Industrial Contaminated Water Network Management Tool

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Abstract

This paper addresses the industrial contaminated water network management problem under the presence of single and multiple contaminants that affect a wide range of industries. The uncontrolled competition for resources is contributing to the increase in industrial production, aimed at supplying the needs of a population of 7 billion, resulting in the generation of effluents and an overall growth of pollution. Governments forced to adopt pollution mitigation strategies to improve water usage efficiency, have legislated water capture and discharge tariffs so as to promote industrial water consumption savings.

The status quo and the complexity of solving such a problem, has provided the opportunity and the motivation to develop software tools to manage the industrial contaminated water networks, based on the water pinch analysis (WPA) methodology and water source diagrams (WSD). Additionally, the developed work allows visualization of the water network diagram (WND), so as to verify the existence of any abnormality in the water flows and the quantities of individual contaminants, so as to evaluate the reuse strategy by calculating the water savings percentage when considered process integration.

Keywords: Industrial Process Integration, Water Network Management, Software Tool, Multiple Contaminants, Water Pinch Analysis

1. Introduction

Water is a scarce and fragile resource where millions of litres can be contaminated with only a drop of a hazardous substance. The growth of industrial production aimed at supplying the needs and lifestyles of the world population, has contributed to the scarcity of natural resources. The unsustainable exploitation of manufacturing a greater variety of products has resulted in an overall growth of pollution and a larger dependency between industries. This has caused major imbalances between the economic, technological and social dimensions of the sustainable industrialization triangle, which impacts by placing pressure on the water.

The world population is expected to grow to 9 billion by 2050, which will lead to a substantial increase in the level of urbanization (UNPF, 2015). The unsustainable growth, in addition to the poor management of the water network, has led to an unfair water distribution across the world, which in some locations has become a commodity. In 2002, the groundwater provided around 65% of water for human consumption in Europe. These reservoirs of water were intensively explored by 60% of the European cities that had committed 50% of wetlands (EC-DGE, 2002).

Water depletion has been encouraged by the absence of water pollution controls, low tariffs applied to the water consumed, and the lack of technological equipment and groundwater catchment restrictions, thus leading to the over exploration of 20% of world aquifers (UNESCO, 2015). This data is alarming since it reveals a pounding water crisis that is translated by the water exploitation index (WEI+) that measures the stress over the hydric resources for each country. The WEI+ index is classified into four categories i) without scarcity, <10%; ii) reduced scarcity, 10-19%; iii) moderate scarcity, 20-40%, and iv) severe scarcity, >40%. Portugal mainland rivers are classified as reduced or moderately stressed, depending on the region (APA, 2015).

Growing concerns on the conservation of natural resources has motivated the governments to shift from the end-of-pipe pollution control strategy to incentive policies for water consumption optimization. This has led to more stringent freshwater capture tariffs and effluent discharge regulations.

A growth of 55% of industrial water consumption is expected by 2050, mainly in the manufacturing and electricity generation (UNESCO, 2015). Industries require large volumes of water to perform their operations, which range from the mass separation agent, heating and cooling utilities to the equipment washing operations. Hence, process integration is a key strategy to minimize the generated effluents and to improve the water consumption efficiency, thereby increasing industries competitiveness.

2. Problem Statement

The industrial contaminated water network management problem can be defined as follows: Given one or many industrial plant processes that use freshwater as a mass separating agent to reduce the concentration of one or more contaminants, determine the water mass exchange network (MEN) that consumes the minimal freshwater, subjected to input and output contaminant concentration bounds as well as water inflow and outflow constraints for each process. Freshwater is considered as the only external water source at 0 ppm and reutilization is the process integration strategy to evaluate.

The purpose of the current paper is to develop the industrial contaminated water network management software tools that implement a contaminant water network management methodology in order to deal with processes that operate in continuous mode for single and multiple contaminants, so as to provide this utility to a maximum number of industries.

3. European Legislation

Over decades, the water abundance, low tariffs and low penalties led to excessive exploration of the water resources which aggravated the scarcity of freshwater because of its contamination by agricultural and industrial units. Since 1975, a lot of effort has been put forth by Europe in order to attenuate and whenever possible, to revert some of the environmental damages caused, through the development of strict measures to sensitize industries and citizens (EC-DGE, 2016). These measures are published in the directives (European Union) and decree-laws (Portugal) which include the definition of exploitation protection zones, the control of volume and pollution level of rivers, the control of climate changes by imposing the allowed limit values for industrial emissions, and finally the development of a pricing system to guarantee that the clean water is kept clean and the polluted water gets cleaned.

3.1. Exploration licensing

The excessive exploration of superficial and groundwater, increased the governments' awareness to invest in the sustainable consumption which resulted in the legalization process of water catchment. For this reason, companies are now required to strictly obtain licenses according to their purpose, since its absence will compromise their activities. The Hydrographic Regional Administration (HRA) became responsible for the duties on taxation and licensing in the hydric resources domain (DR, 2008a). The Decree-Law 46/96 established that only water catchments with extraction equipment and well depths greater than, respectively, 5 horse-power and 20 meters require licensing. In 2017, the annual cost to obtain the license is 1798.27€.

3.2. Protective area delimitation

For groundwater capture, the perimeter delineation criteria were disclosed in Decree-Law 382/99 of 22 of September (DR, 1999) in order to prevent, reduce and control the accidental discharges and aquifers pollution from contaminated water infiltrations. These zones are defined based on the hydrogeological methods that consider the well conditions and the explored aquifer system characteristics. Protective areas are delimited and divided into: i) immediate, ii) intermediate and iii) extended zones (DR,1999). The first delimitation zone directly protects the water origin and depends on the capture morphology, the pressure from anthropological activities and the water quality characteristics. The second zone is based on the aquifer geological conditions, with a focus on the elimination of groundwater pollutants that have a permanence of 50 days. The third protective zone ensures that the groundwater quality is not affected by the presence of persistent pollutants such as organic compounds, radioactive materials and heavy metals for a permanence of 3500 days. The fixed radius method is a common approach to determine the protective area radius.

3.3. The water pricing system

The extensive use of water led the European Union governments to develop sustainable policies in order to penalize who pollutes most, which is known as the polluter pays principle. The National Water Plan approved in 2002, promoted the construction of drainage systems and the domestic and industrial effluent treatment infrastructures as industries faced problems related to inefficient technologies and water treatment systems. The Decree-Law 97/2008 (DR, 2008) developed a tariff system for the hydric resources exploration as a sum of five water charges including the private water usage of State domain, direct or indirect effluent discharge, inert materials extraction of State domain, land and water occupation plans of State domain, and private utilization, regardless of the nature that is subjected to planning. Later, the Water Framework Directive (EC-DGE, 2016) developed a tariff system, indexing water volume usage to the pollution produced to river basins, as a mean to encourage the efficient use of hydric resources, to prevent excessive catchment and to increase the competitiveness of industrial sectors as well as to recover the supply and treatment service costs which encompasses the water capture, storage, distribution to sewage.

3.4. Discharge licensing

The request for effluents rejection is presented in the document of APA (2003). The license is requested by identifying the applicant, followed by the usage characterization, the wastewater origin identification, the residual water allocation for sewage treatment plants, definition of discharge points, the receptor medium, the area of public domain, and the total area required for the industrial project as well as the technical data.

3.5. Emission limit values

The emission limit value (ELV) corresponds to the maximum value for a substance that degrades the physical, chemical, biological and microbiological parameters that define the aquatic environment quality. The ELV must not be exceeded since it is the allowed value for an industrial installation emission to ground or water over a specified period of time. Decree-Law 236/98 establishes the limits beyond which the infringements levy a heavy penalty.

4. Literature Review

The literature on water network management concerning single and multiple contaminants, is classified into two groups: the water pinch analysis and the water allocation problem. The methodologies are divided into techniques for continuous plants assuming a steady state operation and those for batch plants where sources and sinks occur at different points in time, thus requiring water storage and proper activities' scheduling. The current literature review focuses steady state continuous plants based on the water pinch analysis.

The decade of 1980 is marked as the period for concerns for resources conservation. Since then, industries have changed their pollution control strategies from the end of pipe to the water minimization approach. The process integration is defined as the analysis and optimization of large and complex industrial process systems, unit operations and their interactions to maximize the effective use of energy, water and raw materials (NRCAN, 2003). Aimed at reducing the water consumption, it can be achieved in three different forms, specifically: i) water reuse corresponding to direct use of effluents in other operations that may or not be mixed with freshwater to deliver an acceptable level of contamination (Souza *et al.*, 2009); ii) regeneration which involves the partial removal of contamination in the effluent that may be followed by reuse or recycle (Relvas *et al.*, 2004); and iii) process changes by replacing the inefficient equipment (Castro *et al.*, 1999).

Process integration surfaced with the introduction of pinch technology by Linnhoff and Vredeveld (1984). It was first applied to recover heat, and later extended to other areas of process engineering such as water recovery by El-Halwagi and Manousiouthakis (1989), to achieve financial savings by reducing the load of external utilities. In heat exchanger network, the heat is transferred from hot to cold streams. The same reasoning is applied to water networks where the process deals with rich and lean streams defined by its contamination. Later, the limiting water profile was introduced by Wang and Smith (1994) to obtain the minimal water targets for reuse, regeneration-reuse and regeneration-recycle before designing the networks for single and multiple water structures.

The above work concerns fixed load operations for single contaminant networks. Dhole *et al.* (1997) proposed the demand (inlet streams) and source (outlet streams) composite curve to deal with non-mass transfer operations such as reactors and cooling or heating utilities, to account for water losses. Castro *et al.* (1999) developed a targeting methodology for reutilization and regeneration-reuse to deal with single contaminant water networks. Three targeting methods such as mass problem table (MPT), limiting composite curve (LCC) and water source diagram (WSD) are presented. This work introduces the concept of multiple pinch point to overcome the water unavailability at the outlet of the regenerator to perform the mass exchange. A new concept of water surplus diagram was first introduced by Alves (1999) to analyse hydrogen distribution networks in refineries based on the design of demand and source composite curves. Hallale (2002) extended this work for application to water networks.

Most of the work was confined to the reutilization strategy. Relvas *et al.* (2004) developed a Non-Linear Program (NLP) model resorting to GAMS, to determine a set of design parameters for regeneration-reuse. The alfa concept is introduced, corresponding to limiting flowrate fraction before regeneration occurs. The minimal flowrate, water streams at the inlet and outlet of a regenerator, the regenerated pinch and the rejected effluents targets are obtained with NLP and integrated into WSD of AquoMin software developed by Castro *et al.* (1999).

Manan *et al.* (2004) addresses the numerical technique, known as Water Cascade Analysis (WCA), to establish the minimum water targets prior to network design. The trial-and-error iterative step of Hallale (2002) is eliminated by using WCA to achieve those targets and obtain the single or multiple pinch points. Although both approaches seem to obtain the same results, the water surplus diagram does not give the wastewater flowrate. Whenever a process change occurs, WCA not only demands less computational effort since targets are obtained by recalculating the values in a tabular form but can also deal with mass and non-mass transfer operations, respectively quality and quantity controlled.

The heuristic algorithm of WSD for reutilization is explored by Gomes *et al.* (2007) to deal with single contaminant networks. The synthesis of water mass network seeks to minimize the waste generated by allocating the water sources based on three rules: i) freshwater is brought to process if there are unavailable internal sources; ii) maximum possible contamination is transferred within each interval; and iii) operation division should be avoided given that the water streams must continue until the end of an operation. This work includes the presence of multiple water sources, reuse with water losses, regeneration-reuse and regeneration-recycling. Thereafter, the pinch points, minimum freshwater and regenerated water targets are obtained recurring to the proposed algorithm on the final stage of design. Gomes *et al.* (2013) developed a graphical procedure for multiple contaminants water networks, the water source diagram, to help process engineers to cope with and identify reuse possibilities in complex industrial processes. In authors work, the water mass exchange network is simultaneously synthesized while the minimum targets are obtained. The linearity of mass transfer between all contaminants had been adopted by Gomes *et al.* (2013) to account the simultaneous transfer of contamination for each operation.

A lot of effort has been put on the development of new wastewater allocation methods using mathematical models in order to solve the multiple contamination industrial water networks. However, there are no readily available software tools to manage and optimize the contaminated water networks. This has motivated our development of two graphical software tools, WaterGain and WaterGain+, which are based on the methodology proposed in Gomes *et al.* (2013). The main goal of these software tools is to assist industrial experts in analysing the actual network, identifying current opportunities to increase the water consumption efficiency and to verify any abnormality in the water flows and the contamination levels.

5. Industrial Case Study

Under this section, the algorithm of Gomes *et al.* (2013) is detailed for the reutilization strategy. The example shown in table 1 is taken from Doyle and Smith (1997) and concerns a petroleum refinery that has three water using operations and three contaminants, specifically hydrocarbon (A), H_2S (B) and salt (C).

Table 1 Limiting operational data

Operation	Contaminant	$C^{in,max}$ (ppm)	$C^{out,max}$ (ppm)	Flowrate (t/h)
1	A	0	15	45
	B	50	400	
	C	20	35	
2	A	20	120	34
	B	300	12500	
	C	45	180	
3	A	120	220	56
	B	20	45	
	C	200	9500	

Industrial processes generate a lot of effluents with different percentages of pollutants, especially in the oil refineries where the composition of crude varies according to the capture regions. In the absence of integration, the amount of freshwater required by each operation is calculated per contaminant, based on the maximum outlet concentration and the mass load transfer, considering a freshwater concentration of 0 ppm as the maximum inlet value, $\Delta m = F\Delta C$. The absence of process integration implies a higher freshwater consumption of 133.00 t/h, which is the sum of the most restrictive water required per process in order to perform each operation.

5.1. Reutilization

The water source diagram construction for multiple contaminants depends on the reference contaminant as well as the reference operation identification which is the first step of the algorithm. The contaminant having the lowest maximum inlet concentration in more process units is taken as the reference since it is the most restrictive. At first glance from table 1, contaminant A or B could be the reference contaminant. However, only A obeys the monotonic increase rule introduced by Savelski and Bagajewicz (2003), which establishes the increase of outlet concentrations throughout operations. Therefore, A is the reference contaminant. In addition, operation 1 is taken as the reference operation since it requires the cleanest water.

The second step consists of adjusting the non-reference contaminant concentrations in the reference operation. To begin, all reference inlet and outlet concentrations are written in the first row of table 2. Furthermore, as the maximum inlet concentrations of the non-reference contaminants, B and C, in the reference operation are not equal to the clearest water concentration, it is necessary to proceed with their inlet concentration adjustments to 0 ppm as shown in the second and third rows by using square brackets. Focused on maintaining the quantity of mass transferred, the respective outlet concentrations need to be calculated using a linear equation called mass transfer ratio. First, the $K_{A,B,1} = \Delta C_{B,1}/\Delta C_{A,1}$ is computed in order to obtain the outlet concentration of contaminant B, $K_{A,B,1} = (C_{B,1}^{out} - 0)/\Delta C_{A,1}$. The same reasoning is applied for contaminant C.

Table 2 Adjusted values of H_2S (B) and salt (C)

Contaminants	C^{in} (ppm)			C^{out} (ppm)		
A	**0**	**20**	**120**	**15**	**120**	**220**
B (op. 1)	[0]			[350]		
C (op. 1)	[0]			[15]		

In the third step, are evaluated the opportunities for the reutilization of water streams for non-reference operations, based on the condition $C_{c,out1} \leq C_{c,ink}\ \forall_{k,\ni k\geq 2}$. If the inequation returns true, the flow concentration requirements are met. This means that there is no need for further adjustments and hence, the flowrate becomes available to reuse in the reference operation at the outlet concentration. Nevertheless, if the condition is not met for more than one contaminant, the adjustments are made based on the contaminant that presents the worst condition in most operations. As per table 3, the reference contaminant will be adjusted in step 4 based on the concentrations of contaminant B for the operations 2 and 3.

Table 3 Identification of the need for adjustments

$C_{A,out1} \leq C_{A,in2}$	$C_{B,out1} \leq C_{B,in2}$	$C_{C,out1} \leq C_{C,in2}$
$15 \leq 20$	$400 \leq 300$	$35 \leq 45$
$C_{A,out1} \leq C_{A,in3}$	$C_{B,out1} \leq C_{B,in3}$	$C_{C,out1} \leq C_{C,in3}$
$15 \leq 120$	$400 \leq 20$	$35 \leq 200$

In step 2, were adjusted the concentrations of the contaminants in the reference operation. In the fourth step, the mass transfer ratios presented in table 4 are used to proceed with the non-reference operation concentration adjustments, based on the contaminants identified in step 3.

Table 4 Concentration diference ratios

$$K_{A,B,1} = \frac{400-50}{15-0} = 23.3 \qquad K_{A,C,1} = \frac{35-20}{15-0} = 1$$
$$K_{A,B,2} = \frac{12500-300}{120-20} = 122 \qquad K_{A,C,2} = \frac{180-45}{120-20} = 1.35$$
$$K_{A,B,3} = \frac{45-20}{220-120} = 0.25 \qquad K_{A,C,3} = \frac{9500-200}{220-120} = 93$$

First, it is computed the adjusted value of the reference contaminant with respect to the inlet concentration of contaminant B by using the ratio $K_{A,B,1}$ which is based on the reference operation mass transfer. Thereafter, the reference contaminant concentration corresponding to the inlet concentration of contaminant B, is calculated using the ratio $K_{A,B,1} = (C_{B,1}^{out} - C_{B,2}^{in})/(C_{A,1}^{out} - C_{A,1}^{in,adj})$. Once the inlet concentration was changed and this algorithm assumes that the mass transfer is maintained linear, it is required to determine the adjusted value of the reference contaminant of the outlet concentration of contaminant B by using $K_{A,B,2} = (C_{B,2}^{out} - C_{B,2}^{in})/(C_{A,1}^{out,adj} - C_{A,1}^{in,adj})$. The results are shown in table 5 within the square brackets. To conclude, we now repeat the same reasoning for the operation 3.

Table 5 Adjusted inlet and outlet concentration based on the non-reference operations

Pollutant	C^{in}			C^{out}		
A	**0**	**[10.7]**	**[0.84]**	**15**	**[110.7]**	**[100.84]**
B (op. 1)	0			350		
B (op. 2)		300			12500	
B (op. 3)			20			45

Table 6 gathers the adjusted inlet and outlet concentration values based on the required adjustments, identified in the fourth algorithm step. The data is aggregated for contaminant A which is the reference contaminant. In the fifth step, the water source diagram (WSD) is generated.

Table 6 Data for the water source diagram design

Operation	Contaminant	$C^{in,max}$	$C^{out,max}$	Flow rate
1	A	0	15	45
2	A	10.7	110.7	34
3	A	0.84	100.84	56

The water source diagram construction is similar to single contaminant networks where the generation steps are explained in detail in Gomes *et al.* (2007). According to the results obtained with the WSD, the water network is designed in step 6 as shown in figure 4. A concentration balance is performed for each mixer in the water network.

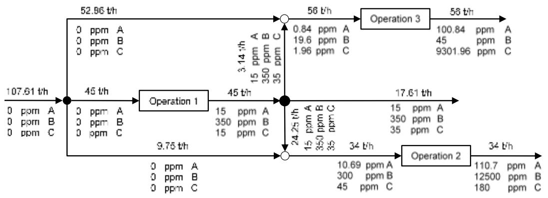


Figure 4. Water network with reuse for table 1 example

After the MEN design, concentration values are inspected by comparing with the original limiting data provided in table 1 to evaluate if the maximum limits are exceeded. Once all values are below or equal to the limiting values, figure 4 is the final water mass exchange network with a minimal freshwater consumption of 107.61 t/h. Thereby, it is not required to proceed for step 7 so as to obtain the optimized water network.

Whenever the concentration limits are not met, there are two possibilities to remove those violations, namely: i) increase the freshwater in case of an operation being supplied by external water, or ii) redirect the water flows upstream to the operation where the flaw will occur if the operation does not receive freshwater directly. This is an iterative step until the maximum inlet and outlet concentration values are not exceeded.

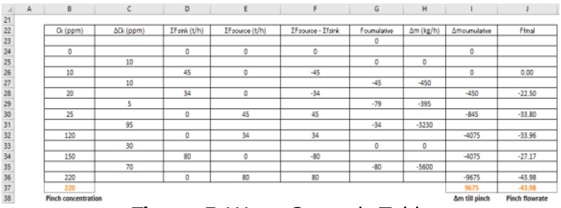
6. Software Tools

The process integration involves introducing process modifications, reuse water streams, water treatment at the source, implement distributed treatment and select the final discharge method to take advantage of the water bodies capacities to receive the water discharged. This work focuses on the reutilization of water streams within an industrial plant. The water reutilization corresponds to direct use of effluents in other operations. The sewage may be mixed with freshwater and/or effluents supplied from other water using operations to result in an acceptable level of contamination, without interfering with the new mass transfer (Souza *et al.*, 2009). This research developed two software tools, which are accessed by executing two macro-enabled workbooks: WaterGain for single contaminant and WaterGain+ for multiple contaminant water networks with reutilization for continuous operating processes. Both software tools deal with fixed load operations wherein the focus is to remove a specific amount of contamination from the water streams, which is controlled by equation 1.

$$\Delta m = F * (C^{out} - C^{in}) \quad (1)$$

6.1. WaterGain

The WaterGain software generates the Water Cascade Table (WCT) for the network with reuse as in figure 5. The WCT shows the concentration levels, the total water demand and source flowrates and the cumulative net water required. The cumulative mass load, in kg/h, is calculated to determine the pinch concentration and the optimal water cascade that ensures the minimal external water consumption.



Ck (ppm)	ΔCk (ppm)	ΣFsink (t/h)	ΣFsource (t/h)	ΣFsource - Σfsink	Fcumulative	Δm (kg/h)	Δmcumulative	Ffinal
					0			
0		0	0	0			0	
	10				0	0		
10		45	0	-45			0	0.00
	10				-45	-450		
20		34	0	-34			-450	-22.50
	5				-79	-395		
25		0	45	45			-845	-33.80
	95				-34	-3230		
120		0	34	34			-4075	-33.96
	30				0	0		
150		80	0	-80			-4075	-27.17
	70				-80	-5600		
220		0	80	80			-9675	-43.98
220							9675	-43.98
Pinch concentration							Δm till pinch	Pinch flowrate

Figure 5. Water Cascade Table

The WaterGain generates the Water Source Diagram (WSD) as presented in figure 6, wherein the total freshwater requirement must equal the target obtained à priori with the WCT. In the WSD, the mass load transferred and the external water source consumption are shown in tons per hour, and the evolution of the contamination in ppm, along the network for each of the operations configured.

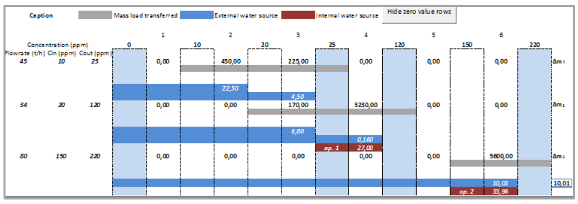


Figure 6. Water Source Diagram

Calculations made for the construction of the WSD are shown so one may perform validations and see the detailed calculations. For each operation, are shown the aggregated flows per interval and the available water for reutilization in tons per hour. The material requirement planning (MRP), which is an integrated system of production planning and inventory control, has been extended and used in the WaterGain software to deal with water systems. The output includes the freshwater requirements per operation and the water streams reutilization from one operation to another. The WaterGain software also projects the Water Network Diagram (WND) as presented in figure 7. The WND shows the water consumption in tons per hour (plotted above the connecting links), and the contaminant concentration in ppm (plotted below the connecting links) between the operations. A comparison of the water savings obtained with and without reutilization is generated.

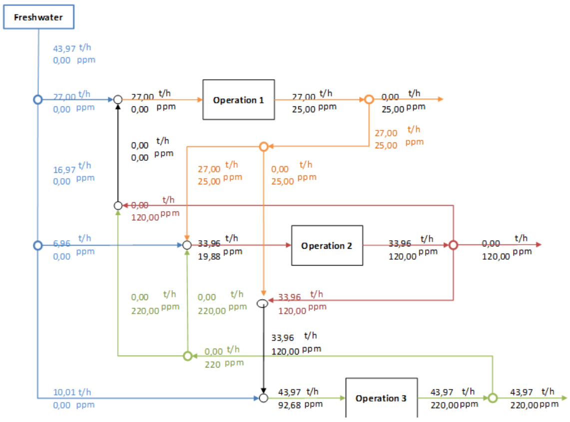


Figure 7. Water Netw ork Diagram

6.2. WaterGain+

An overview of the sequential utilization of the software tool and interpretation of the respective outputs to evaluate the reutilization opportunities are presented in the current section. The user starts by introducing the number of operations and contaminants (green area) as shown in figure 8.

	A	B	C	D
3				
4		Number of operations		4
5				
6		Number of contaminants		3

Figure 8. Select number of operations and contaminants

Thereafter, the Cartesian product of cells D4 and D6 is calculated in order to build the table with the maximum operational data which is instantly generated after the "Create table" button has been clicked. Posteriorly, the user must click on "Insert data" button so as to introduce the general information such as operations, contaminants and mass load transferred. This software feature is intended to save the time of industrial experts, by avoiding the manual introduction of these values, which is cumbersome when large number of operations and/or contaminants are involved. A maximum of 26 contaminants are permitted, which is the number of alphabet letters as defined by arrayC(26). The user has to introduce the limiting flowrate (t/h) and the maximum inlet and outlet concentrations (ppm) data. Thereby, the button "Insert data" must be clicked again to update the mass load transferred (t/h). Figure 9 presents the operational data table, obtained with WaterGain+.

Operations	Contaminants	Limiting flowrate (t/h)	Mass load transferred (kg/h)	Maximum inlet concentration (ppm)	Maximum outlet concentration (ppm)
1	A	34	5440	0	160
1	B	34	15300	0	450
1	C	34	1020	0	30
2	A	75	7500	200	300
2	B	75	12750	100	270
2	C	75	18000	500	740
3	A	80	40000	300	800
3	B	80	37600	460	930
3	C	80	40000	400	900
4	A	20	12800	600	1240
4	B	20	11000	850	1400
4	C	20	23800	390	1580

Create table

Insert data

Figure 9. Limiting operational data

For multiple contaminant water networks, the WSD is developed based on the reference contaminant starting from the reference operation which demands water of pure quality. In order to meet these rules, step1 must be performed to identify which pollutant has the lowest maximum inlet concentration in more processes, so that we reuse water at lower contamination and later determine the equivalent concentration of non-reference contaminants. From figure 10, cells B12 to G15 is a verification table to compare if the contaminant with the higher value of count, is taken as the reference contaminant. Thereby, A is taken as the reference pollutant as well as the first operation is taken as the reference operation. One of the assumptions made in the software tool construction is the availability of at least one operation requiring freshwater to perform the mass exchange.

	A	B	C	D	E	F	G
3							
4		Reference operation					
5							
6		Reference operation	1				
7							
8		Reference contaminant					
9							
10		Reference contaminant	A				
11							
12		Contaminants|Operations	1	2	3	4	Count
13		A	1	0	0	1	2
14		B	0	1	0	0	1
15		C	0	0	1	0	1

Figure 10. Reference operation and contaminant

The second step of WaterGain+ consists of scaling the inlet concentration for each non-reference contaminant in the reference operation to 0 ppm. As the input concentration values were changed, and assuming a linear relationship of contamination transferred in order to guarantee the same amount of contaminant exchanged, the concentration of the outflow has to be calculated. The difference between the outlet and inlet concentrations in figure 8 of the corresponding operation and contaminant, gives the adjusted outlet concentration value for the non-reference contaminants as seen in figure 11.

	A	B	C	D	E	F	G	H	I	J	K
6											
7		Operation	Contaminants	1	2	3	4	1	2	3	4
8		1	A	0.00	200.00	600.00	300.00	160.00	300.00	1240.00	800.00
9		1	B	0.00				450.00			
10		1	C	0.00				30.00			

Figure 11. Adjust reference operation inlet concentration

In order to maintain the equivalence between all concentrations values with respect to the reference operation, the focus shifts to the non-reference operations in order to evaluate the reutilization opportunities. Therefore, an adjustment of the concentrations is required whenever the outlet concentration for a given pollutant in the reference operation is higher than the admissible value at the entrance of other operations, which means that the stream reutilization becomes unfeasible as shown in figure 12. However, if the above condition is not met for more than one contaminant, the selection is based on the contaminant that presents the worst condition that is the pollutant with the highest value of count.

	Reference operation	1	1
Operations	Contaminants	B	C
2	B	1	-
2	C	-	0
3	B	0	-
3	C	-	0
4	B	0	-
4	C	-	0
	Count	1	0
	Contaminant adjust	B	

Figure 12. Adjust non-reference pollutant concentrations

In figure 13, are calculated the key mass transfer ratios that ensure the linearity of the contamination exchange. Those ratios are used to proceed with the inlet and outlet concentration adjustments, based on the contaminant and operation previously identified.

	Non-reference	1	1	1	2	2	2	3	3	3	4	4	4
Reference		A	B	C	A	B	C	A	B	C	A	B	C
1	A	-	2.81	0.19	-	-	-	-	-	-	-	-	-
1	B	0.36	-	0.07	-	-	-	-	-	-	-	-	-
1	C	5.33	15.00	-	-	-	-	-	-	-	-	-	-
2	A	-	-	-	-	1.70	2.40	-	-	-	-	-	-
2	B	-	-	-	0.59	-	1.41	-	-	-	-	-	-
2	C	-	-	-	0.42	0.71	-	-	-	-	-	-	-
3	A	-	-	-	-	-	-	-	0.86	1.86	-	-	-
3	B	-	-	-	-	-	-	1.16	-	2.16	-	-	-
3	C	-	-	-	-	-	-	0.54	0.46	-	-	-	-
4	A	-	-	-	-	-	-	-	-	-	-	0.94	1.00
4	B	-	-	-	-	-	-	-	-	-	1.06	-	1.06
4	C	-	-	-	-	-	-	-	-	-	1.00	0.94	-

Figure 13. Key mass transfer ratios

According to figure 12, it is known the unfeasibility of operation 2 reusing water from operation 1 due to the higher level of contamination, which is expressed by a binary of 1. The main goal of the adjustment, is to obtain both concentrations in the same scale, which is indexed to the reference contaminant. Thereby, the inlet concentration of A in the second operation is determined by using the key mass ration $K_{B,A,1} = 2.81$ (cells E9) based on the mass conditions of reference operation. The corresponding adjusted outlet value of A in the second operation, is calculated based on the mass exchange from operation 2, which is expressed by $K_{B,A,2} = 1.70$ (cell H12). The results obtained with WaterGain+ are presented in figure 14.

Operation	Contaminants	1		2		3		4		1		2		3		4
All	A	0	35.56	200		300		600		160	135.56	300		800		1240
1	B	0								450						
1	C	0								30						
2	B		100								270					
2	C			500								740				
3	B					460								930		
3	C					400								900		
4	B							850								1400
4	C							390								1580

Figure 14. Reference contaminant concentrations scaling for reuse

The data is aggregated for the reference contaminant which is similar to the limiting operational data of the WaterGain software. Figure 15 shows the limiting data required for the construction of the WSD.

Operations	Contaminants	Limiting flowrate (t/h)	Mass load transferred (t/h)	Maximum inlet concentration (ppm)	Maximum outlet concentration (ppm)
1	A	34.00	5440.00	0.00	160.00
2	A	75.00	7500.00	35.56	135.56
3	A	80.00	40000.00	300.00	800.00
4	A	20.00	12800.00	600.00	1240.00

Figure 15. Limiting operational data for WSD

WaterGain+ software now performs the calculations in order to construct the WSD, which is used to validate the values of aggregated flows, freshwater requirement and water streams reused, in tons/h. In Figure 16 are shown the partial calculations for the construction of the WSD.

Aggregated flows from operations (t/h)

Intervals	1	2	3	4	5	6	7	8
Operation1	34.00	34.00	34.00	34.00	34.00	34.00	34.00	34.00
Operation2	0.00	55.33	55.33	55.33	55.33	55.33	55.33	116.78
Operation3	0.00	0.00	0.00	0.00	53.47	61.45	61.45	61.45
Operation4	0.00	0.00	0.00	0.00	0.00	6.02	11.59	11.59

Available water for reutilization (t/h)

Intervals	1	2	3	4	5	6	7	8
Operation1	0.00	0.00	34.00	0.00	0.00	0.00	0.00	0.00
Operation2	0.00	55.33	0.00	0.00	0.00	0.00	0.00	0.00
Operation3	0.00	0.00	0.00	0.00	0.00	61.45	0.00	0.00
Operation4	0.00	0.00	0.00	0.00	0.00	0.00	11.59	0.00

Figure 16. Aggregated flows and water available for reuse

Two major assumptions have been made while developing the calculations in the worksheet. First, the data construction with an MRP structure is constantly measuring the water available in the beginning of the interval, the additional quantity of water required to perform the mass exchange, the water streams reused and the water flowrate available at the end of the interval. With this structure and for a given interval, the WaterGain+ moves backward until it finds the remaining water available from the operations' water flows that are being reused. Therefore, the water streams may bring the first water disposable that is found, instead of the more contaminated water. Secondly, the software deals with a single external water source at 0 ppm which is consumed in the absence of any opportunity to reuse the water flows required.

Subsequently, the WSD is generated as shown in figure 17. This diagram, which is similar to a Gantt chart of the total mass load transferred is plotted as well as the evolution of the contaminant's concentration values in parts per million (ppm), for each of the operations configured.

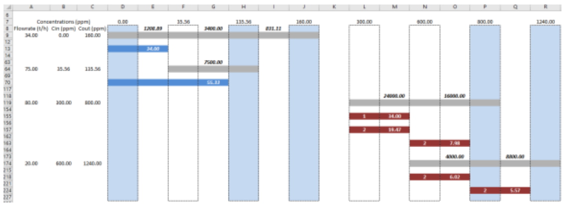


Figure 17. Water source diagram for reutilization strategy

To the best of our knowledge, this methodology required manual calculations to deal with water networks with multiple contaminants. This posed some challenges while developing this methodology into a software. An intermediate step is required to support the construction of the water network. Therefore, the development of WaterGain+ presents yet another contribution by concentrating all the data with respect to the contamination, water flowrate reused, number of operation divisions and the wastewater generated, as shown in figure 18. First, the freshwater requirement for each operation is placed in column C. Secondly, the remaining columns correspond to the water flowrates reused for a given operation. Later, the sum of splitter flows is calculated that corresponds to the water streams at the outlet of each operation (sum in columns). Thereafter, the sum of the mixer flows is obtained by aggregating all flowrates reused for each operation (sum in rows). A condition is introduced to determine the number of splitters and mixers, which is, if the count is greater than 1, a splitter or mixer is placed accordingly. The WaterGain+ software does not consider any water losses across the network and hence, the flows at the inlet equals the flows at the outlet of an operation. Thereby, the total wastewater released, is given by the difference of total flows entering the mixer and total flows reused from an operation going to splitter. Once the flows have been introduced, the attention shifts to the inlet and outlet operational concentrations. From figure 18, operation 3 receives 34 t/h of water from operation 1 (cell D18), and 27.45 t/h from operation 2 (cell E18), with different contaminations. The third operation will receive a flowrate of 61.45 t/h. The weighted average concentration for contaminant A by mixing these two water streams equals $C_{3,A}$ = (34*160 + 27.45*135.56) / 61.45 = 149.08 ppm of A.

	B	C	D	E	F	G	H	I
7								
8	Source operation	0	1	2	3	4	Sum of flows in mixer	Count
9	Destination operation							
10	1	34.00	0.00	0.00	0.00	0.00	34.00	1.00
11	A	0.00					0.00	
12	B	0.00					0.00	
13	C	0.00					0.00	
14	2	55.33	0.00	0.00	0.00	0.00	55.33	1.00
15	A	0.00					0.00	
16	B	0.00					0.00	
17	C	0.00					0.00	
18	3	0.00	0.00	11.59	0.00	0.00	11.59	1.00
19	A	0.00		135.56			135.56	
20	B	0.00		230.44			230.44	
21	C	0.00		325.33			325.33	
22	4	0.00	34.00	27.45	0.00	0.00	61.45	2.00
23	A	0.00	160.00	135.56			149.08	
24	B	0.00	450.00	230.44			351.92	
25	C	0.00	30.00	325.33			161.93	
26	Sum of flows in splitter	89.33	34.00	39.04	0.00	0.00		
27	A	0.00	160.00	135.56	1240.00	800.00		
28	B	0.00	450.00	230.44	1179.54	963.80		
29	C	0.00	30.00	325.33	2378.83	812.86		
30	Count	2.00	1.00	2.00	0.00	0.00		
31	Wastewater		0.00	16.29	11.59	61.45		

Figure 18. Data for water mass exchange network design

Before designing the network, the inlet and outlet concentrations (columns D and E) are compared with their limiting values (columns F and G) in order to verify if the optimal network has been obtained. The optimality condition occurs whenever the sum of all binaryCin (column H) with all binaryCout (column I) equals zero. Although the condition is true for inlet concentrations, there are two concentrations at the outlet that exceed the maximum value as shown in figure 19. Thereby, the water network is not optimal and hence, are required further concentration adjusts.

	B	C	D	E	F	G	H	I
33								
34	Operation	Contaminant	Cin	Cout	Cin max	Cout max	Binary in	Binary out
35	1	A	0.00	160.00	0.00	160.00	0.00	0.00
36	1	B	0.00	450.00	0.00	450.00	0.00	0.00
37	1	C	0.00	30.00	0.00	30.00	0.00	0.00
38	2	A	0.00	135.56	200.00	300.00	0.00	0.00
39	2	B	0.00	230.44	100.00	270.00	0.00	0.00
40	2	C	0.00	325.33	500.00	740.00	0.00	0.00
41	3	A	149.08	800.00	300.00	800.00	0.00	0.00
42	3	B	351.92	963.80	460.00	930.00	0.00	1.00
43	3	C	161.93	812.86	400.00	900.00	0.00	0.00
44	4	A	135.56	1240.00	600.00	1240.00	0.00	0.00
45	4	B	230.44	1179.54	850.00	1400.00	0.00	0.00
46	4	C	325.33	2378.83	390.00	1580.00	0.00	1.00

Figure 19. Contaminant concentration limits verification

The following water network, figure 20, is designed by clicking on the button "Water Network Generation" within the worksheet "Mass Exchange Network".

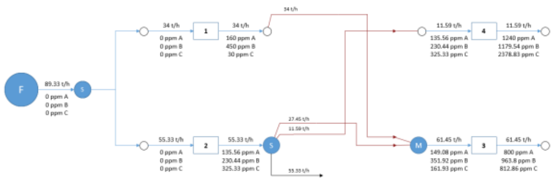


Figure 20. Water mass exchange network

According to figure 19, the third and fourth operations should lower their outlet concentration, respectively for contaminants B and C as they receive internal water from the second operation. Since there is effluent being rejected from operation 2, the flows are redirected to lower the inlet and consequently, the outlet concentration of the contaminants previously identified. A new mass balance has to be performed so as to meet the concentration restrictions, $C^{in} \leq C^{in,max}$ and $C^{out} \leq C^{out,max}$. Thereby, the new flowrate required is determined by equation 2 to overcome those infeasibilities. It is important to consider that the WaterGain+ performs one iteration at a time to remove those concentration violations.

$$\mathrm{dflow} = \frac{\Delta m_{kc} - \mathrm{flowOp} * (C^{out,max}_{kc} - C^{in}_{kc})}{C^{out,max}_{kc} - C^{dflow}} \qquad (2)$$

The work developed by Gomes et al. (2013) had not established any rule to determine the quantity of water to ensure that the concentration restrictions are accomplished. With this work, we intend to overcome this hurdle whenever the limiting concentrations are exceeded. Therefore, equation 2 is developed to calculate the additional flowrate required while meeting the concentration restrictions by ensuring the minimal external water consumption and better exploit the water bodies' capacity and contamination. Unless unavailable, sufficient wastewater with lower concentration than the maximum admissible at the inlet of an operation, freshwater consumption is always the last water source to be consumed. Considering the third operation and contaminant B, recurring to figure 8 the value of $\Delta m_{3,B}$ = 37600 kg/h, the flowOp corresponds to the flowrate that goes to operation 3 which equals 61.45 t/h as shown in figure 17, $C^{out,max}_{3,B}$ = 930 ppm of B, the inlet concentration (C^{in} = 351.92 ppm of B) is taken from mass exchange network, figure 19, and C^{dflow} represents the concentration of the flow that is brought to satisfy the additional water requirement. As can be seen in figure 19, the only wastewater available before operation 3 is 16.29 t/h at 230.44 ppm of B, which is lower than $C^{in}_{3,B}$ = 351.92 ppm of B, and hence, C^{dflow} = 230.44 ppm of B with the corresponding dflow = 2.97 t/h. Therefore, the new value of flowOp will be the sum of the actual flowOp (61.45 t/h) and the dflow (2.97 t/h), which now will be 64.42 t/h. Figure 21 represents the optimized and final water network.

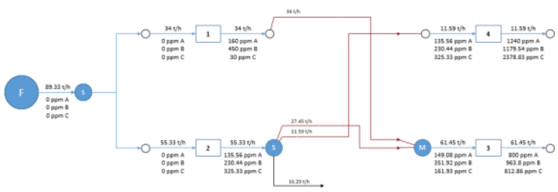


Figure 21. Final water network

7. Conclusions

Increasing the water price and strict environmental regulations, has created challenges for engineers to find solutions to analyse industrial processes in order to increase the water usage efficiency.

Mathematical models have been used to solve industrial contaminated water networks with multiple contaminants, however these are difficult to use. Hence, the research trend has shifted to graphical approaches where the water pinch analysis has proved to be very useful while analysing complex industrial processes with speed and accuracy. Due to its simplicity, the WSD has been used in major sectors as pulp and paper, and oil refining.

The current work focuses the industrial water network management for single and multiple contaminants. The extant European and National legislation as well as the literature are reviewed that provides an overview of the state of the art as also the trends of the developed works. Two software tools are developed to evaluate the water streams reutilization strategy within an industrial plant, having single and multiple contaminants. Two industrial cases are illustrated to evaluate the software tools. These generate the water source diagram, the water mass exchange network, and obtain the percentage of water saved using reutilization strategy.

Each limiting operational data may lead to different network structures, which are affected by factors such as, economic, environmental, safety and level of controllability by industrial experts. Considering the industrial case WSD, the freshwater consumed totals 146.3 t/h in the absence of integration strategy. Reusing the water flows, the external water consumption is lowered to 89.3 t/h, which accounts to a saving of 38.9%. Process integration is a key strategy in industrial sector for increasing productivity through a rational consumption. Lower utilities' consumptions generate lesser effluents, and consequently, lower discharge costs.

Future development could extend the software tools for: regeneration-reuse and regeneration-recycling strategies; continuous mode operations; multiple sources of external water other than freshwater; implement clusters of industrial water consumers to reuse the contaminated water among various industrial plants, sharing costs and utilization of regeneration equipment; external water source selection based on water harvesting costs; implement penalty function for the water network leakages; and develop methodologies to study batch plant operations by introducing time as a variable. It would also be important to study the utilization of these software tools at the factories, with industry specialists, so as to obtain real world design and performance improvement insights.

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