

Water network cost optimization in a paper mill based on a new library of mathematical models

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ABSTRACT

The increasing costs associated with water supply and the disposal of wastewater has stimulated industries to seek more efficient water management systems. Mathematical modelling and simulation can be a very valuable tool for the study of the multiple alternatives available whilst assessing optimum solutions for water management in industry. This study introduces a new steady state model library able to reproduce industrial water circuits. It has been implemented in a novel software framework for the representation, simulation and optimization of industrial water networks. A water circuit representing a paper mill has been modelled and simulated showing the capability to reproduce real case studies. Alternative scenarios for the water network have also been tested to assess the capability of the models to optimize water circuits minimizing total cost.

Key words | mathematical modelling, paper industry, water reuse

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INTRODUCTION

In major water-consuming industries such as paper, food and textiles it is often noted that water is used in a less than efficient manner. In recent years, the rising costs associated with the water supply and disposal has motivated industries to seek more efficient water management approaches. The availability of alternative water sources such as reclaimed municipal wastewater or recycled process water can encourage more efficient water use practices that translate into significant cost savings for many industries (Lens *et al.* 2002).

Finding optimum solutions for reusing water in a water circuit is not a straightforward task as there is a high number of advanced wastewater treatment technologies present in the market and multiple choices of reusing water within a plant. In this context, mathematical modelling and simulation can be a very valuable tool for assessing different alternatives and for seeking optimum solutions taking into account economic and environmental impacts. Over the last decade, industrial water network optimization studies have been performed using different tools that can be categorized as: (i) spreadsheets (e.g. Excel); (ii) Water Pinch Analysis (WPA) software (Manan & Alwi 2007); or

(iii) process simulators (e.g. WinGEMS, IDEAS, WEST ...). Each of these tools has its own particular advantages and disadvantages. Spreadsheets do not support graphical water network representations, but allow their simulation and optimization based on models that mimic reality. Tools based on WPA offer powerful optimization capabilities, albeit only on the basis of simplified linear models, which often do not mimic reality correctly. Finally, process simulators have strong visualization and simulation capabilities, however, they typically lack optimization features. Based on this finding one of the goals of the AquaFitForUse project (www.aquafit4use.eu) is the development of mathematical models and simulation tools that allow the industrial users to explore water reuse options in their plants. In this scope, a new software tool, named Water Quality Management Tool (WQMT), is being developed for the representation, simulation and optimization of water networks in paper, food, textile and chemical industries (Claeys *et al.* 2011).

This paper introduces a new library of steady-state mathematical models able to reproduce a set of traditional and innovative wastewater treatment technologies. These were

implemented in the WQMT, and their capability to reproduce industrial water circuits in paper and food sectors was analysed. The current and alternative scenarios were compared for a paper mill case study with the aim of showing the scope of the mathematical models developed to evaluate the optimum scenario for minimum economical cost in an industry.

INTRODUCTION TO THE MATHEMATICAL MODEL LIBRARY

A mathematical model library that reproduces the most relevant wastewater treatment technologies available in the market was developed (Table 1). These models are steady state, based on the operational variables widely used in engineering (i.e. Hydraulic Retention Time, HRT, Solid Retention Time, SRT, etc.). Due to the need of reproducing water networks as a whole, an integrated modelling methodology was used for the construction of these models in a standardized way based on three principles: (i) definition of a common state vector to guarantee mass and thermal energy continuity and enable an easy connection among different technologies. The components considered within the vector are those necessary to describe the relevant compounds in paper, food and textile industries (Table 2); (ii) next to mass and thermal energy balances, all the unit process models include investment and operational costs equations as functions of operational variables (i.e. treated flow, organic load or chemical additive requirements) that will allow the estimation of the total exploitation cost of the water network and (iii) finally, upper and lower bounds of the components are fixed to

Table 1 | Mathematical model library

Biological treatments	Solid-liquid separation treatments		Chemical treatments
Activated Sludge Unit (ASU)	Settler	NF and RO	Advanced oxidation
Membrane Bioreactor (MBR)	DAF	Electrodialysis	Disinfection (O ₃ , Cl ₂ and UV)
Moving Bed Bioreactor (MBBR) and Denitrifier	3FM	Evapoconcentrator	Coagulation-flocculation
Anaerobic Reactor (UASB)	MF and UF		FACT

ensure water quality for machinery requirements, product quality, workers safety and legislation limits. This way a specific technology will not be allowed to be used in water streams with concentrations out of the bounds specified for that technology.

Table 2 | State vector

n	Symbol	Description	Unit
1	S _a	Soluble biodegradable COD	g COD/m ³
2	S _f	Soluble biodegradable COD	g COD/m ³
3	S _i	Soluble inert COD	g COD/m ³
4	S _h	Protons	mol H/m ³
5	S _{oh}	Hydroxyl ions	mol OH/m ³
6	S _{po4-3}	Phosphate	mol P/m ³
7	S _{hpo4=}	Hydroxyl phosphate	mol P/m ³
8	S _{h2po4-}	Dihydroxyl phosphate	mol P/m ³
9	S _{nh4+}	Ammonium	mol N/m ³
10	S _{nh3}	Ammonia	mol N/m ³
11	S _{co2}	Dissolved carbon dioxide	mol C/m ³
12	S _{hco3-}	Bicarbonate	mol C/m ³
13	S _{co3=}	Carbonate	mol C/m ³
14	S _{Na+}	Sodium ion	mol Na/m ³
15	S _{k+}	Potassium ion	mol k/m ³
16	S _{Mg2+}	Magnesium ion	mol Mg/m ³
17	S _{Ca2+}	Calcium ion	mol Ca/m ³
18	S _{Ba2+}	Barium ion	mol Ba/m ³
19	S _{Mn2+}	Manganese ion	mol Mn/m ³
20	S _{Fe2+}	Ferrous ion	mol Fe/m ³
21	S _{Al3+}	Aluminium ion	mol Al/m ³
22	S _{Cl-}	Chloride	mol Cl/m ³
23	S _{SO4=}	Sulphate	mol S/m ³
24	S _{no3-}	Nitrate	mol N/m ³
25	C _b	Colloidal biodegradable COD	g COD/m ³
26	C _i	Colloidal inert COD	g COD/m ³
27	X _b	Particulate biodegradable COD	g COD/m ³
28	X _i	Particulate inert COD	g COD/m ³
29	X _{ii}	Particulate inorganic matter	g/m ³
30	X _{CaCO3}	Calcium carbonate	mol CaCO ₃ /m ³
31	X _{MgCO3}	Magnesium carbonate	mol MgCO ₃ /m ³
32	X _{FeCO3}	Iron (II) carbonate	mol FeCO ₃ /m ³
33	X _{BaCO3}	Barium carbonate	mol BaCO ₃ /m ³

(continued)

Table 2 | continued

n	Symbol	Description	Unit
34	X_{MnCO_3}	Manganese carbonate	mol $MnCO_3/m^3$
35	X_{CaSO_4}	Calcium sulphate	mol $CaSO_4/m^3$
36	X_{BaSO_4}	Barium sulphate	mol $BaSO_4/m^3$
37	X_{CaPO_4}	Calcium phosphate	mol $Ca_3(PO_4)_2/m^3$
38	X_{BaPO_4}	Barium phosphate	mol $Ba_3(PO_4)_2/m^3$
39	X_{MgPO_4}	Magnesium phosphate	mol $Mg_3(PO_4)_2/m^3$
40	X_{MnPO_4}	Manganese phosphate	mol $Mn_3(PO_4)_2/m^3$
41	X_{AlPO_4}	Aluminium phosphate	mol $AlPO_4/m^3$
42	X_{SiO_2}	Silica	mol SiO_2/m^3
43	S_{Vi}	Virus	units/ m^3
44	$X_{E. coli}$	Bacteria <i>E. coli</i>	units/ m^3
45	$X_{Legionella}$	Legionella	units/ m^3
46	X_{Cyst}	Cyst-Giardia	units/ m^3
47	X_{Crypt}	<i>Cryptosporidium</i>	units/ m^3
48	X_{Egg}	Nematode eggs	units/ m^3
49	Temp	Temperature	$^{\circ}C$
50	TSS	Total Suspended Solids	g/m^3
51	TCS	Total Colloidal Solids	g/m^3
52	TDS	Total Dissolved Solids	g/m^3
53	COD	Chemical Oxygen Demand	$g\ COD/m^3$
54	COD_sol	Soluble Chemical Oxygen Demand	$g\ COD/m^3$
55	BOD	Biological Oxygen Demand	$g\ COD/m^3$
56	cond	Conductivity	$\mu S/cm^2$
57	CD	Cationic Demand	meq/L
58	sulph	Sulphates	$g\ S/m^3$
59	pH	pH	dimensionless

Models representing biological treatments describe the organic matter removal under different environmental conditions and for different configurations, depending on HRT, SRT and specific stoichiometric and kinetic parameters. The activated sludge unit (ASU) is based on the model proposed by Marais & Ekama (1976) (Table 3). The other biological models are variations of the ASU model with differences in mass transport definition (Figure 1) and some cost parameter values.

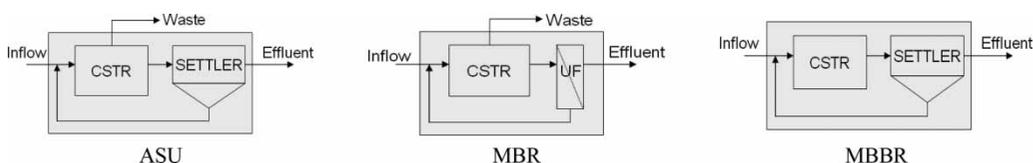


Figure 1 | Mass transport representation of the biological units.

Table 3 | Stoichiometry and kinetics for aerobic COD removal (Marais & Ekama 1976)

Component → Process ↓	S_s	X_{BH}	X_{end}	O_2	Kinetic rate
X_{BH} growth	-1	Y_H		$-(1 - Y_H)$	$\rho = \frac{\mu_H}{Y_H} \cdot \frac{S_s}{K_s + S_s} X_{BH}$
X_{BH} decay		-1	f_{end}	$-(1 - f_{end})$	$\rho = b_H \cdot X_{BH}$

As an example, the adaptation of the model proposed by Marais & Ekama (1976) (Table 3) to the MBBR configuration presented in Figure 1 results in the model presented in Table 4.

In the UASB model, biological sulphate and organic matter removal are modelled under anaerobic conditions in the biological tank, and the same mass transport configuration as for the ASU has been considered (Lizarralde et al. 2010). For all the unit processes described above, the investment and operational costs have been related to the organic load to be treated (Henze et al. 1995). The cost parameter values proposed are the results of fitting the curve to the treatment prices proposed by a particular provider.

The solid-liquid separation treatments are considered as ideal splitters. The separation is characterized by two general parameters: the fraction of inflow recovered and the fraction of solids removed. The settler model describes the solid separation by the fraction of non-settleable suspended matter. In the dissolved air flotation unit (DAF) model, the solid separation is described by the fraction of floated particles, which depends on the air flow applied to the process. Membrane separation units (Flexible Fibre Filter module (3FM), microfiltration (MF), ultrafiltration (UF), nanofiltration (NF) and reverse osmosis (RO)) models describe the solid retention as a percentage of solids retained by the membrane, as a function of the membrane pore size. In the case of RO, scaling likelihood and antiscalant usage are measured. The investment and operational cost of the solid-liquid separation treatments are in general proportional to the flow treated. The operational costs considered are related to pumping energy but also to antiscalant dosage in the case of RO (Purchas 1977), using data from a specific provider to adjust the model parameter values.

Table 4 | Example of the model for MBBR unit

State	Output	Lower limit	Upper limit	
Q	$Q_{ef} = Q_{in}$	0	Inf	
X_b	$X_{b,ef} = f_{bulk_TOT} \cdot \left(\frac{Y_H}{f_{bulk_TOT}} (BOD_{in} - BOD_{max_ef}) \right)$	0	Inf	
X_i	$X_{i,ef} = f_{bulk_TOT} \cdot \left(\frac{HRT}{(f_{bulk_TOT})^2} \cdot f_{end} \cdot b_H \cdot Y_H (BOD_{in} - BOD_{max_ef}) + X_{i,in} \right)$	0	Inf	
C_b	$C_{b,ef} = f_{bulk_TOT_R} \cdot (f_{C_COD} \cdot BOD_{max_ef})$	0	Inf	
C_i	$C_{i,ef} = f_{bulk_TOT_R} \cdot (C_{i,inf})$	0	Inf	
S_f	$S_{f,ef} = (1 - f_{C_COD}) \cdot BOD_{max_ef}$	0	Inf	
S_a	$S_{a,ef} = 0.0$	0	Inf	
Investment costs (€)	$IC = C_{MBBR} \cdot \left(\frac{Q_{in} \cdot COD_{in}}{1,000} \right)^{K_{MBBR}}$	Operational costs (€/year)		
		$OP = P_{MBBR} \cdot \left(\frac{Q_{in} \cdot COD_{in}}{1,000} \right)^{K_{op}}$		
Model parameters	Description	Unit	Value	Reference
BOD_{max_ef}	Objective effluent BOD	g COD/m ³	10	Estimated for each case study
f_{bulk_TOT}	Bulk particulate/total particulate ratio	–	0.2	Estimated for each case study
$f_{bulk_TOT_R}$	Bulk colloid/total colloid ratio	–	0.05	Estimated for each case study
f_{C_COD}	C_b /COD ratio in effluent	–	0.3	Estimated for each case study
K_s	So consumption semi saturation constant	g COD/m ³	10	Henze <i>et al.</i> (2000)
b_H	Heterotrophic biomass decay rate	d ⁻¹	0.24	Henze <i>et al.</i> (2000)
Y_H	Heterotrophic biomass yield	–	0.67	Henze <i>et al.</i> (2000)
μ_H	So consumption rate constant	d ⁻¹	5	Henze <i>et al.</i> (2000)
f_{end}	Fraction of inert matter in biomass	–	0.08	Henze <i>et al.</i> (2000)
C_{MBBR}	Cost parameter for design	–	295	Adjusted to fit provider value
K_{MBBR}	Cost parameter for design	–	0.95	Adjusted to fit provider value
P_{MBBR}	Cost parameter for design	–	88.6	Adjusted to fit provider value
K_{OP}	Cost parameter for design	–	0.83	Adjusted to fit provider value

Taking into account the features explained above, the model for the DAF unit is presented in Table 5.

Four different chemical treatments are considered in the mathematical model library built for this work. The advanced oxidation process (AOP) model describes the transformation of a fraction of inert organic matter into biodegradable organic matter depending on the dosage of the oxidizing agent used. The disinfection unit models (O_3 , Cl_2 and UV) reproduce the pathogen removal as a function of the HRT, the disinfectant used and the operating conditions such as temperature and pH based on Chick's law (Asano et al. 2007). The coagulation unit model describes the fraction of colloidal and dissolved matter that coagulates depending on the quantity of coagulant added to the

process. Finally the Filtration Assisted Crystallization Technology (FACT) is modelled. FACT achieves hardness removal as a hybrid process combining precipitation and filtration. Precipitation is modelled based on the prediction of saturation of dissolution and the filtration is described as a fraction of crystals retained by the membrane. The investment costs of all the processes are proportional to the treated water flow, whilst operational costs are described as a function of the water flow and chemical agent dosage (Henze et al. 1995, 2008).

The mathematical model library described above has been implemented in the WQMT. Models implemented in this tool allow the assessment by simulation of different water network configurations and finding optimum

Table 5 | Example of the model for DAF unit

DAF model State	Clarified output (clar)	Floated output (float)	Lower limit	Upper limit
Q	$Q_{\text{clar}} = r \cdot Q_{\text{in}}$	$Q_{\text{float}} = (1 - r) \cdot Q_{\text{in}}$	0	Inf
TSS	$TSS_{\text{clar}} = (1 - f_{\text{float}}) \cdot TSS_{\text{in}} \cdot \frac{Q_{\text{in}}}{Q_{\text{clar}}}$	$TSS_{\text{float}} = f_{\text{float}} \cdot TSS_{\text{in}} \cdot \frac{Q_{\text{in}}}{Q_{\text{float}}}$	0	4,000
TCS	$TCS_{\text{clar}} = (1 - f_{\text{float}}) \cdot TCS_{\text{in}} \cdot \frac{Q_{\text{in}}}{Q_{\text{clar}}}$	$TCS_{\text{float}} = f_{\text{float}} \cdot TCS_{\text{in}} \cdot \frac{Q_{\text{in}}}{Q_{\text{float}}}$	0	8,000
X_j	$X_{j,\text{clar}} = \frac{X_{j,\text{in}}}{TSS_{\text{in}}} \cdot TSS_{\text{clar}}$	$X_{j,\text{float}} = \frac{X_{j,\text{in}}}{TSS_{\text{in}}} \cdot TSS_{\text{float}}$ where $j \in 27 - 42$	0	6,000
C_j	$C_{j,\text{clar}} = \frac{C_{j,\text{in}}}{TCS_{\text{in}}} \cdot TCS_{\text{clar}}$	$C_{j,\text{float}} = \frac{C_{j,\text{in}}}{TCS_{\text{in}}} \cdot TCS_{\text{float}}$ where $j \in 25, 26$	0	12,000
Investment costs (€)		Operational costs (€/year)		
$IC_{\text{DAF}} = C_{\text{DAF}} \cdot Q_{\text{inf}}^{K_{\text{DAF}}}$		$OP_{\text{DAF}} = P_{\text{DAF}} \cdot Q_{\text{inf}}^{K_{\text{OP}}} + P_{\text{AIR}} \cdot Q_{\text{AIR}}^{K_{\text{AIR}}}$		
Model parameters	Description	Unit	Value	Reference
r	Fraction of water recovered	–	0.78	Estimated for each case study
a_s	Air to solids ratio	mL/mg	0.005 – 0.06	Asano et al. (2007)
f_{float}	Fraction of particulate matter removed	–	$f_{\text{float}} = 0.66 \cdot a_s + 0.79$	Asano et al. (2007)
Q_{AIR}	Air flow required	–	$a_s \cdot TSS_{\text{in}} \cdot Q_{\text{in}}$	Asano et al. (2007)
C_{DAF}	Cost parameter for design	–	12,200	Adjusted to fit provider value
K_{DAF}	Cost parameter for design	–	0.45	Adjusted to fit provider value
P_{DAF}	Cost parameter for design	–	970	Adjusted to fit provider value
K_{OP}	Cost parameter for design	–	0.33	Adjusted to fit provider value
P_{AIR}	Cost parameter for design	–	280	Adjusted to fit provider value
K_{AIR}	Cost parameter for design	–	0.33	Adjusted to fit provider value

solutions considering effluent restrictions and economical costs. This WQMT is completely open for users to modify the existing model library or add new models to create their own model library in a user-friendly environment adapted to wastewater systems (Claeys *et al.* 2011).

DESIGN OF THE OBJECTIVE FUNCTION FOR WATER NETWORK COST OPTIMIZATION

The comparison of the alternative scenarios is carried out in terms of an objective function specifically defined for this work. The objective function takes into account the investment costs of the new treatments added to the network, operational costs of the operating devices, the cost associated with sludge production and the cost of fresh water consumption. The general equation of the objective function was defined as follows:

$$\begin{aligned} \text{COST} = & \sum_{i=\text{new treat}} \left(\text{IC}_i \cdot \frac{N}{\text{LS}_i} \right) + \sum_{i=\text{treat}} (\text{OP}_i \cdot N) \\ & + \left(73,000 \cdot \frac{\text{TSS}_w \cdot Q_w}{10^6} + 5,475 \cdot Q_w \right) \cdot \\ & N + 515 \cdot Q_{\text{FW}} \cdot K \cdot N \end{aligned}$$

where IC: Investment cost, N : No of years, LS: Lifespan, OP: Operational cost, TSS: Total suspended solids, Q_w : Waste flow, Q_{FW} : Fresh water flow.

A further upgrade of this work could be the consideration of both the economical costs and environmental impact in the objective function.

CASE STUDY: ASSESSMENT OF THE OPTIMUM SOLUTION FOR THE HOLMEN PAPER MADRID WATER NETWORK

The objective of this study is to check the capability of the model library to reproduce real water circuits and the capability of assessing optimum water networks using the WQMT. Using the model library presented above, a simulation model was constructed to reproduce the real water network in Holmen Paper Madrid (www.holmenpaper.com).

Description of the case study

Holmen Paper Madrid a user of approximately 10,000 m³ of fresh water per day no longer regards water as a consumable

or utility but as a highly valuable asset. Rather than discharge, the study of different scenarios in which wastewater is treated and internally reused to the municipal WWTP, it is a high priority for the mill itself.

The case study (Figure 2) includes four specific parts of paper production (Drum Pulper, Loop 1, Loop 2 and a Paper Machine), a heat exchanger, cooling tower, three DAFs and one thickener and finally the wastewater treatment plant existing in the mill (four MBBRs and one DAF). The internal circuit of the production line is closed, minimizing water consumption in the drum pulper, loop 1 and loop 2 (Blanco *et al.* 2009). Therefore, the only point at which water consumption can be reduced is the paper machine. There, water is spread in showers and it may be in contact with personnel, this factor is the reason why workers safety is the most demanding limitation for water quality for reuse. Moreover, conductivity has to be lower than 500 $\mu\text{S}/\text{cm}$ and solids free. The point from which water can be withdrawn is the effluent of the WWTP, but further treatments are needed to meet the quality requirements. The points from 1 to 14 marked in the water network are the sampling points (SP) at which experimental data are available. Data corresponding to the real plant have been provided by Holmen Paper Madrid and Complutense University of Madrid.

Modelling and verification of the existing water network

The model of the water network that describes the Holmen Paper water circuit was implemented in the WQMT and experimentally verified. The model has been constructed based on the mathematical model library introduced in this article and additional models that describe the processes of the production line in a paper mill ('black box' models where the outflows are expressed as function of water inflow and operational parameters). The experimental verification was done by monitoring throughout the whole circuit the following measurements: soluble chemical oxygen demand (COD), total suspended solids (TSS), sulphates and temperature. In order to fit these variables the model parameters need to be adjusted.

For the MBBR the stoichiometric, kinetic and operational parameters have been adopted from literature as shown in Table 4. Using these values the simulation results have been satisfactory regarding soluble COD and TSS in the WWTP effluent. Default values for the DAF model parameters are taken from literature (Table 5). However in this study the values of the air to solids ratio in each DAF have been adjusted to reproduce correctly the TSS at each point

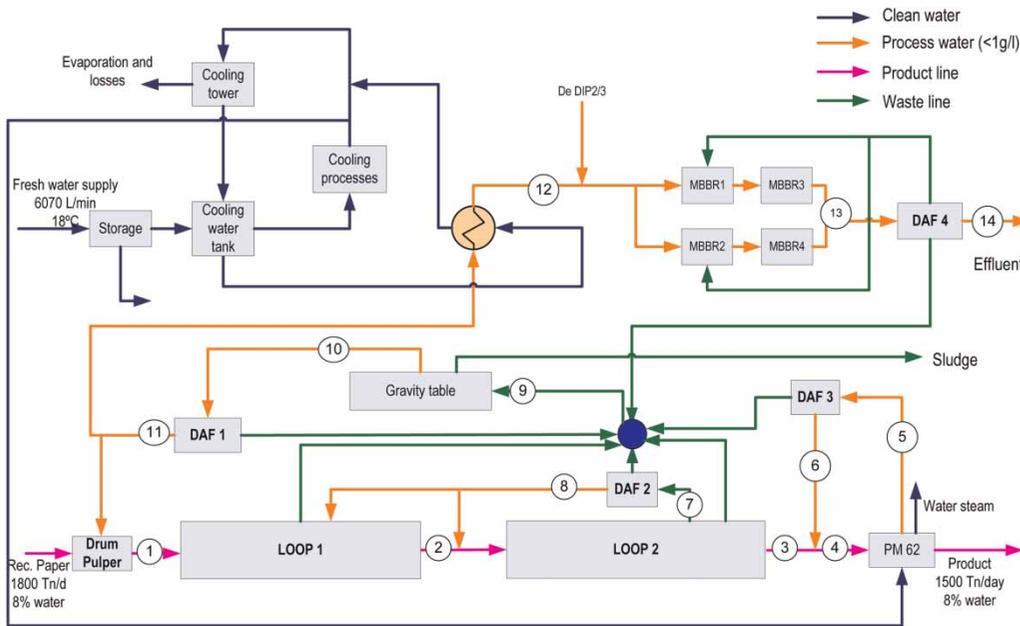


Figure 2 | Existing water network.

of the water network. The gravity table was designed as an ideal splitter and adjusted to reproduce the removal of TSS. The heat exchanger is modelled to calculate the fresh water required to cool the water going to the WWTP to a certain temperature. The processes of the production line were designed specifically for this case study, and all the model parameters were estimated to fix simulated data to the experimental data available in terms of the four measurements monitored.

Figure 3 shows that the simulation reproduces soluble COD and TSS throughout the circuit reasonably well. However, there is a mismatch regarding soluble COD between experimental and simulated data after the gravity table. In experimental data it is seen that there is an increase in

soluble COD in contrast to simulated data in the clarified outflow of the gravity table (SP10) possibly caused by the partial solubilization of the particulate matter in the gravity table. This error is transmitted to SP 11, the outflow of the DAF as it can be noticed that the difference between experimental and simulated data in SP 10 and 11 is similar.

In Figure 4 it can be seen that, in general, the model is able to reproduce the water network behaviour in terms of sulphates and temperature. In the case of the sulphates there is a difference in the simulated and experimental data in SP 10, the outflow of the gravity table. This reduction in the real network could be explained by precipitation of sulphates in the thickener. However, the model considers the thickener as an ideal splitter and therefore does not

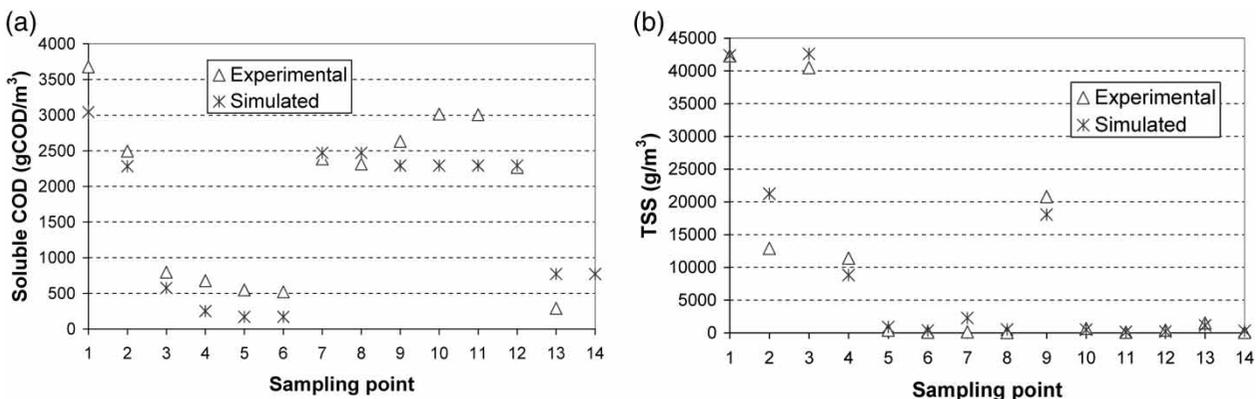


Figure 3 | (a) COD and (b) TSS monitoring through the circuit.

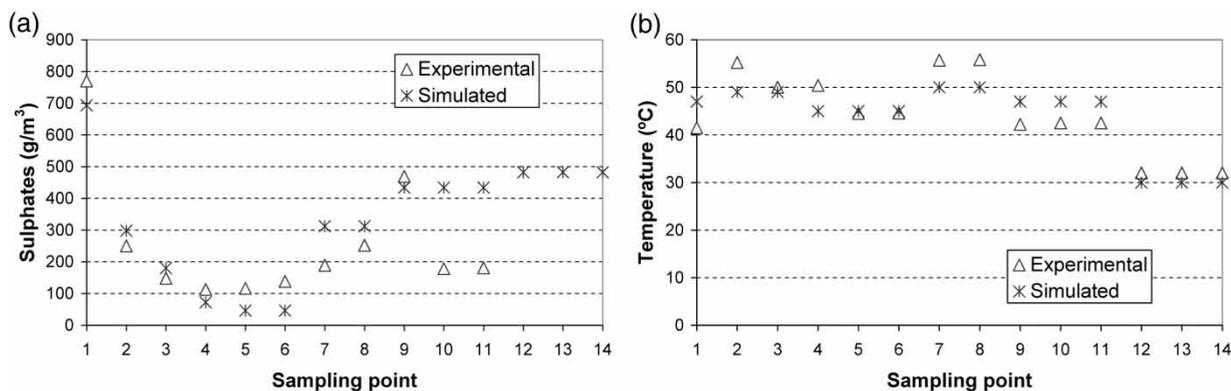


Figure 4 | (a) Sulphates and (b) Temperature monitoring through circuit.

predict precipitation. This error is again propagated to the outflow of the DAF. There are no experimental data available for sulphates in the wastewater treatment plant.

Based on these results, it can be said that the model is able to reproduce reasonably well the water network in the paper mill. Although it does not reproduce some effects happening in the gravity table, it must be pointed out that the overall objective of the model library presented is to make a first approach to assess how the economical cost of the mill could be reduced and not to accurately reproduce the process performance. If more detailed studies were required, models could be enhanced by considering for instance partial solubilization of the particulates or precipitation of sulphates.

Optimization by exploration of the water network

Once the capability of the model to reproduce the real circuit was checked, three different alternative scenarios for water reuse were compared: (i) the first scenario studied is the existing plant, discharging the effluent to the municipal WWTP; (ii) the second scenario incorporates a completely

new wastewater treatment plant including a UASB reactor, where COD and sulphates are biologically removed, an MBR to remove COD that could not be removed under anaerobic conditions and an evapoconcentrator to remove ions and possible pathogens present in the wastewater. The outflow of the evapoconcentrator meets the quality requirements so that it can be considered as an alternative water source for the paper machine; and (iii) the third scenario is a modification of the second scenario where the evapoconcentrator is substituted by a RO membrane to reduce conductivity and a disinfection unit to remove pathogens. The outflow of the disinfection unit meets the quality requirements of the paper machine and it can be considered as an alternative water source (Figure 5).

The three scenarios were implemented in the WQMT and a grid based exploration of the parameters has been carried out. A set of 1,295 simulations were run by different combinations of the three scenarios and by changing the fractions of water to be discharged and reused in each of the combinations. All the fractions of water considered have a discrete uniform distribution ranging from 0 to 1 with a spacing of 0.2.

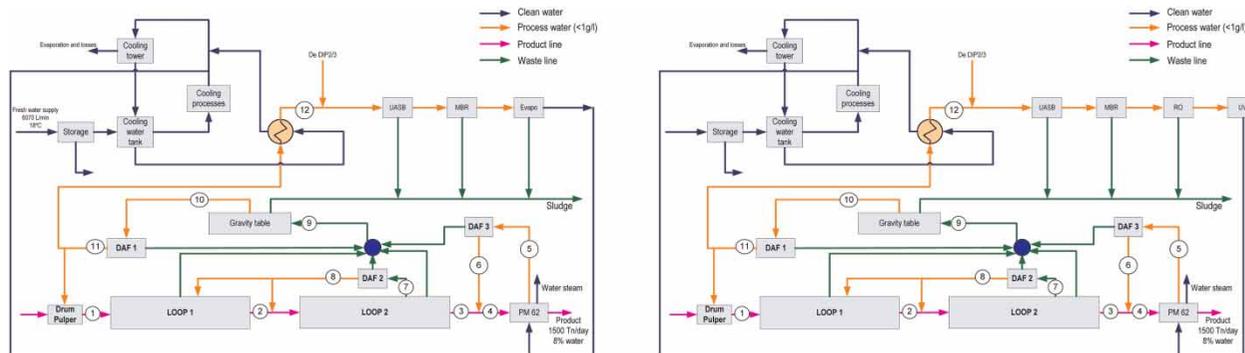


Figure 5 | Representation of the alternative scenarios.

Table 6 | Comparison of three alternatives

	Scenario 1		Scenario 2		Scenario 3	
	Investment cost (€)	Operational cost (€/y)	Investment cost (€)	Operational cost (€/y)	Investment cost (€)	Operational cost (€/y)
Drinking water	–	7,210,210	–	3,272,310	–	2,354,615
Sludge production	–	57,019,935	–	53,071,419	–	51,307,320
MBBR	–	348,605	–	–	–	–
DAF	–	19,434	–	–	–	–
UASB	–	–	2,453,025	11,754	2,593,192	12,405
MBR	–	–	3,326,701	77,324	3,643,882	83,524
Evapoconcentrator	–	–	2,685,131	177,755	–	–
RO	–	–	–	–	1,110,224	68,853
UV	–	–	–	–	189,863	56,959
Objective function	1,291,963,680 €		1,140,676,097 €		1,085,210,681 €	

The results obtained in this study show that even if an initial investment cost is needed; the exploitation costs are reduced when all the water is treated as in the third scenario and all the effluent of the disinfection process is internally reused for the paper production in the mill, reducing the total objective function. A brief summary of the results for each scenario can be seen in Table 6. In both scenarios the reduction of the objective function is mainly due to the reduction of the drinking water consumption as well as the reduction in sludge production. Moreover it should be kept in mind that even if new technologies need to be added, if these technologies allow recovery of energy or resources, as is the case of the UASB where energy is recovered as methane production, this situation will contribute to the sustainability of closed water networks.

Note that the objective function of the three scenarios presented differs in a small percentage, that is, slight changes in model parameters could lead to a different solution. To this respect, an uncertainty analysis of model parameters would be a very suitable study for assessing the robustness of the obtained optimum scenario. Although this study has not been tackled in this paper, a further version of the WQMT will allow carrying out this uncertainty analysis by means of Monte Carlo simulations.

CONCLUSIONS

The minimization of water consumption in industry entails a great deal of complexity because of the high number of alternatives. This study has shown with a first example the

benefits of using mathematical models for analysing different choices for water reuse in industry.

According to this, a new mathematical model library able to reproduce water circuits in the paper industry has been built. The ability of the models to reproduce real water circuits and the capability of obtaining optimum solutions considering economical aspects using the WQMT have been shown by means of the Holmen Paper Madrid case study analysis.

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REFERENCES

- Asano, T., Burton, F. L., Leverenz, H. L., Tsuchihashi, R. & Tchobanoglous, G. 2007 *Water Reuse: Issues, Technologies, and Applications*. McGraw-Hill, New York.
- Blanco, A., Ordóñez, R. & Hermosilla, D. 2009 *100% Reutilización de agua para fabricar 100% papel recuperado*. Infoenviro, Septiembre 2009.

- Claeys, F. H. A., Benedetti, L., Lizarralde, I. & de Gracia, M. 2011 WQMT: a software framework for representing and solving water quality issues in industry. In: *Proceedings from Watermatex '11*, June 20–22, San Sebastián, Spain.
- Henze, M., Harremoës, P., la Cour Janses, J. & Arvin, E. 1995 *Waterwater Treatment, Biological and Chemical Processes*. Springer, Heidelberg.
- Henze, M., Gujer, W., Mino, T. & van Loosdrecht, M. C. M 2000 *Activated Sludge Models ASM1, ASM2, ASM2d and ASM3*. Scientific and Technical Report N°9, IWA Publishing, London, UK.
- Henze, M., Van Loosdrecht, M., Ekama, G. A. & Brdjanovic, D. 2008 *Biological Wastewater Treatment: Principles, Modelling and Design*. IWA Publishing, London, UK.
- Lens, P., Hulshoff, P. & Asano, T. 2002 *Water Recycling and Resource Recovery*. IWA Publishing, London, UK.
- Lizarralde, I., de Gracia, M., Sancho, L., Ayesa, E. & Grau, P. 2010 New mathematical model for the treatment of wastewaters containing high sulphate concentration. In: *Proceedings from 1st Spain National Young Water Professionals*.
- Manan, Z. A. & Wan Alwi, S. R. 2007 [Water Pinch analysis evolution towards a holistic approach for water minimization](#). *Asia-Pacific Journal of Chemical Engineering* **2**, 544–553.
- Marais, G. v. R. & Ekama, G. A. 1976 The activated sludge process part 1 – steady state behaviour. *Water SA* **2** (4), 163–200.
- Purchas, D. B. 1977 *Solid/Liquid Separation Equipment Scale-Up*. Uplands Press Ltd.

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