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Water Reuse and Wastewater Minimization in Chemical Industries Using Differentiated Regeneration of Contaminants

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ABSTRACT: There is currently a great demand for tools that allow the analysis of water networks in a practical and objective way. In the modern scenarios chemical industries need to consume water in more rational forms to minimize the risk of water scarcity caused by pollution. Some of the alternatives for reducing water consumption involve the reuse and/or recycling of wastewater, such as the methodology based on the water source diagram (WSD), which is a flexible and dynamic alternative approach to generating viable scenarios for the management of water networks. In this study the implementation of the WSD to support the optimization software (GAMS) in a process of differentiated regeneration is studied, treating the operation of a chemical process of interest in an objective and systemic way. The method can be applied to resource networks with multiple impurities, even when the utility contains impurities. The possibilities for maximum reuse of water and differentiated effluent regeneration are studied, aiming to minimize the total flow of wastewater being treated inside the treatment units and the global cost of the network. The application of this methodology is illustrated through two case studies. The results show that this procedure allows the successful identification of different scenarios which present a condition of minimum water consumption together with a minimum network operation cost.

1. INTRODUCTION

The growth of the world population and concurrent economic development mean that the demands for natural resources such as natural gas, crude oil, and water are increasing rapidly. In this context, process integration techniques are well-recognized as a promising tool in resource conservation associated with cost reduction and sustainable process development.

The chemical, petrochemical, textile, and paper and cellulose industries consume large quantities of water, and there are increasing requirements to minimize this consumption as natural resources become ever scarcer. The global tendency is toward an increase in the cost of water and of the treatment of effluents, due to new restrictions regarding discharges to the environment. This scenario has led to the need to minimize industrial water consumption, favoring the development of new methodologies for the optimization of the use of these resources.[1,2]

Pollution is of international concern in relation to human health, and this has led to an increase in environmental awareness in all social segments. At the industrial level, the first attempt to control the pollution of water resources was the use of end-of-pipe (centralized) treatments, in which all of the effluents are combined and sent to a final treatment system. In this type of treatment, the total cost is higher and the system is very large scale.[3−6]

Since industrial facilities require large quantities of fresh water and thus produce considerable amounts of wastewater, it is important to reduce their fresh water consumption and wastewater generation, which can be achieved by means of water reuse and wastewater regeneration for reuse or recycling. Regeneration and reuse or recycling allows a lower fresh water consumption and wastewater production than that associated only with water reuse to be obtained.[7]

All operational practices whose objective is to minimize the generation of effluents require a change in the way in which the process is approached. In industry the greatest incentives for this change are a reduction in the costs associated with the disposal of discharges, tax incentives associated with gains in the sustainability of the process, and an improvement in the image of the company.[4]

Modern industrial plants are faced with the challenge of reducing effluent generation and reaching sustainable standards for their operation, incorporating into their design economic solutions which consider wastewater segregation systems and differentiated regeneration, which are predicted to be important to allow maximum reuse of water within their processes.[5]

Many researchers have developed procedures, techniques, algorithms, and computational programs to aid in the solving of environmental problems. The minimization of water consumption and reduction of effluent discharge are issues which are being increasingly studied.[8−12]

The main objective of this study is to investigate global optimization scenarios for the chemical industry and to propose solutions which allow a reduction in water consumption in the transformations involved, leading to an economy of scale and less aggressive environmental conditions in relation to water use. Thus, the procedure involving the algorithmic−heuristic water source diagram (WSD)[4,7] is used to analyze water networks considering the differentiated regeneration of multiple contaminants and wastewater recycling within the industrial plant. After

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application of the WSD the response is improved by using mathematical programming to evaluate the situations which lead to minimum flow rate and lowest cost.

In this study, such a procedure is investigated using two examples, where the possibilities for the reuse of water in chemical processes through the differential regeneration of processes with multiple contaminants are explored and the results obtained compared with data available in the literature.[3] To this aim, a methodology was developed to represent the problem in a water source diagram for the analysis and synthesis of the network.

2. OPTIMIZATION MODELS

Technical options for the minimization of wastewater involve the following: the choice of raw materials; the introduction of modifications in the production process, the recycling of wastewater streams, treatment at the source and reuse of treated effluents within a process, the implementation of distributed treatments, and the selection of final discharge methods which better exploit the capacity of the receiving water bodies.[2]

To achieve rational management of liquid effluent, in the first instance, companies need to systematically measure the current water consumption and the generation of effluents which are subsequently discarded for each of their operations and identify which points of the process are candidates for a reduction in water consumption. This approach provides a baseline for the evaluation of risks, the prioritization of efforts, and the measurement of operational progress in the water management system.[13]

Nowadays, the designers of water supply systems need to create more efficient designs, based on the development of systematic methods for the integration of water at an industrial plant,[14,15] and research in the area of the global optimization of chemical processes has led to an increase in the scope of the field of interest of industrial optimization.[16]

Considering all of these factors, it is clear that the development of methodologies to minimize the use of water in industrial plants is an important area of process integration.[4]

Water pinch technology was developed in order to achieve process integration in relation to water use, and this has led to process designs which are cost-effective and which reduce the generation of liquid effluents and conserve water with the application of two approaches to resolve these issues:[4,17,18] algorithmic—heuristic procedures; procedures based on mathematical programming.

2.1. Algorithmic—Heuristic Procedures. Wang and Smith[19] began the research in the field of water integration, developing the water pinch technology for mass integration, based on the more generalized problem of mass exchange network synthesis.[20] These authors presented the concepts of direct water reuse, reuse with regeneration, and regeneration with recycling as an approach to minimize the generation of effluents. On the basis of this approach, it became possible to improve the design of effluent treatment systems where the residue is treated in a distributed way.[3]

Water pinch technology evolved together with the broader concept of the integration of process, of materials, of energy, and of the minimization of emissions and discharges associated with chemical processes. This technology can be considered as a type of integration of mass transfer between water-using operations, allowing process engineers to deal with important questions regarding the updating of existing units and the design of new water consumption networks.[21]

Water pinch technology consists of three basic tasks:[21] the identification of the minimum water consumption and effluent generation in operations, the design of a water utilization network aiming to fulfill the objectives for water consumption and effluent generation, and the modification of an existing water utilization network to maximize direct reuse and to minimize effluent generation through effective changes in the process.

In the first phase, the targets of the network design are established on the basis of a graphical procedure which uses data from a limiting composite curve and vertical transfer in order to determine the minimum fresh water and wastewater flows; this stage is followed by the detailed network design stage.

The flow restrictions and the integration of regeneration units were later considered.[22,23]

The studies carried out by Dhole et al.,[24] Hallale,[25] and Manan et al.[26] showed that not all of the processes can be modeled as mass-transfer operations. Some examples are boilers, cooling towers, and reactors. Water network synthesis for these units is generally viewed as a fixed flow rate problem.

The first generation of source and sink composite curves to resolve fixed flow rate problems were proposed by Dhole et al.[24] and later improved by Polley and Polley.[27]

Water pinch technology traditionally minimizes the fresh water flow rate which is incorporated into the system, using the mass balance and the contaminant concentrations at the inlet and outlet of the water-using operations as process restrictions. Due to the diverse types of operations, efficiencies and costs associated with regenerative processes, as well as the different types of contaminants present in the streams, the criteria for efficient water use are inherently nonlinear, multiple, and very restrictive.[21]

Many techniques for the design of water networks and for reaching the flow rate targets have been proposed.[7,19,23,28−32]

Once the flow rate targets are established, the water network can be studied in order to reach the minimum targets. Subsequently, a preliminary network synthesis can be performed in order to obtain the simplified network.[32,33]

2.2. Mathematical Programming. Takama et al.[34] introduced the water allocation problem (WAP) in a refinery using nonlinear programming and considering fixed removal rates specified for each contaminant.

Alva-Argáez et al.[35] developed an integrated approach which combines the fundamentals of the water pinch technique and mathematical programming to investigate fixed mass load problems.

The optimization technique based on nonlinear programming (NLP) was presented to address fixed load[36] and fixed flow rate[37] problems. Huang et al.[38] developed individually the mathematical approximation to include water treatment in water network synthesis. Bagajewicz and colleagues used linear programming and algorithmic procedures to design water networks in monocontaminant[39,40] and multiple contaminant[41] systems.

Advanced mathematical optimization techniques, such as fuzzy programming,[42] the genetic algorithm,[43−45] and random search optimization,[46] have been used to study water network synthesis.

The mathematical optimization technique serves as a supplemental tool for the graphical pinch technique in the study of more complex systems, such as those with a large number of water-using processes,[39] multiple impurities,[14,34] mass load uncertainty,[47] capital cost evaluation,[35,48] and integration with a network with waste interception,[49] and a water treatment system[3,38] or evaluation of the possibility for zero discharge.[50]

A useful review of the various techniques available for the study of the water network synthesis problems was presented by Bagajewicz.[8]

Another area in which water reuse/recycling has made significant advances in recent years is the synthesis of the water network in batch processes.

3. METHODOLOGY

ITo apply the WSD procedure, the process needs to be studied in order to (i) identify the operations which use water, (ii) determine the water balance of these operations (water-transfer network), (iii) ascertain the flow limit of the operations, and (iv) identify all of the contaminants and determine their concentrations.[2,4,6]

To address systems with differentiated regeneration, the WSD methodology needs to be adapted and the minimum level of effluent which requires treatment must be determined in order to establish the targets for the minimization of aqueous streams.

Observation 1: Primary water will be consumed only by operations which are not attended by regenerative processes, other operations being supplied by reuse, regeneration, and regeneration with recycling strategies.

Observation 2: The greatest quantity of contaminants possible is transferred in each concentration interval. After minimizing the primary water consumption, the second objective is to rationalize the flow rate of the effluent which passes to the regenerators.

Observation 3: It is necessary to establish the limit values for the regeneration in order to minimize the flow to be treated in differentiated regeneration processes. In multiple regeneration equipment it is possible to reduce the level of some contaminants to concentrations below the maximum permissible limits.[2,6]

The methodology is divided into five analysis steps:

Step 1: Calculate or obtain equations for the value of ΔC for each contaminant and for each stage of the network, establishing the optimal conditions for each case.

(step 1a) global balance:

$$\overbrace{\Delta m_j^F}^{Inlet} + \overbrace{\sum_p \Delta m_j^p}^{Source} = \overbrace{\sum_r \Delta m_j^r + \Delta m_j^W}^{Outlet} \tag{1}$$

for fresh water sources:

$$\Delta m_j^{\text{regeneration}} = \Delta m_j^{\text{processes}} - \Delta m_j^{\text{W}} \tag{2}$$

(step 1b) for the discharge conditions:

$$\Delta m_j^{\text{W}} = \frac{f^{\text{F}} \Delta C_j^{\text{W}}}{1000} \tag{3}$$

$$\Delta m_j^{\text{W}} = \frac{f^{\text{W}}(C_j^{W} - C_j^{\text{F}})}{1000} \tag{4}$$

optimality condition:

$$\Delta m_{j,\max}^{\text{W}} = \frac{f^{\text{F}}(C_{j,max}^{\text{W}} - C_j^{\text{F}})}{1000} \tag{5}$$

(step 1c) for the units of the process:

$$\Delta m_j^p = \frac{f^p(C_j^{\text{out},p} - C_j^{\text{in},p})}{1000} \tag{6}$$

$$\Delta C_j^p = C_{j,\max}^{\text{out},p} - C_{j,\max}^{\text{in},p} \tag{7}$$

$$\Delta m_j^{\text{processes}} = \sum_p \Delta m_j^p \tag{8}$$

(step 1d) for the regenerationunits:

$$\Delta m_j^r = \frac{f^r(C_j^{\text{out},r} - C_j^{\text{in},r})}{1000} \tag{9}$$

$$\Delta C_j^r = (1 - \varepsilon_j^r) C_j^{r,\text{out}} - C_j^{r,\text{in}} \tag{10}$$

optimality condition:

$$\Delta m_{j,\min}^{\text{regeneration}} = \Delta m_j^{\text{processes}} - \Delta m_{j,\max}^{\text{W}} \tag{11}$$

Step 2: Construct the stream allocation diagram to represent the evolution of the calculations and the possible connections between currents.

Step 3: Identify in the diagram all of the operations which need to consume primary water and calculate the flow required to attend to the needs of the process.

Step 4: Calculate the outlet concentration and the predicted flow available for each regeneration unit. Recalculate the inlet and/or outlet concentration for each process unit ordered from the lowest to the highest flow rate, always allowing the limit value for the input concentration to be reached. If necessary, use regeneration with recycling in the process to complement the flow. On allocating the flows, the following priority rules are valid: first maximum reuse, second differentiated regeneration, and finally regeneration with recycling.

Step 5: Verify the restrictions of the process and the mass balances, updating the calculations, and obtain a flow diagram of the process with the proposed solutions.

Step 6: Repeat steps 4 and 5 if any restriction is violated until the limit values for the regenerative treatments are reached. Present the flow diagram of the process with the final solution.

By applying the WSD adapted to deal with differentiated regeneration processes, it was possible to obtain a viable solution for the two proposed problems. These solutions were used as an initial value for the search process in the program GAMS (general algebraic modeling system, developed by Brooke et al.[51]) using the nonlinear programming algorithm SNOPT. The results of these processes can be seen in Tables 6 and 13.

4. CASE STUDIES

The two examples explored herein were studied by Karuppiah and Grossmann,[3] and the plant operates at 8000 h·a (hour per year),[1] the AR value is 0.1, and the α value is 0.7. In these case studies, the objective functions chosen can deal with either the minimum flow or the minimum cost.

4.1. Case 1. This network has two process units which use water during their operation. In the processing two contaminants

Table 1. Process Data for Case 1

unit	f (t·h^{-1})	contaminant	Δm_j^p (kg·h^{-1})	$C_{j,\max}^{p,\text{in}}$(ppm)
P1	40	A	1.0	0
		B	1.5	0
P2	50	A	1.0	50
		B	1.0	50

Table 2. Contaminant Removal Efficiencies for the Regenerative Processes Proposed in Case 1

	removal efficiency, ε_j^r (%)	
unit	A	B
R1	95	0
R2	0	95

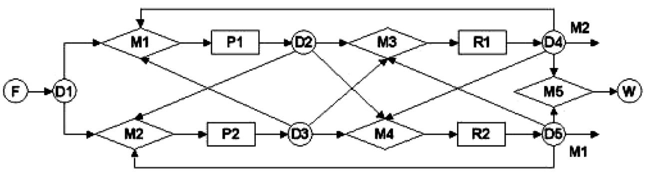


Figure 1. Representation of superstructure in case 1.

are incorporated (A and B), and their mass loads and maximum concentrations at the inlet and outlet are given in Table 1.

In this network, the fresh water source is free of contaminants and the discharge conditions must be such that both contaminants A and B have concentrations below 10 ppm. To reach this discharge limit, two regeneration units are available and Table 2 shows the data relating to the regenerative processes. The superstructure for case 1 is shown in Figure 1.

As the objective function two equations can be used: one to minimize the captured water flow and the need for regeneration and the other specifically to monitor the total cost of the effluent capture and regeneration process.

minimum flow:

$$\min \text{FO} = f^{\text{F,D1}} + f^{\text{M3,R1}} + f^{\text{M4,R2}} \tag{12}$$

minimum cost:

$$\min FO = \underbrace{H.CF.f^{F,D1}}_{Freshwater\ \ cost} + \underbrace{AR\left[CI^{R1}\left(f^{M3,R1}\right)^{\alpha} + CI^{R2}\left(f^{M4,R2}\right)^{\alpha}\right]}_{Investment\ \ cost} + \underbrace{H\left[CO^{R1}.f^{M3,R1} + CO^{R2}.f^{M4,R2}\right]}_{Operational\ \ cost} \tag{13}$$

The investment costs and those for the operational of the regeneration units are shown in Table 3.

The preliminary calculations for application of the water source diagram are as follows: maximum outlet concentration and value for the concentration variation for each of the process units. Table 4 summarizes these preliminary results.

Once the ΔC_j^p values for the process units are known, the values for the maximum contaminant loads removed from the

Table 3. Coefficients of Investment and Operational Costs Associated with the Regenerative Processes Proposed in Case 1

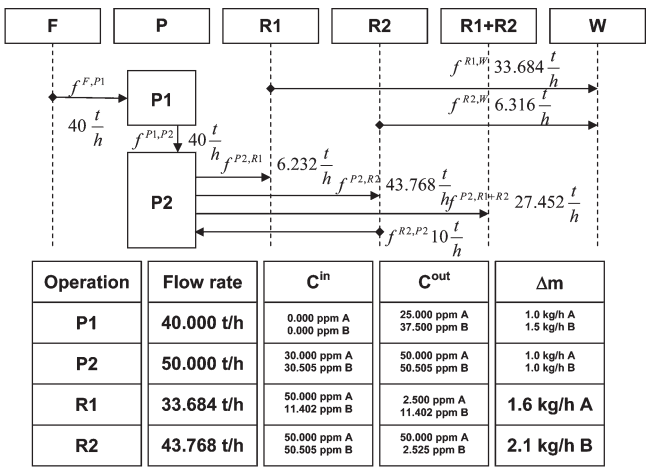
unit	CI^r (investment cost coefficient)	CO^r (operational cost coefficient)
R1	16 800	1.0000
R2	12 600	0.0067

Table 4. Calculated Maximum Output Concentration and Value for the Variation in Concentration for the Process Units in Case 1

unit	f^p (t·h^{-1})	contaminant	$C_{j,\max}^{p,\text{out}}$(ppm)	ΔC_j^p (ppm)
P1	40	A	25.0	25.0
		B	37.5	37.5
P2	50	A	70.0	20
		B	70.0	20

Table 5. Calculated Values for the Contaminant Load in the Process, in the Discharge, and in the Regenerative Processes for Case 1

contaminant	$\Delta m_j^{\text{processes}}$ (kg·h^{-1})	$\Delta m_{j,\max}^{\text{W}}$ (kg·h^{-1})	$\Delta m_{j,\min}^{\text{regeneration}}$ (kg·h^{-1})
A	2.0	0.4	1.6
B	2.5	0.4	2.1



Operation	Flow rate	C$^{\text{in}}$	C$^{\text{out}}$	Δm
P1	40.000 t/h	0.000 ppm A 0.000 ppm B	25.000 ppm A 37.500 ppm B	1.0 kg/h A 1.5 kg/h B
P2	50.000 t/h	30.000 ppm A 30.505 ppm B	50.000 ppm A 50.505 ppm B	1.0 kg/h A 1.0 kg/h B
R1	33.684 t/h	50.000 ppm A 11.402 ppm B	2.500 ppm A 11.402 ppm B	1.6 kg/h A
R2	43.768 t/h	50.000 ppm A 50.505 ppm B	50.000 ppm A 2.525 ppm B	2.1 kg/h B

Figure 2. Implementation of step 5 of the WSD for Case 1.

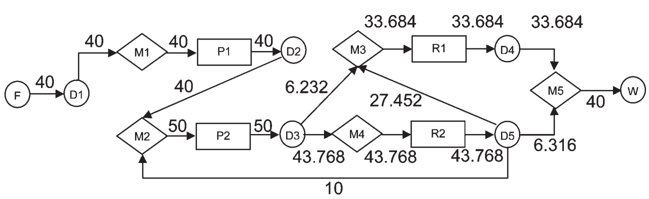


Figure 3. Process diagram of the solution proposed in the WSD for case 1.

Table 6. Comparison of Results Obtained in This Study (Case 1) with Those of Karuppiah and Grossmann[3]

	this study (case 1)			Karuppiah and Grossmann,[3] for given objective
methodology	WSD	GAMS	GAMS	
objective	min flow rate	min flow rate	min cost	min flow rate
captured water ($t \cdot h^{-1}$)	40.000	40.000	40.000	40.000
regeneration ($t \cdot h^{-1}$)	77.453	77.050	79.510	77.050
total flow rate ($t \cdot h^{-1}$)	117.453	117.050	119.510	117.050
total cost (U.S. dollars)	632 705.02	693 546.49	596 183.53	693 546.49

Table 7. Process Data for Case 2

unit	f ($t \cdot h^{-1}$)	contaminant	Δm_j^p ($kg \cdot h^{-1}$)	$C_{j,max}^{p,in}$ (ppm)
P1	40	A	1.0	0
		B	1.5	0
P2	50	A	1.0	50
		B	1.0	50
P3	60	A	1.0	50
		B	1.0	50

Table 8. Contaminant Removal Efficiencies for the Regenerative Processes Proposed in Case 2

	removal efficiency, ε_j^r (%)	
unit	A	B
R1	95	0
R2	80	90
R3	0	95

Table 9. Coefficients of Investment and Operation Costs Associated with the Regenerative Processes Proposed in Case 2

unit	CI^r (investment cost coefficient)	CO^r (operational cost coefficient)
R1	16 800	1.0000
R2	24 000	0.0330
R3	12 600	0.0067

system through discharge and the values for the minimum contaminant loads to be removed by the regenerative processes can be calculated, as shown in Table 5.

Figure 2 shows the stream allocation diagram obtained with the application of the proposed methodology, and Figure 3 shows the flow diagram of the process with the proposed solution. The results of this process for case 1 can be seen in Table 6.

4.2. Case 2. This case is an integrated network comprising three process units (P1, P2, and P3) which generate contaminants A and B at defined rates. To remove contaminants A and B, there are three regenerating units (R1, R2, and R3), R1 being specifically for contaminant A and R3 specifically for contaminant B, and R2 can, with a certain efficiency, remove both

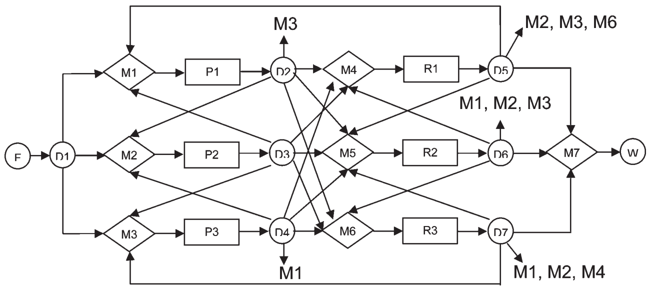


Figure 4. Representation of superstructure in case 2.

Table 10. Calculated Value for the Maximum Output Concentration and the Value for the Variation in the Concentration for the Process Units of Case 2

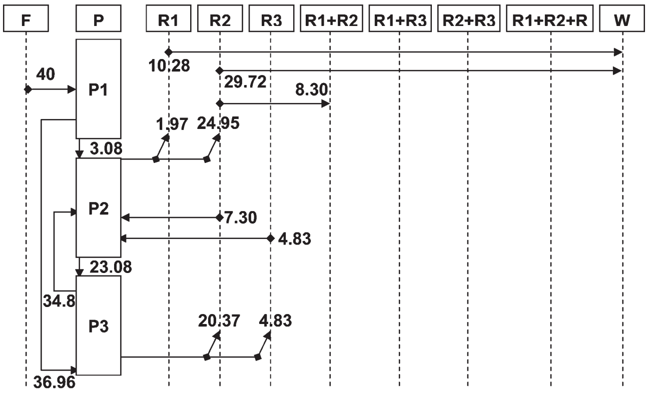
unit	f^p ($t \cdot h^{-1}$)	contaminant	$C_{j,max}^{p,out}$ (ppm)	ΔC_j^p (ppm)
P1	40	A	25.00	25.00
		B	37.50	37.50
P2	50	A	70.00	20.00
		B	70.00	20.00
P3	60	A	66.67	16.67
		B	66.67	16.67

Table 11. Calculated Values for the Contaminant Loads in the Process Units, the Discharge, and the Regenerative Processes for Case 2

contaminant	$\Delta m_j^{processes}$ ($kg \cdot h^{-1}$)	$\Delta m_{j,max}^{W}$ ($kg \cdot h^{-1}$)	$\Delta m_{j,min}^{regeration}$ ($kg \cdot h^{-1}$)
A	3.0	0.4	2.6
B	3.5	0.4	3.1

Table 12. Contaminant Loads Removed by the Regenerative Processes in Relation to the Problem Stream Allocation in Case 2

		ΔC (ppm)		Δm ($kg \cdot h^{-1}$)	
regenerator	flow ($t \cdot h^{-1}$)	A	B	A	B
R1	10.278	22.884	0.000	0.2352	0.0000
R2	45.322	52.187	61.674	2.3652	2.7952
R3	4.829	0.000	63.346	0.0000	0.3059



Operation	Flow rate	C^{in}	C^{out}	Δm
P1	40.00 t/h	0 ppm A 0 ppm B	25.0 ppm A 37.5 ppm B	1.0 kg/h A 1.5 kg/h B
P2	50.00 t/h	50 ppm A 50 ppm B	70 ppm A 70 ppm B	1.0 kg/h A 1.0 kg/h B
P3	60.00 t/h	43.308 ppm A 50.000 ppm B	58.975 ppm A 66.667 ppm B	1.0 kg/h A 1.0 kg/h B
R1	10.28 t/h	24.085 ppm A 18.988 ppm B	1.204 ppm A 18.988 ppm B	0.2352 kg/h A
R2	45.32 t/h	65.233 ppm A 68.528 ppm B	13.047 ppm A 6.853 ppm B	2.3652 kg/ A 2.7952 kg/h B
R3	4.83 t/h	59.075 ppm A 66.681 ppm B	59.075 ppm A 3.334 ppm B	0.3059 kg/h B

Figure 5. Implementation of WSD for case 2.

contaminants A and B. In this study one of the limitations imposed is that the maximum discharge concentration of either contaminant A or B must not surpass 10 ppm.

In this study, the flows for the operations P1−P3, the maximum admissible input concentrations for the process operations, and the contaminant load added in the permanent regime are previously imposed. These process data are summarized in Table 7.

The contaminant removal efficiencies of the regeneration units are known for the regenerators R1−R3 (Table 8), as well as the costs associated with the investment and the regeneration operation (Table 9).

Since there is a set of three process units which generate contaminants and a set of three regenerative units which selectively remove these contaminants, the problem addressed aims to synthesize an integrated water network for the use and/or reuse of water for these units through a set of connections with mixers and dividers of the process streams. In this study one of the limitations imposed is that the maximum discharge concentration of either of the two contaminants A or B must not surpass 10 ppm. The superstructure for this case study is shown in Figure 4.

In this case, as the objective function, two equations can be used: one to minimize the captured water flow and the need for regeneration and the other specifically to monitor the total cost of the effluent capture and regeneration process.

Minimum Flow: On using this type of objective function, it is necessary to minimize the sum of the flows which represent primary water consumption ($f^{F,D1}$) and the total water flow of the process sent for regenerative treatment ($f^{M4,R1}$, $f^{M5,R2}$, and $f^{M6,R3}$).

In this case the objective function of the minimum flow is described by

$$\min \mathrm{FO} = f^{F,D1} + f^{M4,R1} + f^{M5,R2} + f^{M6,R3} \tag{14}$$

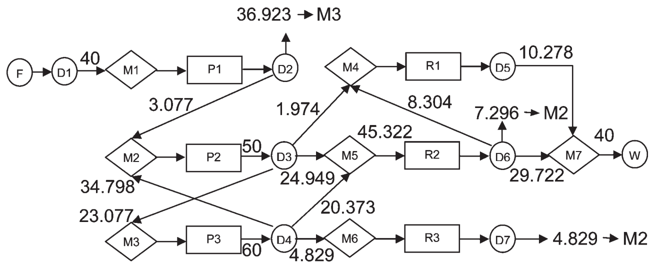


Figure 6. Flow chart of the process with the proposed solution applying the WSD to case 2.

Minimum Cost: In this case the objective function of the minimum cost is described by

$$\begin{aligned} \min FO = {} & \underbrace{H.CF.f^{F,D1}}_{\text{Freshwater cost}} + \\ & \underbrace{AR\left[CI^{R1}\left(f^{M4,R1}\right)^{\alpha} + CI^{R2}\left(f^{M5,R2}\right)^{\alpha} + CI^{R3}\left(f^{M6,R3}\right)^{\alpha}\right]}_{\text{Investment cost}} + \\ & \underbrace{H\left[CO^{R1}.f^{M4,R1} + CO^{R2}.f^{M5,R2} + CO^{R3}.f^{M6,R3}\right]}_{\text{Operational cost}} \end{aligned} \tag{15}$$

For this case, the maximum output concentration and the value for the variation in the concentration for each of the process units are shown in Table 10.

Once the Δm_j^p values for the process units are known, the values for the maximum contaminant loads removed from the system by the discharge and the minimum contaminant loads to be removed by the regenerative processes can be calculated, and the results are shown in Table 11.

The contaminant loads removed in each of the regenerative processes can be observed in Table 12.

Figure 5 summarizes the WSD, and the flow chart of the process and the proposed solution is given in Figure 6.

In the following, the solution presented by the proposed WSD procedure was used as the initial value to improve the solution using the algorithm of the nonlinear program SNOPT for the resolution of the computational code implemented.

The first stage in the investigation carried out to improve the solution was to use the computational code to verify the solution presented by Karuppiah and Grossmann[3] and calculate the cost associated with the operation, in order to calibrate and eliminate in advance the occurrence of errors associated with the programming. The solution proposed by Karuppiah and Grossmann[3] and the other solutions obtained in the study reported herein are presented below, and the results are summarized in Table 13.

The solution proposed by Karuppiah and Grossmann[3] to minimize the flow is presented in Figure 7, where all of the mass flows involved are clearly identified.

Using the configuration proposed by the WSD and with the aim of minimizing the cost of the process, the configuration for the process streams shown in Figure 8 is obtained.

To evaluate the use of this methodology to find the lowest level for the regenerated flow, the flow chart of the process shown in Figure 9, with the respective mass flows calculated in the computational code, was obtained.

In Table 13 the results for captured water, regeneration, total flow rate, and total cost for case study 2 for different methodologies and the objective function employed in this study are summarized.

When the objective is to determine the minimum fresh water flow and/or minimum cost, the WSD methodology showed a

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Table 13. Comparison of Results Obtained in This Study with Those of Karuppiah and Grossmann[3] for Case 2

	this study (case 2)				Karuppiah and Grossmann[3]
methodology	WSD	GAMS	GAMS	GAMS	
objective	min flow rate	min flow rate	min flow regeneration	min cost	min flow rate
captured water ($t \cdot h^{-1}$)	40.000	40.000	40.000	40.000	40.000
regeneration ($t \cdot h^{-1}$)	60.429	65.000	65.011	65.011	65.000
total flow rate ($t \cdot h^{-1}$)	100.429	105.000	105.011	105.011	105.000
total cost (U.S.dollars)	461 468.70	381 759.21	455 820.73	381 759.21	381 759.21

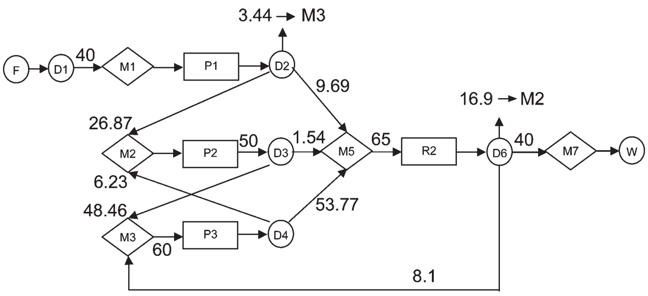

Figure 7. Flow chart of the process with the solution proposed by Karuppiah and Grossmann[3] in case 2.

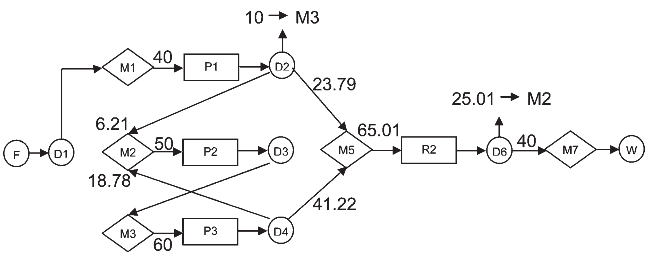

Figure 8. Flow chart of the process (proposed based on the WSD) related to the minimum cost for case 2 (GAMS).

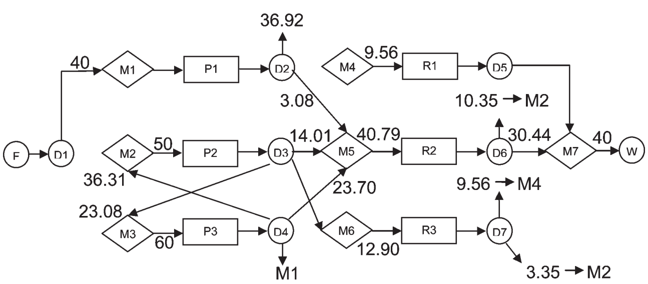

Figure 9. Flow chart of the process (proposed based on the WSD) relation to the minimum regenerated flow for case 2 (GAMS).

total cost 21% higher than that obtained by Karuppiah and Grossmann[3] and using GAMS. However, when the results of this methodology are used as initial values in the optimization with GAMS, the total cost obtained is identical to that reported in the literature, indicating the potential of this methodology.

Even having obtained the same minimum flow for fresh water, resulting in a lower water flow for the regeneration, the results for this case indicated that when the objective function was to minimize the regeneration, the total cost is 19.4% higher than that obtained by Karuppiah and Grossmann[3] and using GAMS and (it is) 1.23% lower than that obtained with the WSD. This behavior is the result of the regeneration costs, which were not minimized in this scenario.

The solution for this case, summarized in Table 13, shows that the methodology proposed herein gives similar results to those reported in the literature and that a minimum consumption of water can be obtained through different solution methodologies, resulting in different flow scenarios for the process. Depending on the most important parameter to be minimized, a different water network will be obtained.

These scenarios allow the process engineer to opt for one or another modification without adversely affecting the water consumption and the costs of the operation of the industrial plant.

5. CONCLUSIONS

The global optimization of the water network with differentiated regeneration using the adapted WSD methodology was shown to be an efficient means to determine the opportunities for water reuse and regeneration, leading to the obtainment of a viable solution to the problem, not very distant from the minimum point in terms of flow.

The contribution of this study is associated with the adaptation of the WSD (heuristic method) to deal with water networks which rely on differentiated regeneration, establishing values close to those of the operation, and the use of these as initial data in the commercial optimization software (GAMS). The results obtained showed the potential of this methodology.

The mathematical optimization process using the optimization software allowed, on the basis of this solution, progress toward the minimum flow point reported by Karuppiah and Grossmann[3] and a significant reduction in the operational costs.

This paper presents a new approach to the problem of a global analysis of chemical processes with differentiated regeneration, preestablishing regeneration targets for each unit and contaminant as a means to minimize the flow to be regenerated and to monitor these targets through a quick look at the stream allocation diagram in relation to the violation of some restriction in the process according to the allocations applied.

The results show that this procedure allows the successful identification of different scenarios which present a condition of minimum water consumption together with a minimum operation cost for the network.

Because the model formulation is linear, there are no major computational difficulties, and global optimality is ensured once a solution is found.

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NOMENCLATURE

S = stream splitter
F = fresh water source
M = stream mixer
max = maximum
min = minimum
P = process unit
R = regeneration unit
W = wastewater sink

Indices

s = splitter
j = contaminant
m = mixer
p = process
r = regenerator

Continuous Variables

C = concentration
f = flow
Δm = contaminant load

Parameters

AR = updated factor for investment in treatment units
CF = cost of fresh water, U.S$/t
C_j^{F} = concentration of contaminant j in fresh water stream, ppm
$C_{j,\max}^{W}$ = upper boundary for concentration of contaminant j in wastewater stream, ppm
$C_{j,\max}^{p,\text{in}}$ = upper boundary for concentration of contaminant j in input stream of process p, ppm
$C_{j,\max}^{p,\text{out}}$ = upper boundary for concentration of contaminant j in output stream of process p, ppm
CI^r = investment cost coefficient for regeneration unit r
$\text{CI}^r(f^{m,r})^{\alpha}$ = investment cost, U.S.$
CO^r = operating cost coefficient for regeneration unit r
$\text{CO}^r f^{m,r}$ = operating cost, U.S.$/h
f^p = flow required for process p, $\text{t}\cdot\text{h}^{-1}$
$f^{\text{F,D1}}$ = Captured water flow, $[\text{t.h}^{-1}]$
$f^{\text{M4,R1}}$ = flow of effluent sent to regenerator 1, $\text{t}\cdot\text{h}^{-1}$
$f^{\text{M5,R2}}$ = flow of effluent sent to regenerator 2, $\text{t}\cdot\text{h}^{-1}$
$f^{\text{M5,R3}}$ = flow of effluent sent to regenerator 3, $\text{t}\cdot\text{h}^{-1}]$
FO = objective function (minimum flow), $\text{t}\cdot\text{h}^{-1}$
FO = objective function (minimum cost), U.S.$
H = hours of plant operation per annum, h
α = exponential cost function ($0 \leq \alpha \leq 1$)
Δm_j^p = load of contaminant j in process unit p, $\text{kg}\cdot\text{h}^{-1}$
ε_j^r = removal efficiency for contaminant j in regeneration unit r

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