

## Conceptual design and comparative assessment of WWTP layouts based on plant-wide model simulations

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### Summary of key findings

Model-based explorations are a very useful tool for the fast and rigorous assessment of any new wastewater treatment plant (WWTP) layout, and especially suitable in the preliminary analysis of the interrelations among leading-edge technologies and the other processes of the plant. This abstract presents the usefulness of mathematical models and simulation tools to describe the behaviour of advanced WWTPs taking into account technical, environmental, energetic and economic aspects. The main challenge of this work is the model-based assessment of different configurations using the Plant-wide modelling methodology: i) a conventional WWTP; ii) the combination of a high rate activated sludge system, operating at short SRT, coupled with an autotrophic (ADN) system for nitrogen removal; iii) an ADN system for the reject water treatment; and iv) the use of a Thermal Hydrolysis reactor as sludge pre-treatment. In the analysis, it has been seen that in a conventional WWTP configuration the energy content utilization is minimal, using only 7% of the available energy. Also it has been concluded that the most appropriate way to reduce operational costs is to decouple the carbon removal from the nitrogen removal using an ADN system in the water line.

### Background and relevance

In the last years, a new paradigm is emerging in which urban wastewater -traditionally considered as a pollution problem- is starting to be conceived as a continuous and sustainable source of resources. To address this shift, new and innovative combinations of emerging and conventional technologies and configurations in WWTPs can offer sustainable solutions for obtaining the required effluent quality, optimising the recovery of valuable by-products and energy. In this context, model-based explorations are a very useful tool for the fast assessment of any new WWTP layout. The main challenge of this work is to compare WWTPs configurations by simulation, taking into account energetic, economic and environmental aspects and analysing the use of the potential energy content of wastewaters. The complexity of the configurations and processes with recirculations and interrelations among the units makes it necessary to consider a plant-wide perspective in order to establish an optimum solution for the design or operation of the entire plant (Jeppsson *et al.*, 2007; Grau *et al.* 2007).

The PWM model library based on the Plant-wide modelling (PWM) methodology (Grau *et al.* 2007; Fernández-Arévalo *et al.*, 2014; Lizarralde *et al.*, 2015) is a suitable tool to construct compatible and directly connectable mathematical models so as to analyse the WWTP layouts as a whole. The PWM methodology is based on selecting the set of process transformations required to model all unit-process elements incorporated into each specific WWTP. The unification of these set of transformations permits the definition of a unique component vector for the whole plant, without the need to develop specific transformers to interface the unit-process models. The accurate definition of the stoichiometry ensures the elemental mass (in terms of C, N, O, H, P or other elements) and charge continuity in all these transformations, while the definition of the enthalpies of formation of each component allows the estimation of the reaction heat of each transformation. Thus, this methodology allows the straightforward construction of compatible mathematical models, being especially suitable for the comparative assessment of any combination of existing or under development technologies.

The PWM library is divided into three different parts: (1) Categories or transformations lists, which gather all components and biochemical, chemical and physic-chemical transformations needed to model all Unit Processes throughout the entire plant, (2) Unit process models that can be part of an advanced or conventional WWTP and (3) actuator models required in the costs estimation (Table 1.1).

**Table 1.1 Description of actuator models**

Actuator	Equations	Definition of parameters
Agitation engine model	$W_{\text{agit}} = \frac{N_p \phi_S N_{js}^3 D_{\text{stir}}^5}{\eta_{\text{agit}}} F_{\text{oversize}}$ $N_{js} = S \left( \frac{g(\phi_S - \phi_W)}{\phi_W} \right)^{0.45} \frac{X_{TSS}^{0.13} d_p^{0.2} \nu_W^{0.1}}{D_{\text{stir}}^{0.85}}$	<p><math>W_{\text{agit}}</math> (Electrical consumption of stirring [kJ d<sup>-1</sup>]); <math>F_{\text{oversize}}</math> (Oversize factor [-]); <math>\phi_S</math> and <math>\phi_W</math> (Solid and aqueous phase densities [g m<sup>-3</sup>]); <math>N_p</math> (Power number [-]); <math>N_{js}</math> (Impeller rotational speed required to just suspend the particles [Hz]); <math>D_{\text{stir}}</math> (Impeller diameter [m]); <math>\eta_{\text{agit}}</math> (Efficiency of agitation engines [%]); <math>S</math> (Impeller/tank geometry factor [-]); <math>X_{TSS}</math> (Weight percentage of solids in the suspension [%]); <math>g</math> (Gravitational acceleration [m s<sup>-2</sup>]); <math>d_p</math> (Particle size [m]); <math>\nu_W</math> (Kinematic viscosity of the aqueous phase [m<sup>2</sup> s<sup>-1</sup>]).</p>
Cogeneration unit model	$W_{\text{therm,w}} = (\dot{m}_{g,\text{in}})_{G_{CH4}} \Delta h_r \eta_{\text{therm,w}}$ $W_{\text{therm,g}} = (\dot{m}_{g,\text{in}})_{G_{CH4}} \Delta h_r \eta_{\text{therm,g}}$ $W_{\text{elect}} = (\dot{m}_{g,\text{in}})_{G_{CH4}} \Delta h_r \eta_{\text{elect}}$	<p><math>W_{\text{therm,i}}</math> (water and gas phase thermal energy production [kJ d<sup>-1</sup>]); <math>W_{\text{elect}}</math> (Electrical energy production [kJ d<sup>-1</sup>]); <math>\dot{m}_{g,\text{in}}</math> (Inlet gas phase mass flux [gE d<sup>-1</sup>]); <math>\Delta h_r</math> (Specific reaction enthalpy [kJ gE<sup>-1</sup>]); <math>\eta_{\text{therm,i}}</math> (Thermal degree of efficiency to produce water and gas phases [-]); <math>\eta_{\text{elect}}</math> (Electrical degree of efficiency [-]).</p>
Blower or compressor model	$W_{\text{blow}} = \sum_{i=1}^m \left[ \frac{(\dot{m}_{g,\text{in}})_i R T_{g,\text{in}}}{(MW)_i \left( \frac{\gamma_{g,i}-1}{\gamma_{g,i}} \right) \eta_{\text{blow}}} \right] \left[ \left( \frac{P_{g,\text{out}}}{P_{g,\text{in}}} \right)^{\frac{\gamma_{g,i}-1}{\gamma_{g,i}}} - 1 \right]$ $k_{L,a} = \alpha_{kLa} F_{kLa} \theta_{kLa} T_w^{-293} \frac{OTE_{293} (\dot{m}_{g,\text{in}})_{G_{O2}}}{V_w C_{\infty}^*}$	<p><math>W_{\text{blow}}</math> (Electrical consumption of blower or compressors [kJ d<sup>-1</sup>]); <math>R</math> (Ideal gas constant [kJ mol<sup>-1</sup> K<sup>-1</sup>]); <math>T_{g,\text{in}}</math> (gas phase inflow temperature [K]); <math>MW_i</math> (Molecular weight of <math>i</math> gaseous phase components [g mol<sup>-1</sup>]); <math>\gamma_{g,i}</math> (Heat capacity ratio of the <math>i</math> gaseous phase components [-]); <math>\eta_{\text{blow}}</math> (Efficiency of blowers/compressors [-]); <math>P_{g,\text{in}}</math> and <math>P_{g,\text{out}}</math> (Absolute gas pressure at the blower inlet and outlet [bar]); <math>k_{L,a}</math> (Mass transfer coefficient [d<sup>-1</sup>]); <math>\alpha_{kLa}</math> (ratio of process water to clean water mass transfer coefficient [-]); <math>F_{kLa}</math> (Fouling factor [-]); <math>\theta_{kLa}</math> (Constant for temperature effect on <math>k_{L,a}</math> [-]); <math>T_w</math> (water temperature [K]); <math>OTE_{293}</math> (Oxygen transfer rates at 293 K [-]); <math>V_w</math> (Volume of the water phase [m<sup>3</sup>]); <math>C_{\infty}^*</math> (Saturation concentration [gE m<sup>-3</sup>]).</p>
Pump model	$W_{\text{pump}} = \phi_W g Q_W HL \eta_{\text{pump}}$ $HL = HL_s + HL_f + HL_l$ $HL_f = f_{\text{coeff}} \left( \frac{L_{\text{pipe}}}{D_{\text{pipe}}} \right) \left( \frac{u_W}{2g} \right)$	<p><math>W_{\text{pump}}</math> (Electrical pump consumption [kJ d<sup>-1</sup>]); <math>Q_W</math> (Water flow rate [m<sup>3</sup> d<sup>-1</sup>]); <math>HL</math> (Total head loss [m]); <math>HL_s</math> (Static head [m]); <math>HL_f</math> (Friction head loss [m]); <math>HL_l</math> (Minor losses [m]); <math>f_{\text{coeff}}</math> (Friction coefficient [-]); <math>L_{\text{pipe}}</math> and <math>D_{\text{pipe}}</math> (Pipe length and diameter [m]); <math>u_W</math> (Liquid velocity [m s<sup>-1</sup>]).</p>
Boiler model	$W_{\text{steam}} = (\dot{m}_{g,\text{in}})_{G_{CH4}} \Delta h_r \eta_{\text{steam}}$	<p><math>W_{\text{steam}}</math> (steam thermal energy production [kJ d<sup>-1</sup>]); <math>\eta_{\text{steam}}</math> (Thermal degree of efficiency to produce steam [-]).</p>

## Results

Several innovative plant layouts, incorporating conventional and leading-edge technologies have been simulated and compared. As a basis scenario for comparisons, an optimised conventional WWTP layout based on the Benchmark Simulation Model No. 2 (BSM2) has been taken (Jeppsson *et al.*, 2007). The other configurations are, ii) the combination of a high rate activated sludge system, operating at short retention time, coupled with an autotrophic system (ADN) for nitrogen removal; iii) a Thermal Hydrolysis (TH) reactor as sludge pretreatment; and iv) the incorporation of an ADN system for the reject water treatment. Thus, the preliminary results obtained are shown in Table 1.2.

In the TH process, a rise in electric power production has been observed due to the increase of the sludge biodegradability. At low temperatures, it was necessary to oxidize part of biogas to use it in the steam production, achieving a lower electric energy than expected (6-10%). It is for this reason, that the temperature of the water stream is an important factor in the TH process viability. An increase in aeration costs have also been observed due to the 20% increase of N-NH<sub>4</sub> concentration in the sludge digester effluent. The smaller sludge production in case of the incorporation of an ADN system for the reject water treatment is the reason why a little less electric energy has been produced. Even so, the ADN system has reduced the aeration costs by 16% because of the Anammox process. Finally, it has been seen that the optimum way to reduce operational costs considerably, was disengaging the carbon removal from the nitrogen removal. Anoxic zones are removed, reducing agitation costs; aeration costs are minimized by 60% thanks to the ADN process; and the SRT is reduced increasing the electrical energy production, with a surplus of thermal energy unlike the preceding cases. Nonetheless, the disadvantage compared with the other layouts is the difficulty to maintain a stable population of Anammox bacteria at low temperatures and the difficulty of obtaining low effluent N-NH<sub>4</sub> values.

Table 1.2 Comparison of different configurations at 13°C of water temperature

		Optimized BSM2	BSM 2 + TH	BSM 2 + ADN (sludge line)	BSM 2 + ADN (water line)
Effluent quality	N-NH <sub>4</sub> (gN/m <sup>3</sup> )	1.92	1.8	2	3
	N-NO <sub>2</sub> (gN/m <sup>3</sup> )	-	-	0.0	0.0
	N-NO <sub>3</sub> (gN/m <sup>3</sup> )	7.9	8.2	8	3 - 3.2
Operational variables	SRT in the water line (d)	20	20	28	3.15
	Steam needed (ton/h)	-	0.19	-	-
Energy needed	Aeration energy activated sludge (kW)	184	1.5%	-16%	-60%
	Digester Heating / steam (kW)	0	0%	0%	0%
	Agitation (kW)	41	0%	0%	-58%
Energy produced	Cogeneration elec. Energy (kW)	242	6-10%	-6%	10-20%
	Surplus thermal energy (kW)	0	0	0	0 - 10%

Additional analyses of elemental mass and energy fluxes for each plant configuration have been also carried out, to evaluate the optimal use of the energy and to identify the possible areas for energy improvement. Figure 1.1 shows an example of this for the prediction of the different energy fluxes in a conventional WWTP. As can be seen, only 7% of the mass energy content of the wastewater (0.5% of the total mass and thermal energy content) is converted into electricity. This electricity produced can supply 77% of the operational costs analysed. In the analysed operational costs, the aeration represents 70% of the costs, followed by the pumping energy with 11% (without including in the analysis the raw water pumping) and the digester and anoxic tanks agitation (7% and 10% respectively). So, it has been observed that through a better use of energy, it could be reached to have a self-sufficient plant.

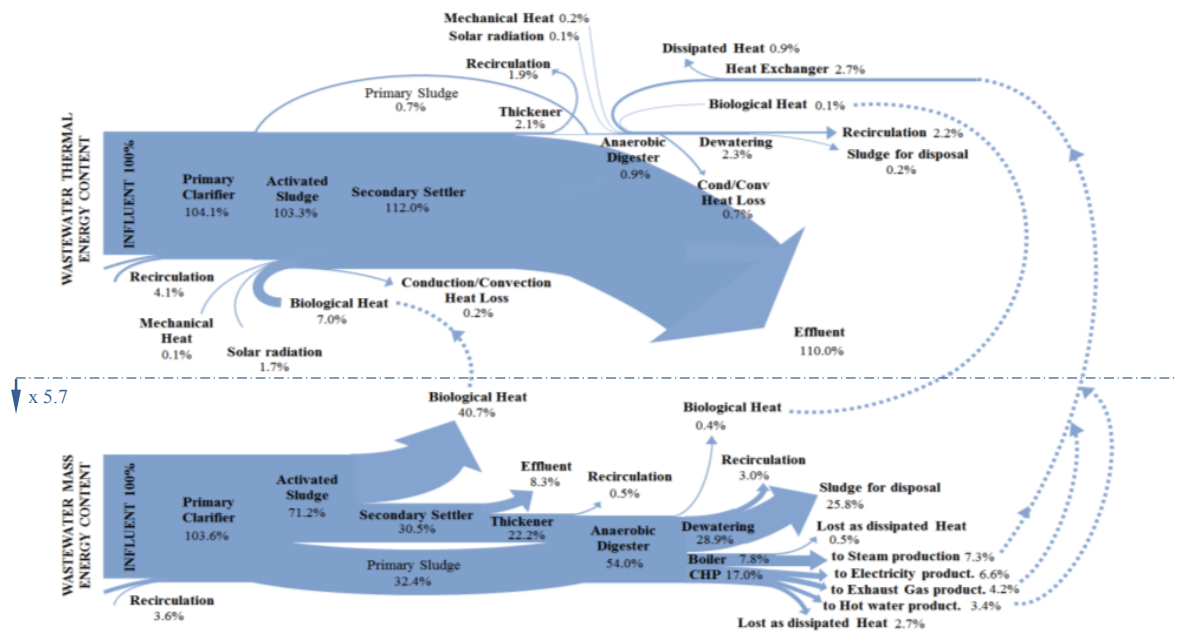


Figure 1.1 Simulation example of the wastewater mass and thermal energy content throughout a plant

## Discussion

Simulation results have demonstrated the usefulness of the proposed model-based methodology to identify the most appropriate combination of conventional and leading-edge technologies for each specific treatment scenario, taking into account effluent quality, energy balance, resources recovery and economy in a holistic approach. This result opens the door to develop a new generation of WWTPs: from waste to products.

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