/h–159.92 ppm) has a lower concentration (other authors: 83.33 t/h–162.8 ppm), representing lower cost in terms

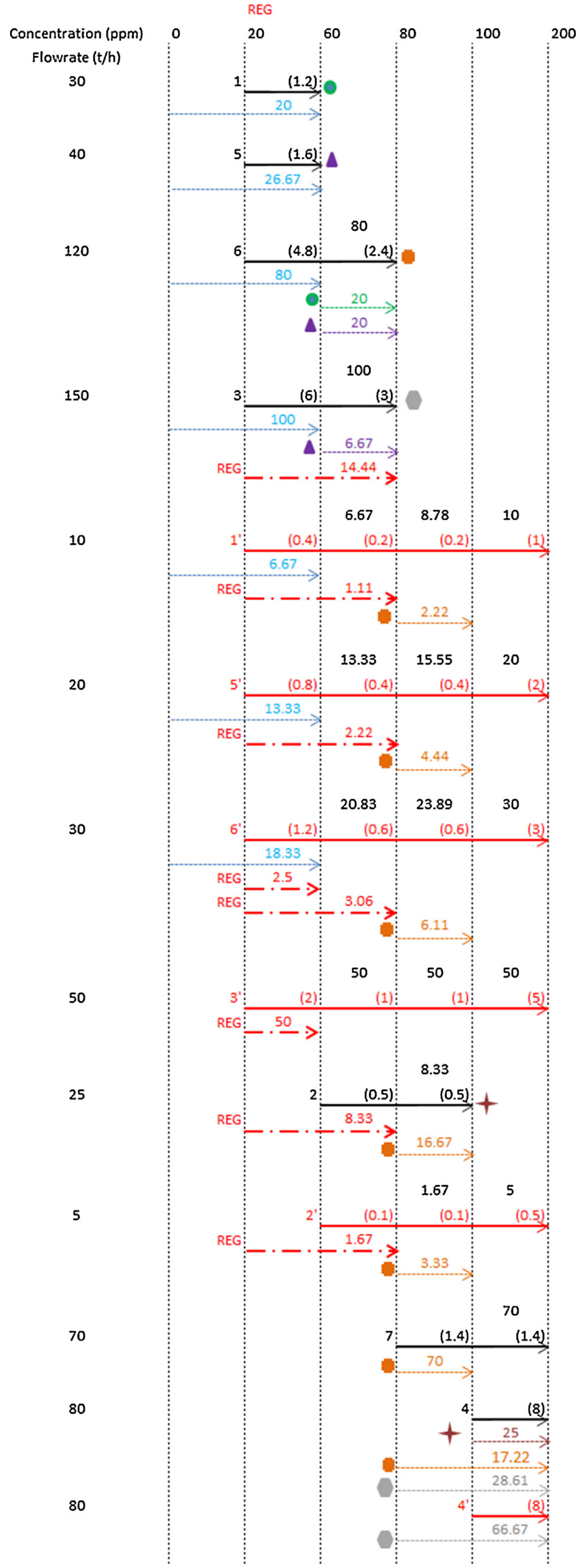

Fig. 12 – WSD with zero water discharge – Case Study 03.

of regeneration to achieve the regeneration concentration goals.

Case Study 4: This Case Study aims to show that processes represented by water sources and sinks can also be treated by the WSD algorithm with small adaptations. The process data

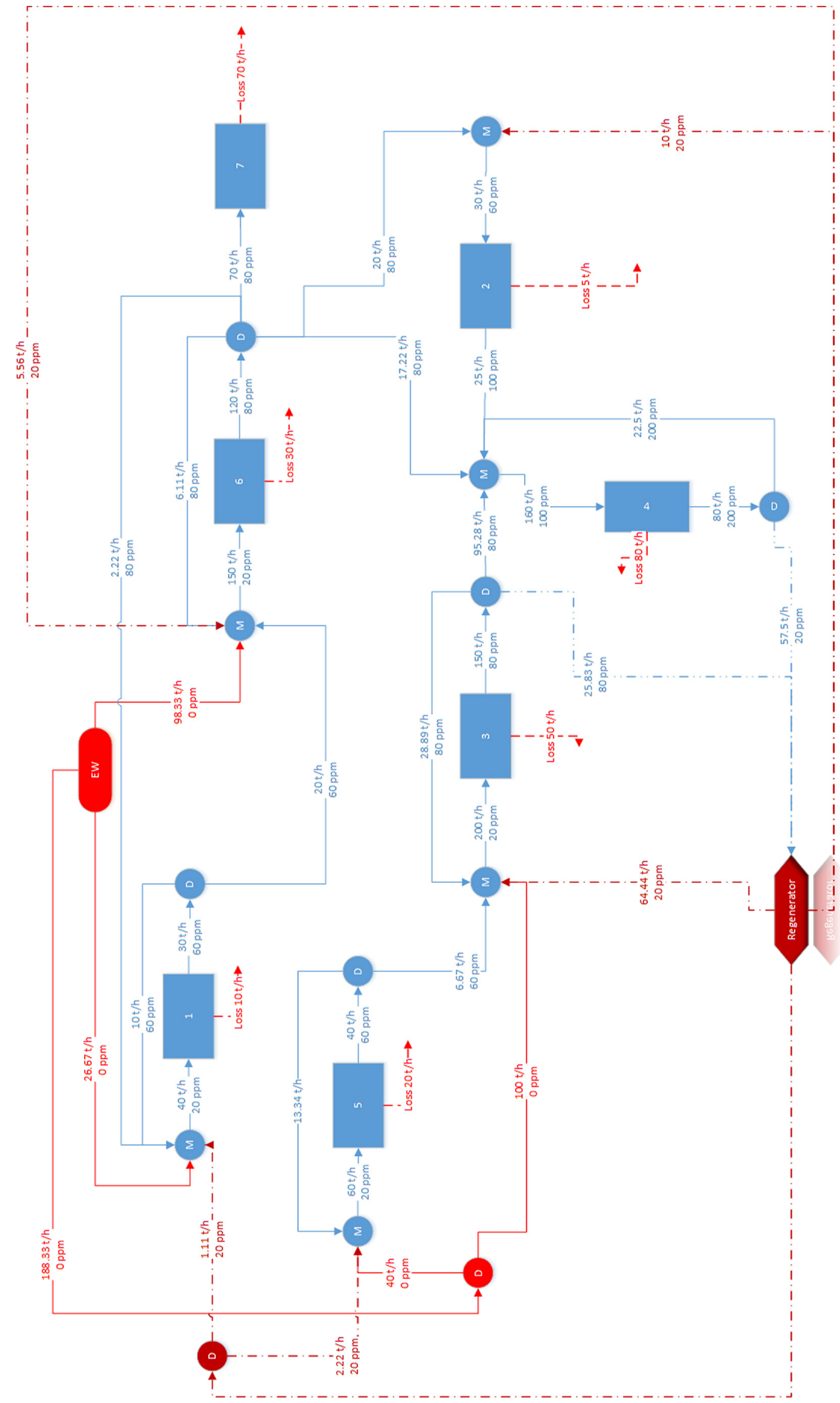

Fig. 13 – Case Study 3. Water system structure for maximum reuse.

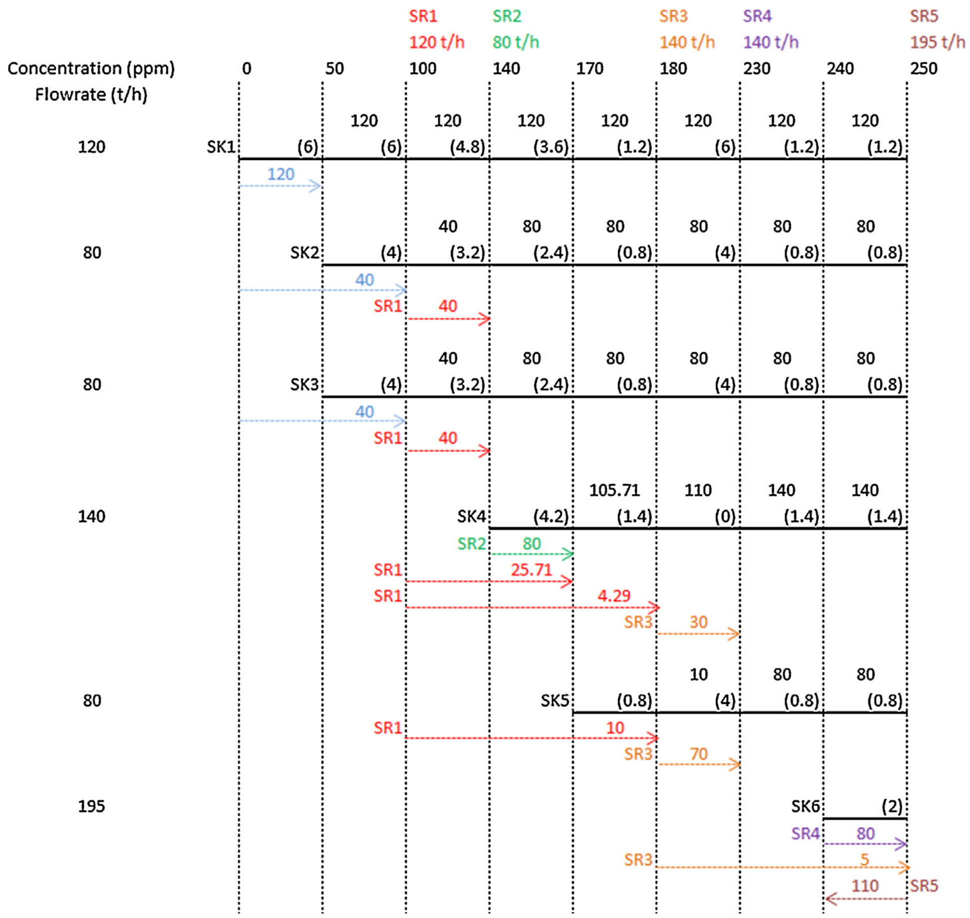

Fig. 14 – Final WSD – Case Study 4.

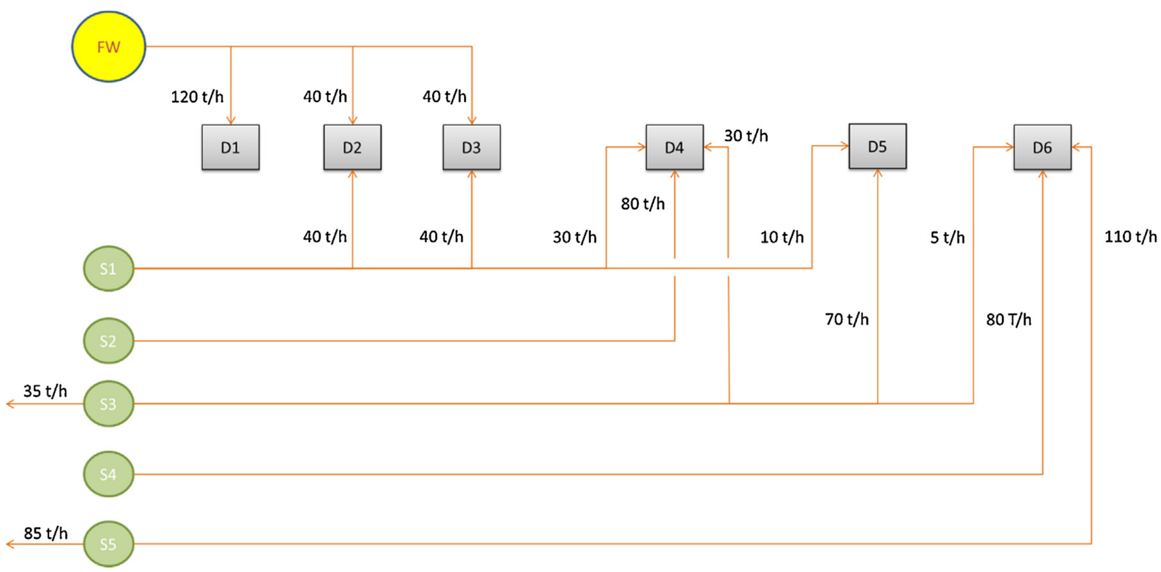

Fig. 15 – Case Study 4. Water system structure for maximum reuse.

are taken from Sorin and Bédard (1999), and are presented in Table 8. The final WSD is shown in Fig. 14 and the corresponding network is shown in Fig. 15.

The WSD obtained is analyzed and when the flowrate in an operation (actual sink) is not achieved (SK6), the source with low and nearest concentration (SR5) is then used to complete the specified flowrate.

The WSD algorithm indicates external water and wastewater flowrates of 200 t/h and 120 t/h, respectively. The same values are reported by other authors using different techniques (Sorin and Bédard, 1999; Hallale, 2002; El-Halwagi et al., 2003; Manan et al., 2004; Prakash and Shenoy, 2005; Ng et al., 2007a; Saw et al., 2010). According to Poplewski et al. (2010) this is the minimum global and they reached this value with a minimum of 14 connections. The same number of connections was obtained by Ng and Foo (2006). Using WSD it is obtained the same targets but with 13 connections. To reach the same number of connections, Poplewski et al. (2010) applied the penalty of 11.43 t/h, while Ng and Foo (2006) applied the penalty of 30 t/h on increasing freshwater

Table 9 – Limiting operational data – Case Study 05.

Process number	Operation	Demand flowrate (t/h)	C_{in} (mg L^{-1})	C_{out} (mg L^{-1})	Water loss (t/h)	Water gain (t/h)
1	Washing/depuration	160	0	45	144.4	*
2	Recovery boiler	400	15	*	400	*
3	Washing filters	200	38.5	*	200	*
4	Acid stage	400	26	379	*	4.5
5	Alkali stage	200	112	483	*	4.7
6	Drying	1000	0	*	1000	*

Source: Marques (2008).

Table 10 – Rearranged limiting operational data – Case Study 05.

Process number	Operation	Demand flowrate (t/h)	C_{in} (mg L^{-1})	C_{out} (mg L^{-1})
1′	Washing/depuration	144.4	0	483
1	Washing/depuration	15.6	0	45
2	Recovery boiler	400	15	*
4	Acid stage	400	26	379
3	Washing filters	200	38.5	*
5	Alkali stage	200	112	483

External water sources	C_{in} (mg L^{-1})	Available (t/h)
EW	12	*
OP6	0	1000
F4	379	4.5
F5	483	4.7

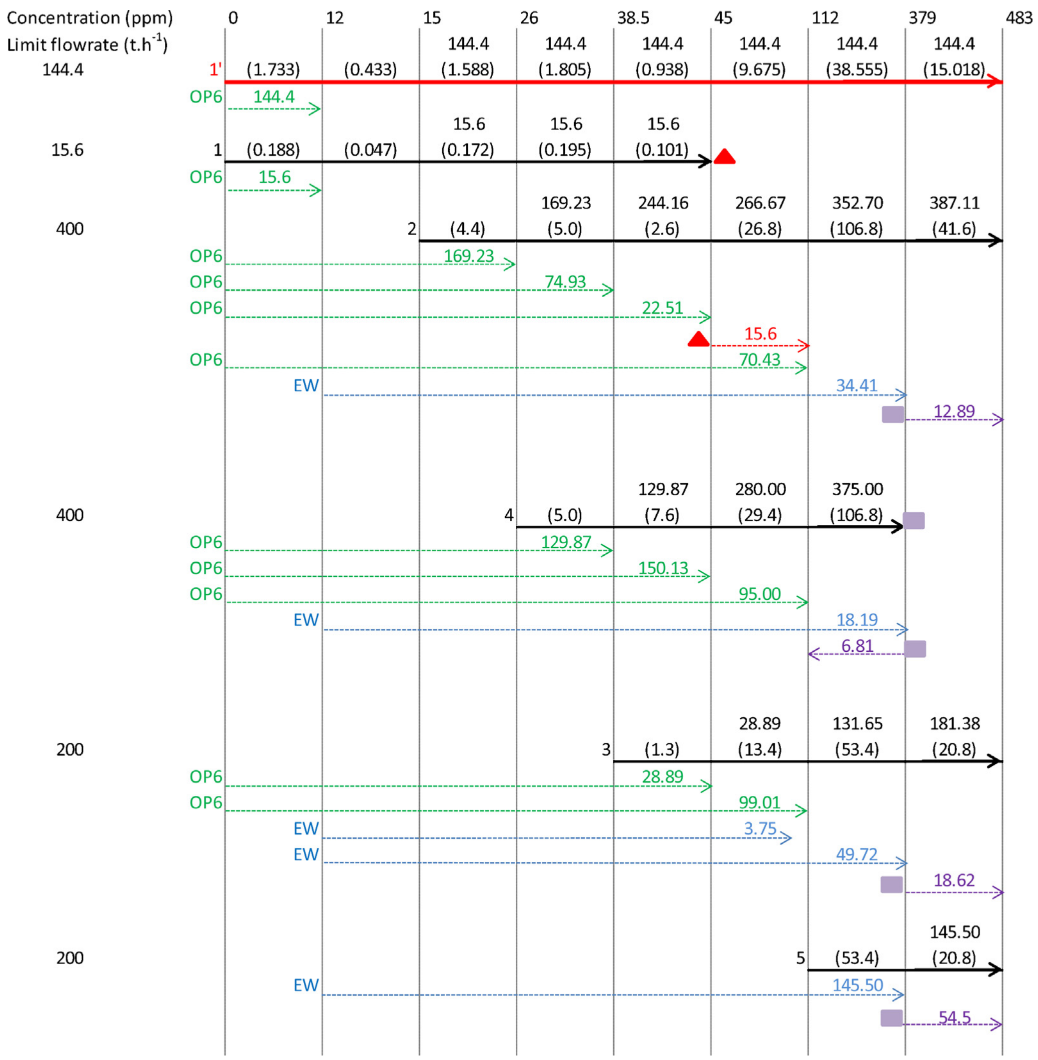

Fig. 16 – Final WSD – Case Study 5.

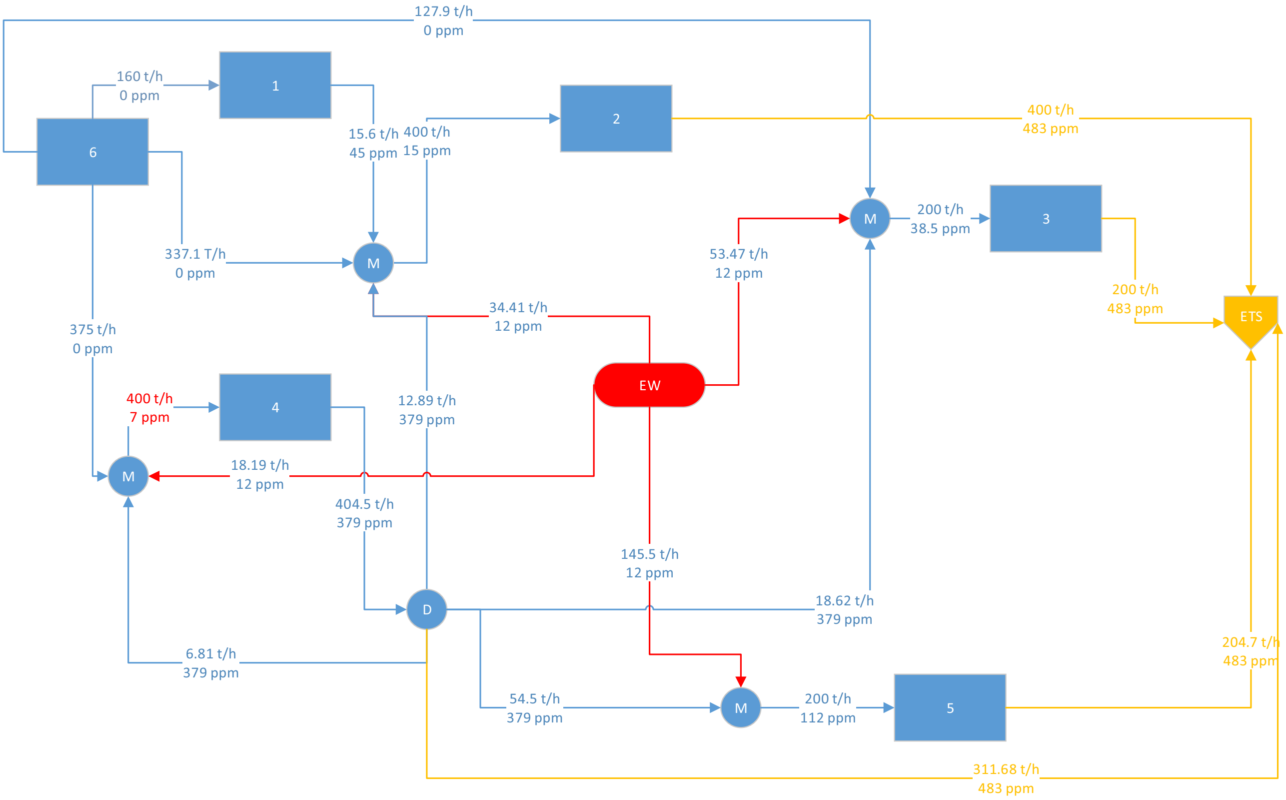

Fig. 17 – Case Study 5. Water system structure for maximum reuse. (For interpretation of the references to color in text, the reader is referred to the web version of the article.)

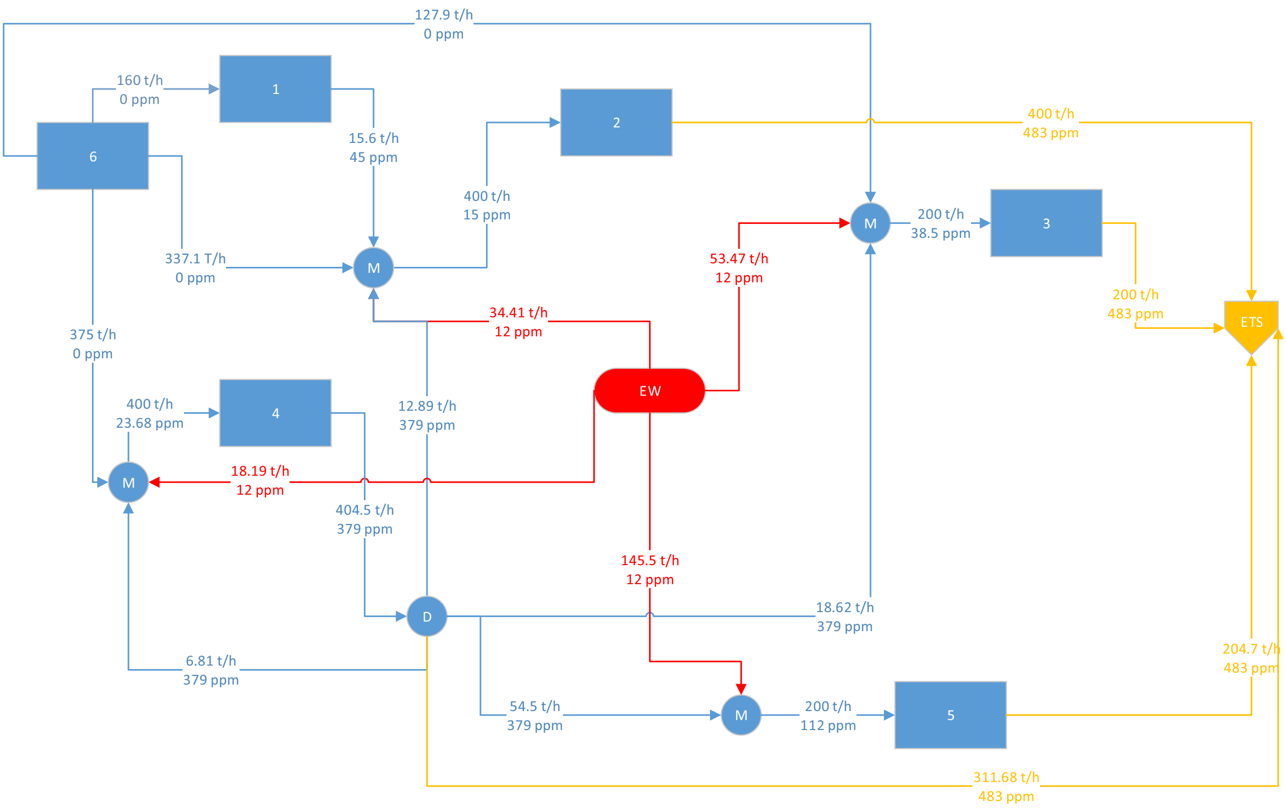

Fig. 18 – Case Study 5. Water system structure for maximum reuse – final result.

consumption. The pinch point (100 ppm) reported by WSD is the limiting pinch point of the problem as reported by others authors (El-Halwagi et al., 2003; Hallale, 2002; Manan et al., 2004).

Case Study 5: This case study involves a retrofit of a Brazilian pulp mill, with real data taken from Marques (2008). The analysis focuses on maximum reuse and only one contaminant is considered: chloride. All the operations are considered as fixed flowrate operations.

The production process of this industry consumes 1360 t/h of freshwater as can be seen in Table 9, which also presents the data for each operation that consumes water. The drying operation is a source of clean water, with limited flowrate. Note that washing/depuration operation has water loss and the alkali and acid stages present water gain. Table 10, shows the rearranged data after adding the equivalent operations and the new sources. An external water source with unlimited flowrate and concentration of 12 ppm is originally available. The source OP6 represents the water gain in drying process, and sources F4 and F5 represents the water gain in the alkali and acid stages, respectively.

Based on data from Table 10 and using the proposed algorithm, the obtained WSD with maximum reuse is presented in Fig. 16 and the correspondent water system structure in Fig. 17.

There is no violation in the water system of Fig. 17, but the inlet concentration in operation 4 (in red) is lower than the respective limit (see Table 9). As commented on Case Study 3, an opportunity of external water consumption reduction is present. This reduction is possible through the increasing of the local recycle flowrate in operation 4–25 t/h, which decreases the external water consumption in this operation to 0 t/h, with inlet concentration equal to 23.7 ppm. Fig. 18 shows the final water system, which has external water consumption of 233.4 t/h and an effluent discharge (after mixing) equal to 1116.38 t/h at 483 ppm, representing a reduction of 82.84% and 8.85% of external water consumption and effluent discharge, respectively.

5. Conclusions

The extension of the WSD procedure for WAPs in single contaminant processes is presented and its application in five different Case Studies shows that this algorithm can be used successfully in several processes, involving fixed contaminant load operations (FL operations), fixed flowrate operations (FF operations), water loss/gain operations, hybrid water systems (with both types of operations), and also in water systems described only by sources and sinks. This extension involves the introduction of equivalent operations and/or water sources to adapt the representation of the FF operations to FL operations, which can be handled using the traditional WSD approach. It is important to note that this extended algorithm keeps the capability of the original one, simultaneously determining a minimum external water consumption goal and synthetizing the respective water system. Moreover, as the WSD procedure can generate different water system structures, its results can be easily adapted to typical industrial constrains.

The broad applicability and simplicity of the extended WSD for FL and FF operations are shown using four Case Studies with data from previous studies of other authors. In all these studies the extended WSD achieves similar results. The fifty Case Study uses real data from a Brazilian pulp mill, showing the WSD application in this industry and obtaining an important proposal to water consumption reduction.

It is important to note that in a study involving cost analysis, a tradeoff in the specification of the regeneration process outlet concentration can be conducted using the WSD procedure by organizing a recursive algorithm.

It is also shown that the WSD algorithm can be used in WAPs focusing zero effluent discharge. An example using regeneration with fixed outlet concentration is presented and the results obtained are similar to the ones obtained by other authors.

Finally, real data of a Brazilian pulp mill was used to show the application of the WSD in this industry. The results showed the possibility of a great reduction of water consumption.

In multiple contaminant problems, the proposed methodology can be applied using the concept of a reference contaminant (see Gomes et al., 2013). Present researches are directed toward a general approach to identify the reference contaminant in order to minimize the work on extending the results based on the reference contaminant to the others ones in multiple contaminants systems.

Acknowledgments

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