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Quantitative assessment of energy and resource recovery in wastewater treatment plants based on plant-wide simulations

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ABSTRACT

The growing development of technologies and processes for resource treatment and recovery is offering endless possibilities for creating new plant-wide configurations or modifying existing ones. However, the configurations' complexity, the interrelation between technologies and the influent characteristics turn decision-making into a complex or unobvious process. In this frame, the Plant-Wide Modelling (PWM) library presented in this paper allows a thorough, comprehensive and refined analysis of different plant configurations that are basic aspects in decision-making from an energy and resource recovery perspective. In order to demonstrate the potential of the library and the need to run simulation analyses, this paper carries out a comparative analysis of WWTPs, from a techno-economic point of view. The selected layouts were (1) a conventional WWTP based on a modified version of the Benchmark Simulation Model No. 2, (2) an upgraded or retrofitted WWTP, and (3) a new Wastewater Resource Recovery Facilities (WRRF) concept denominated as C/N/P decoupling WWTP. The study was based on a preliminary analysis of the organic matter and nutrient energy use and recovery options, a comprehensive mass and energy flux distribution analysis in each configuration in order to compare and identify areas for improvement, and a cost analysis of each plant for different influent COD/TN/TP ratios. Analysing the plants from a standpoint of resources and energy utilization, a low utilization of the energy content of the components could be observed in all configurations. In the conventional plant, the COD used to produce biogas was around 29%, the upgraded plant was around 36%, and 34% in the C/N/P decoupling WWTP. With regard to the self-sufficiency of plants, achieving self-sufficiency was not possible in the conventional plant, in the upgraded plant it depended on the influent C/N ratio, and in the C/N/P decoupling WWTP layout self-sufficiency was feasible for almost all influents, especially at high COD concentrations. The plant layouts proposed in this paper are just a sample of the possibilities offered by current technologies. Even so, the library presented here is generic and can be used to construct any other plant layout, provided that a model is available.

1. Introduction

The purpose of the design and upgrade of conventional waste(water) treatment plants (WWTPs) has traditionally been to remove the residual organic compounds and nutrients contained in the water to fulfil quality standards. Resource or energy recovery was focused exclusively on obtaining energy from the biogas produced in anaerobic sludge digestion. This biogas production can supply from a quarter to half of the energy requirements for a

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Nomenclature

$Cost_{actuator}$	Actuator cost (€ d^{-1})
$Cost_{Chem}$	Chemical agent specific cost (€ kg^{-1})
$Cost_{dosage}$	Chemical agent globalcost (€ d^{-1})
$Cost_{poly}$	Polyelectrolyte specific cost (€ kg^{-1})
d_p	Particle size (m)
D_{pipe}	Pipe diameter (m)
D_{sti}	Impeller diameter (m)
f_{moody}	Friction coefficient
$F_{oversize}$	Oversize factor
G	Gravitational acceleration (m s^{-2})
G	Velocity gradient (s^{-1})
$\overline{H}_{in}$	Input enthalpy (kJ d^{-1})
$\overline{H}_{out}$	Output enthalpy (kJ d^{-1})
HL	Total head loss (m)
HL_f	Friction head loss (m)
HL_l	Minor losses (m)
HL_s	Static head (m)
k_{Chem}	Dosage constant (g_{chem} m^{-3})
$k_{poly,i}$	Polyelectrolite and Total solids concentration ratio for the sludge type i (g_{poly} kg^{-1}_{TSS})
L_{pipe}	Pipe length (m)
$\overline{m}_{i,in}$	Inlet i phase mass flux (gE d^{-1})
MU	Monetary unit (€ d^{-1})
MW_i	Molecular weight of i gaseous phase components
n_{CEPT}	Chemically Enhanced Primary Treatment constant
N_{js}	Impeller rotational speed required to just suspend the particles (Hz, revolutions per sec.)
N_P	Power number
$P_{g,in}$	Absolute gas pressure at the blower/compressor inlet
$P_{g,out}$	Absolute gas pressure at the blower/compressor outlet
Q_w	Water flow rate (m^3 d^{-1})
R	Ideal gas constant (kJ mol^{-1} K^{-1})
S	Impeller/tank geometry factor
Submergence	Submergence (m)
$T_{i,in}$	i phase inflow temperature (K)
$T_{i,out}$	i phase outflow temperature (K)
TSS_i	Total suspended solids concentration in the phase i (gSS m^{-3})
u_w	Average liquid velocity (m s^{-1})
V_i	Volume of the i phase (m^3)
$W_{actuator}$	Electrical consumption of actuators (W_{blow}, W_{pump}, W_{stir}, $W_{turbine}$, etc.) (kJ d^{-1})
W_{blow}	Electrical consumption of blower or compressors (kJ d^{-1})
W_{pump}	Electrical consumption of pump (kJ d^{-1})
W_{stir}	Electrical consumption of stirring (kJ d^{-1})
$W_{turbine}$	Electrical consumption of turbine (kJ d^{-1})
X_{TSS}	Weight percentage of solids in the suspension

Greek Symbols

$gamma_{g,i}$	Heat capacity ratio of the i gaseous phase components
η_i	Dynamic viscosity (kg m^{-1} s^{-1})
η_{blow}	Efficiency of blowers/compressors
η_{CEPT}	Chemically Enhanced Primary Treatment efficiency
η_{max}	Chemically Enhanced Primary Treatment maximum efficiency
η_{min}	Chemically Enhanced Primary Treatment minimum efficiency
η_{pump}	Efficiency of pumps
η_{stir}	Efficiency of agitation engines
η_{turb}	Efficiency of turbines
υ_i	Kinematic viscosity of the i phase (m^2 s^{-1})
φ_i	Density (g m^{-3})

Subscripts

Comp	Phase components
G	Gaseous phase
M	No. of state variables in the off-gas phase
S	Solid phase
W	Aqueous phase

WWTP with an activated sludge (AS) process (WERF, 2010; McCarty et al., 2011; Puchongkawarin et al., 2015), which needs between 0.3 and 0.6 kWh $m^{-3}_{treated\ water}$ (Foley et al., 2010) to fulfil the energetic needs of the plant. Nevertheless, this value is only one tenth of that associated to the heat of combustion of organic compounds contained in the wastewater (McCarty et al., 2011; Shoener et al., 2014; Kokabian and Gude, 2015). Hence, if a greater proportion of this energy was recovered, treatment plants could become self-sufficient and producers of energy (Logan, 2004; Guest et al., 2009).

Recent concerns about climate change or sustainability have led to an increasing awareness of the importance of resource recovery, energy minimization and environmental impact assessment, which in turn has resulted in tightening effluent standards. Under this changing context, a new paradigm has emerged in which municipal wastewater (MWW), traditionally considered to be a pollution problem and an energy- and chemical-intensive activity with excess sludge disposal issues (Gude, 2015), is starting to be thought of as a continuous and sustainable source of chemical energy and resources (Frijns et al., 2013). As a result, WWTPs are now considered to be Wastewater Resource Recovery Facilities (WRRF) from which valuable products like chemicals, nutrients (mainly phosphorus, P), bioenergy (methane from anaerobic digestion) and bioproducts can be obtained (Keller, 2008; Guest et al., 2009). To make this change possible, the water sector is developing new and innovative treatment technologies, such as energy-efficient nutrient removal or recovery technologies with Anammox, struvite crystallisers, phototropic bacteria, high rate algae systems, sludge pre-treatment processes, or systems for the production of microbial polymers.

The most immediate step for reaching this goal is the updating of existing plants in order to reduce overall operating costs and recover resources. Thanks to the incorporation of new technologies or different plant layouts, energy self-sufficient WWTPs is a feasible goal (Jeppsson et al., 2007). Proof of this comes from the Strass and Wolfgangsee-Ischl WWTPs in Vienna (Wett et al., 2007; Nowak et al., 2011). As stated in the work of Batstone et al. (2015), currently there are two extended philosophies to address the transition from WWTPs to WRRF's. One is the low energy mainline (LEM) configuration, which focuses on using low strength anaerobic digestion processes for treating raw domestic sewage, followed by nutrient removal processes (McCarty et al., 2011). The other is the Partition-Release-Recover (PRR) configuration, which focuses on a first stage of chemical oxygen demand (COD) and nutrient accumulation in the solids, a second stage of release through the digestion process, and a final stage of digestate treatment (Verstraete et al., 2009).

In the literature there are numerous studies comparing different plant layouts and analysing the energy consumption of conventional WWTPs (Nowak, 2003; Gude, 2015; Tchobanoglous et al., 2014; Mininni et al., 2015), and fewer studies analysing advanced WWTPs (Garrido et al., 2014; Batstone et al., 2015; Khiewwijit et al., 2015), many of which use life cycle analysis (LCA) methods and decision support system (DSS) tools (Foley et al., 2010; Garrido-Baserba et al., 2014; Bisinella de Faria et al., 2015; Castillo et al., 2016). Even so, virtually all these studies are based on operating cost analysis and are largely dependent on the quality of the ratio used and their specifications. The use of ratios brings simplicity to mathematical models, while streamlines the simulation process. However, these indicators can only be used near the operating point where they were estimated, under similar operating conditions (solids concentration, temperature, etc.) or for units or processes with the same characteristics (drive type, elevation changes, number of diffusers, diffusers submergence, etc.). Consequently, an improper use of these ratios can lead to underestimates or overestimates of operating costs. One of the main problems found in these energy assessments is the limited information available to reproduce disturbances or unusual situations (Jenkins and Wanner, 2014). Many of these ratios are function of the flow only (collected in units of kWh m^{-3}) and they do not consider the load variations. It is for this reason that the best tool for overcoming all these obstacles is to conduct mass balances for COD, nitrogen (N), and phosphorus (P) for the whole plant (Spindler and Vanrolleghem, 2012; Jenkins and Wanner, 2014), and to use, as far as possible, detailed cost models that depend on operational process variables (flowrates, enthalpy changes of reaction, solids concentration, etc.). The detailed analysis of each stream allows for better understanding of the process, identifying areas for improvement and opportunity for resource and energy recovery. Among existing approaches in the literature, the Plant-Wide Modelling (PWM) methodology proposed by Ceit-IK4 (Grau et al., 2007a; Fernández-Arévalo et al., 2014; Lizarralde et al., 2015) constitutes a very suitable tool for rigorously and globally assessing the incorporation of new leading-edge technologies in conventional plant layouts (as was verified in a preliminary analysis carried out in Fernández-Arévalo et al., 2015) or selecting the most appropriate operating strategies at existing full-scale facilities (Fernández-Arévalo et al., 2017b).

The main objective of this paper is to conduct a comparative analysis of WWTPs, from a techno-economic point of view, analysing in turn organic matter and nutrient energy use and recovery options. To do this, an upgraded plant and a newly designed plant have been analysed and compared against a conventional plant (based on the Benchmark Simulation Model No. 2 configuration; Jeppsson et al., 2007) using the PWM methodology described in Grau et al. (2007a) Fernández-Arévalo et al. (2014), and Lizarralde et al. (2015). In the upgraded or retrofitted WWTP, thermal hydrolysis (TH) technology and a nitritation/Anammox process have been incorporated into the reference plant, and the new plant is a C/N/P decoupling WWTP, which is based on the PRR configuration proposed by Batstone et al. (2015).

2. Modelling tool: Plant-Wide Modelling library

The Plant-Wide Modelling (PWM) methodology (Grau et al., 2007a; Fernández-Arévalo et al., 2014; Lizarralde et al., 2015) allows for rigorous and systematic construction of compatible unit-process models (UPM) in order to describe the dynamic behaviour of different processes and technologies in the water and sludge lines in an integrated way. This PWM methodology is based on selecting, from a global list, the set of process transformations required to describe all unit-processes incorporated into each specific WWTP. Thus, the model will be constituted by a unique set of transformations and components vector that will allow for the description of all relevant processes occurring in the plant (Grau et al., 2007a; Fernández-Arévalo, 2016). An accurate definition of the stoichiometry and the enthalpies of formation ensures the elemental mass, charge and energy continuity through the whole plant (Fernández-Arévalo et al., 2014; Fernández-Arévalo, 2016). This methodology allows for the straightforward construction of different plant-wide models, which is especially suitable for the comparative assessment of any combination of existing technologies and configurations or those that are under development.

Following the guidelines proposed by Grau et al. (2007a), Fernández-Arévalo et al. (2014) and Lizarralde et al. (2015) and with the goal of simplifying plant-wide models construction, this paper uses the PWM library (Fig. 1). The users can construct their own plant-wide models by the means of the appropriate selection of the category, unit-process models and cost models depending on the case under study (Fernández-Arévalo et al., 2017a).

2.1. *Category selection*

Each category includes equations describing a set of biochemical, chemical and physico-chemical transformations. Depending on the complexity of the WWTP and the goals and scope of the modelling study users could select one category or another. The model categories have been developed combining conventional biological processes described in ASM (Henze et al., 2000) and ADM (Batstone et al., 2002) models with chemical and physico-chemical processes. All of them are represented by means of the definition of a stoichiometric matrix and kinetics vector (Grau et al., 2007a; Lizarralde et al., 2015). The nomenclature used to define the categories is as follows: “C”, “N” and “P” describe biological organic matter biodegradation, N biodegradation, and biological and chemical P removal, respectively, all of them in aerobic and anoxic conditions at low and high temperatures (TH reactions); “2N” specifies two-step N removal and Anammox reactions; “chem” denotes chemical P but not biological P removal; “prec” includes precipitation reactions; and finally, “AnD” describes anaerobic conditions at low and high temperatures (fermentation and digestion).

The organised structure that the methodology presents enables the straightforward development of categories, allowing the library to be continuously updated (the latest version of the categories can be found in Fernández-Arévalo, 2016).

2.2. *Unit-process model selection*

The Ceit PWM library contains a set of unit-process models that describes the mass and energy transport in each unit. According to the features of novel technologies and processes analysed in advanced WWTPs, these models consider in most of the cases aqueous, gas and solid phases and mass and energy exchange among them (Fernández-Arévalo et al., 2014; Lizarralde et al., 2015).

2.3. *Cost model selection*

Lastly, the library includes a set of actuator models, specific energy ratios and dosage cost models in order to estimate in detail the costs of each element (see Table 1). Cost models parameters can be found in the Supplemental Information Sections 1 (Tables A.1-A.8). All actuator models are developed based on engineering expressions instead of directly using cost curves or fixed values. The models are standardised, so they can be used interchangeably in any category.

The model presented in this paper is part of a series of papers already published. The calibration and validation of the model has

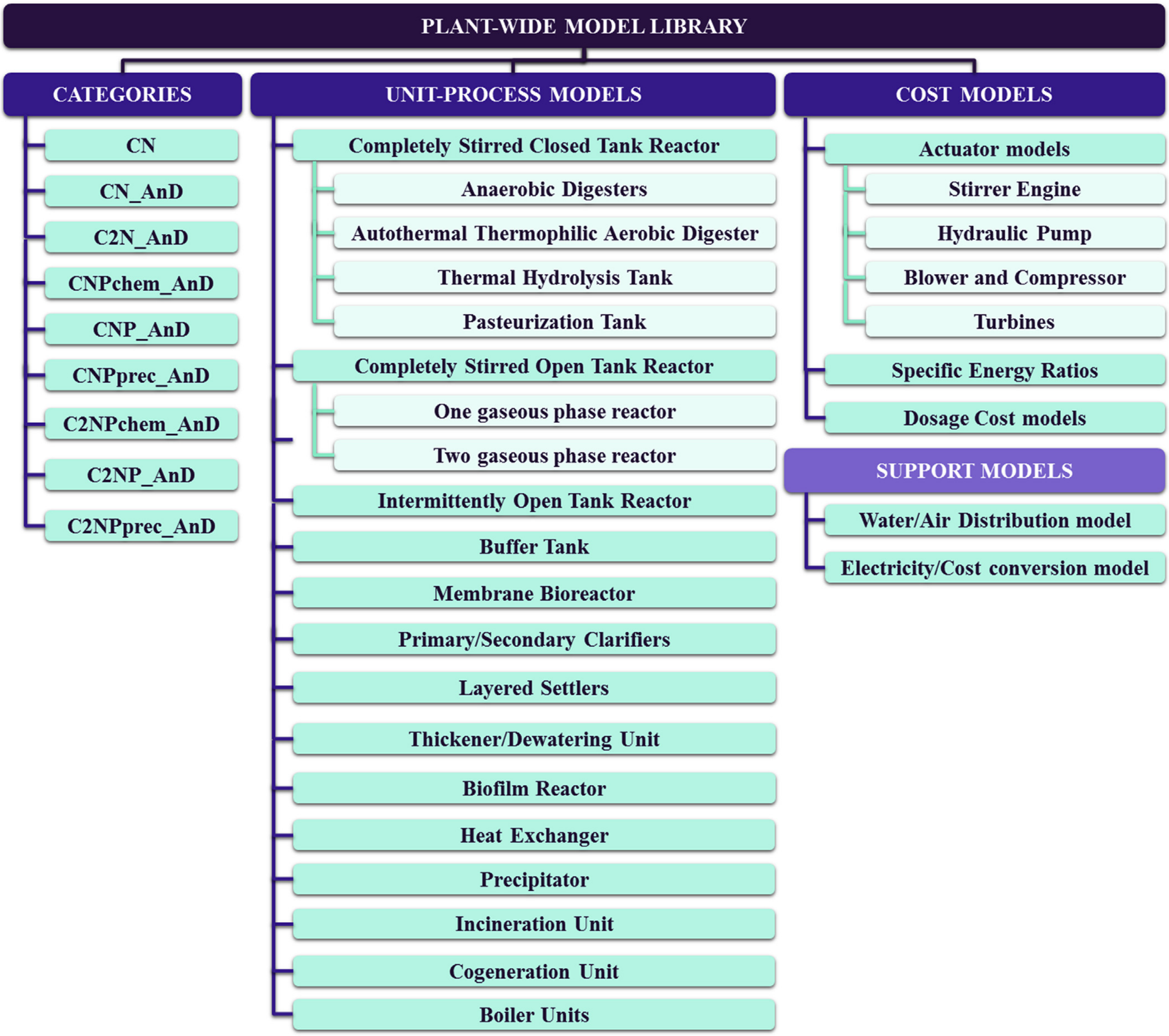

Fig. 1. Schematic representation of the Ceit Plant-Wide Model library.

previously been done (Grau et al., 2007b; Fernández-Arévalo et al., 2014; Lizarralde et al., 2015, 2016; Sainz et al., 2015; Fernández-Arévalo, 2016; Fernández-Arévalo et al., 2017b) and consequently this paper focuses on the application of the model.

3. Description of the scenarios

The comparative analysis of the three configurations selected (conventional WWTP, upgraded WWTP and C/N/P decoupling WWTP) has been based on PWM simulations. To a greater or lesser degree, all simulations have taken the Benchmark Simulation Model No. 2 (BSM2; Jeppsson et al., 2007) configuration as a reference. As a novelty regarding the BSM2 configuration, a dissolved air flotation (DAF) unit has been added to the configuration to replace the secondary sludge thickener, a cogeneration unit for the estimation of the thermal and electrical energy obtained from the biogas, and a chemical and/or biological treatment of phosphorus to consider a complete nutrients removal (the BSM2 configuration only considers COD and N removal). Finally, a total suspended solids removal of 60% in the primary sedimentation has been considered. This section details the description of these plant layouts and the steps followed to build the model.

3.1. Plant layouts definition

3.1.1. Conventional WWTP

The plant layout (Fig. 2) is constituted by a primary clarifier for the pre-treatment step, an AS process for C and N removal based on a Modified Ludzack-Ettinger configuration (2 anoxic and 3 aerobic tanks and a secondary clarifier), a DAF unit to treat the secondary sludge, an anaerobic digestion process and a dewatering step. A ferric chloride dosage is delivered to the output from the third aerobic tank for chemical P removal. Besides adding the chemical agents for P removal, ferric chloride can also be added to enhance the settling characteristics of the primary sludge for cases in which the production of primary sludge needs to be maximised. Finally,

Table 1
Description of cost models (Actuators, Specific Costs and Dosage Cost models).

	Equations	
Actuator Models		
Stirrer Engine Model	For maintaining solids in suspension	$W_{stir} = \frac{N_P \varphi_s N_{js}^3 D_{stir}^5}{\eta_{stir}} F_{oversize}; \quad N_{js} = S\left(\frac{g(\varphi_s - \varphi_w)}{\varphi_w}\right)^{0.45} \frac{X_{TSS}^{0.13} d_p^{0.2} v_w^{0.1}}{D_{stir}^{0.85}}$
	For rapid mixing or flocculation	$W_{stir} = G^2 \eta_w V_w$
Hydraulic pump model	$W_{pump} = \varphi_W g Q_W HL \eta_{pump} H_{w,out} = H_{w,in} + W_{pump} (1 - \eta_{pump})$	
Blower and Compressor model	$W_{blow} = \sum_{comp=1}^{m} \left[\frac{(\dot{m}_{g,in})_{comp} R T_{g,in}}{(MW)_{comp} \left(\frac{\gamma_{g,comp}-1}{\gamma_{g,comp}}\right) \eta_{blow}}\right] \left[\left(\frac{P_{g,out}}{P_{g,in}}\right)^{\frac{\gamma_{g,comp}-1}{\gamma_{g,comp}}} - 1\right]$ $T_{g,out} = \frac{T_{g,in}}{\eta_{blow}} \sum_{comp=1}^{m} \left(\frac{(\dot{m}_{g,in})_{comp}}{\sum_{comp=1}^{m} (\dot{m}_{g,in})_{comp}} \left(\frac{P_{g,out}}{P_{g,in}}\right)^{\frac{\gamma_{g,comp}-1}{\gamma_{g,comp}}} - (1 - \eta_{blow})\right)$	
Turbine model	$W_{turbine} = \sum_{comp=1}^{m} \left[\frac{(\dot{m}_{g,in})_{comp} R T_{g,in}}{(MW)_{comp} \left(\frac{\gamma_{g,comp}-1}{\gamma_{g,comp}}\right)}\right] \left[\eta_{turb} - \left(\frac{P_{g,in}}{P_{g,out}}\right)^{\frac{1-\gamma_{g,comp}}{\gamma_{g,comp}}}\right]$ $T_{g,out} = T_{g,in} \sum_{comp=1}^{m} \left(\frac{(\dot{m}_{g,in})_{comp}}{\sum_{comp=1}^{m} (\dot{m}_{g,in})_{comp}} \left(\frac{P_{g,out}}{P_{g,in}}\right)^{\frac{\gamma_{g,comp}-1}{\gamma_{g,comp}}} + (1 - \eta_{turb})\right)$	
Support Models		
Water/Air Distribution model	Detailed Model	$HL = HL_S + HL_f + HL_l; \quad HL_f = f_{moody} \left(\frac{L_{pipe}}{D_{pipe}}\right) \left(\frac{u_w^2}{2g}\right)$
	Approximation	$P_{g,out} = \varphi_W g (Submergence + 1) 10^{-5}$
Electricity/cost conversion model	$Cost_{actuator} = W_{actuator} MU$	
Dosage Cost Models		
Chemically Enhanced Primary Treatment (CEPT)	$Cost_{dosage} = Cost_{Chem} \left[\frac{€}{kg}\right] \cdot \left(\frac{k_{Chem}^{n_{CEPT}} \left(1 - \frac{\eta_{max} - \eta_{CEPT}}{\eta_{max} - \eta_{min}}\right)}{\frac{\eta_{max} - \eta_{CEPT}}{\eta_{max} - \eta_{min}}}\right)^{1/n_{CEPT}}$	
Poly-electrolyte dosage costs	$Cost_{dosage} = Cost_{poly} \left[\frac{€}{kg}\right] \cdot \sum_{i=1}^{N^o\ of\ kinds\ of\ sludge} \left(TSS_i Q_W k_{Poly,i} \left[\frac{g_{poly}}{kg_{TSS}}\right]\right)$	

(Camp and Stein, 1943; CEDEX, 2004; Tchobanoglous et al., 2014; Tik and Vanrolleghem, 2017; Weisbach, 1845; Zaher et al., 2009; Zweitering, 1985).

two other chemical additions are required in the flotation and dewatering processes: ferric chloride and polyelectrolyte polymers to improve flocculation in the DAF unit, and polyelectrolyte for enhancing sludge dewaterability.

3.1.2. Upgraded WWTP

This second layout is based on the reference case (conventional WWTP), but with two advanced technologies being incorporated in the sludge line: a thermal hydrolysis (TH) reactor and a nitritation/Anammox process for treating the rejected supernatants (Fig. 3).

The aim of the TH process is to maximise biogas production by increasing the biodegradability of the sludge. To achieve this, pressurised steam must be fed to the reactor to maintain the chamber at 170 °C (Fernández-Polanco et al., 2008). In this scenario, part of the biogas produced in the anaerobic digestion was diverted to a boiler to cause combustion and produce the required steam. The amount of biogas required for the TH and consequently, the benefits in electricity generation will depend on the incoming sludge temperature and concentration that will be crucial for the profitability of the process. The increase in sludge biodegradability also involves an extra release of ammonium (NH_X-N), which must be treated *in situ*. To remove this surplus of N and the NH_X-N released in the anaerobic digestion, a nitritation/Anammox process is an interesting approach. In the Anammox process, ammonium is oxidised with the nitrite formed in the previous nitritation process, without oxygen and COD consumption, raising the stoichiometric aeration cost savings up to 63% (Volcke et al., 2006).

3.1.3. New WRRF concept: C/N/P decoupling WWTP

The partition-release-recover (PRR) concept proposed by Batstone et al. (2015) was used as an example of a new WRRF concept. This configuration completely decouples COD and nutrient treatments in order to seek greater process performance. For this, the water line secondary bioreactors are operated at a very short sludge retention time (SRT) of 2–4 days (depending on the temperature; Mamais and Jenkins, 1992) to consume only the strictly necessary N for the growth of the microorganisms. The configuration (Fig. 4) consists of a Phoredox (A/O) process for the biological soluble COD and orthophosphates (ortho-P) accumulation in the solids (heterotrophic organisms, polyphosphate (polyP) accumulating organisms (PAO), polyhydroxyalkanoates (PHA) and polyP), a thermal hydrolysis technology to increase the biodegradability and dewaterability of sludge, an anaerobic sludge digestion process for the COD removal and P and N release, a crystalliser for P precipitation as struvite ($MgNH_4PO_4 \cdot 6H_2O$), and a partial nitritation/Anammox process in the mainstream and side stream to treat the N. The pH at the crystalliser has been controlled by NaOH addition to maintain it at a value of 8.1, above which struvite precipitation is favoured. The $MgCl_2$ dosage has been controlled keep the effluent concentration of Mg at the value of 0.5 gMg m^{-3}.

3.2. Plant-wide model construction

Based on the Ceit PWM library, the models describing the three above-mentioned scenarios were constructed and implemented in

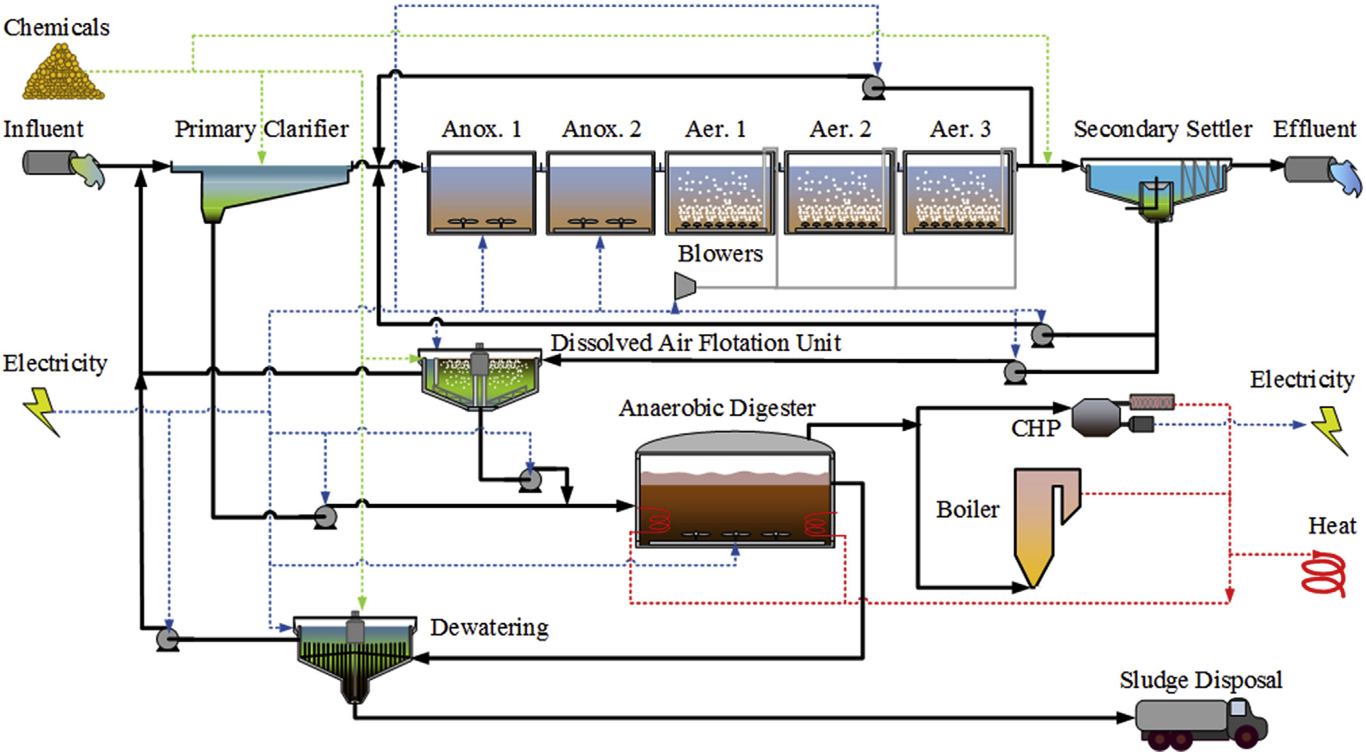

Fig. 2. Conventional wastewater treatment plant (based on BSM2 layout).

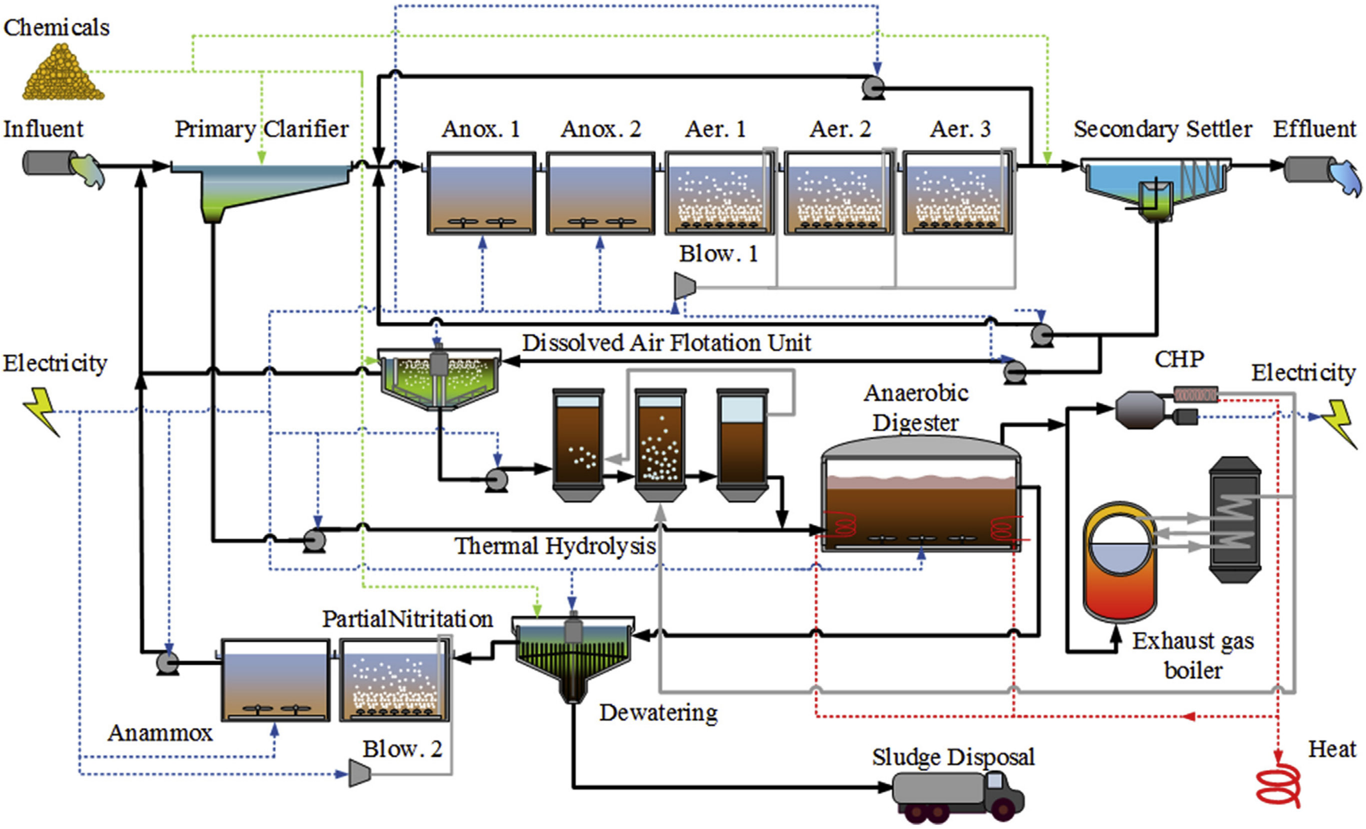

Fig. 3. Upgraded wastewater treatment plant.

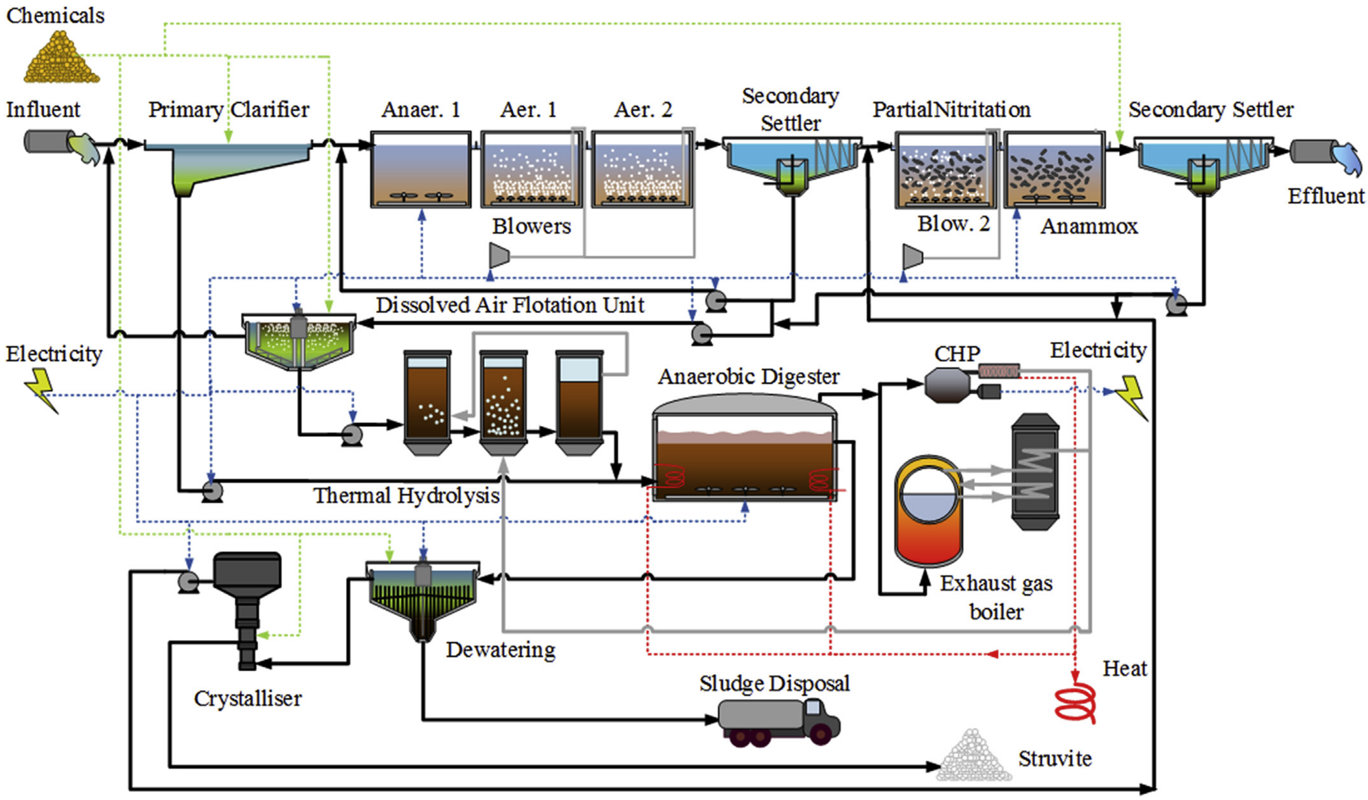

Fig. 4. New WRRF concept: C/N/P decoupling WWTP.

the WEST simulation platform (www.mikebydhi.com) following the steps described below.

3.2.1. *Category selection and influent characterization*

Given the characteristics of the three plant layouts, the CNPchem_AnD, the C2NPchem_AnD and the C2NPprec_AnD categories from the Ceit PWM library were selected to reproduce the behaviour of all plants. The biochemical reactions considered in the model were the ones that are necessary to describe biological organic matter, P and two-step N removal under different environmental conditions (aerobic, anoxic and anaerobic). The chemical transformations considered in the model were the weak acid-base and complex ion-pairing equilibrium reactions between volatile fatty acids (VFAs), inorganic carbon, N, P, calcium, magnesium and potassium. Finally, two types of physico-chemical transformations were considered: (1) liquid-gas transfer, regulated by gaseous partial pressure according to Henry's law of dissolution, and (2) the precipitation-redissolution equilibrium. The kinetic and stoichiometric constants used in the simulations are the proposals for the simulation of the BSM2 configuration adapted to the PWM methodology. All these constants can be found in Fernández-Arévalo (2016).

Influent wastewater was simulated using the average flow-weighted influent concentrations calculated for one year of influent defined in BSM2 (Gernaey et al., 2014), with some minor modifications and additions. Maintaining the 100,000 population equivalent proposed by BSM2, the influent total COD (TCOD) has been divided into soluble (SCOD), particulate (PCOD) and colloidal (CCOD) organic matter. The (SCOD + CCOD)/TCOD ratio (SCOD/TCOD ratio in the original BSM2 influent) was increased from 0.14 to 0.44 to allow for the complete denitrification and fermentation processes. The VFA concentration was set to 15% of the soluble and colloidal COD (Henze and Comeau, 2008). The colloidal fraction of the slowly biodegradable matter remained at 25%, and the VSS/TSS at 0.76. Finally, the original BSM2 influent does not have the ortho-P components; therefore, a theoretical value of 5 has been set to the TKN/TP ratio in order to add the P to the standard influent.

3.2.2. *Unit-process and actuator model selection*

In each configuration, the units were selected to describe the detailed layouts in the previous section (Completely stirred open and closed tank reactors, primary and secondary clarifiers, thickener and dewatering units, biofilm reactors to simulate the partial nitrification and Anammox processes in the third configuration, CHP units, boilers, heat exchangers and precipitation units). To describe the major costs of the system the following models were selected: blowers, pumps, stirrer engines, gas and water distribution systems, specific energy ratios, dosage costs and electricity/cost conversion models. The dehydration process is described from specific energy ratios and dosage costs, and in the case of flotation the process is described by specific energy ratios and pumping, aeration and dosage costs. All these cost models were calibrated from standard engineering values.

4. Simulation analysis: energy and nutrient management exploration

Once the models for the three scenarios proposed were constructed, (steady state) simulations were carried out to analyse the potential use of the energy contained in the organic matter and nutrients and/or its recovery. Furthermore, a cost analysis of these plants for different influent C/N/P ratios was carried out. To avoid possible interferences from other factors that affect plant operation (plant oversising, unit-process efficiencies, environmental factors, etc.), reactor volumes and recycle flows have been optimised for each plant layout and for each influent in order to fulfil a fixed effluent quality of 10 gN m^{-3}, 1 gP m^{-3}, 125 gCOD m^{-3} and 35 gSS m^{-3}, according to the European Directive 91/271/EEC.

4.1. General considerations about the potential use of the energy contained in COD and nutrient and/or its recovery options in WWT processes

In analysing the different conventional options of getting energy from COD removal, the most effective and typical way is to transform the organic matter into CH_4 (the $\Delta h_r{}^{o}{}_{CH4}$ is 13.91 kJ $gCOD^{-1}$ or 890 kJ mol^{-1}) and use its combustion to produce thermal and electric energy. The anaerobic COD biodegradation presents three advantages compared to aerobic or anoxic oxidation in AS: (1) the heat of the reaction is higher, 11.86–13.37 kJ $gCOD_{rem}^{-1}$ against 4.07 kJ $gCOD_{rem}^{-1}$-5.27 kJ $gCOD_{rem}^{-1}$ for aerobic and 3.52 kJ $gCOD_{rem}^{-1}$-4.74 kJ $gCOD_{rem}^{-1}$ for anoxic biodegradation (calculated from the model), (2) the energy recovery from biogas combustion is more effective because of the heat dissipated when oxidation occurs in the aqueous phase, and (3) aeration costs are reduced. Thus, the clearest alternative to maximise the recovery or reuse of the COD energy potential is to minimise the COD oxidation in AS processes. This can be obtained by producing more primary sludge and working at lower SRT in the secondary biological treatment.

Although, as it has been abovementioned, the energy recovery from compounds is more efficient when they are in a gaseous phase. In the case of the ammonia, its solubility in water is very high, necessitating stripping methods for transferring it from water into gas phase. This, added to the fact that ammonia requires a catalyst for its oxidation in gas phase (Jones et al., 1999), makes this process economically unfeasible. Moreover, the nitrogen recovery techniques (ion exchange methods or stripping processes) consume more energy than removal processes, with the exception of struvite recovery technologies. Consequently, from an economic perspective, the destruction of nitrogen compounds to nitrogen gas appears the most logical route (Matassa et al., 2015) and low-energy alternatives can be proposed, such as the use of Anammox bacteria, anaerobic phototropic bacteria or high-rate algae (Batstone and Virdis, 2014). Comparing the N oxidation reactions in the aqueous phase, the Anammox reaction is the one that releases more energy to the medium (23.32 kJ gN_{rem}^{-1}), followed by nitritation (15.46 kJ gN_{rem}^{-1}) and nitratation (6.09 kJ gN_{rem}^{-1}) reactions. Thus, Nitritation/Anammox reactions maximise the energy utilization of the N and minimise oxygen consumption in the process that leads to a reduction in the aeration costs.

Finally, the scarcity of natural phosphorus resources converts the recovery of P into the first alternative for use. Currently, P recovery methods from municipal wastewater (MWW) include the agricultural use of sludge, production of struvite, particularly in enhanced biological P removal (EBPR) plants, and the recovery of P from ash (Wilfert et al., 2015). Furthermore, P is a component that is extracted from the treatment plant only within the liquid streams (effluent and sludge). Therefore, efficient extraction of the energy content of inorganic P components is not viable.

4.2. Analysis of the energy use of a conventional wastewater treatment plant

To analyse the degree of utilization of thermal energy content (energy associated with the fluid temperature) and mass energy content (energy associated with the composition of water), a global plant-wide simulation of a conventional plant was carried out under steady-state conditions for a critical temperature of 13 °C.

Based on the mass and energy fluxes proposed by Pagilla and Nouri (2004), Fig. 5 shows the maximum energy potential of the wastewater in each point of the plant. The top of the figure shows the total thermal energy or enthalpy (not exergy) associated with temperature, while the bottom part reflects the maximum energy potential of the constituents in the water, that is the energy released upon oxidation of all water components to CO_2 (g), H_2O (aq.), NO_3, H_3PO_4, P_2O_5, Fe_2O_3, and $Mg_2P_2O_7$ (Fernández-Arévalo, 2016).

As shown in Fig. 5, the biological heat and the solar and atmospheric radiations increase the temperature of the aqueous phase by 0.5–2° (1.5 °C for this case study) and the thermal energy output of the plant by 10% (energy loss through the effluent). Heat recovery technologies (Wanner et al., 2005; Corbala-Robles et al., 2016) could be an appropriate solution for taking advantage of this thermal energy. However, the obtained heat (55–75 °C, Alekseiko et al., 2014) is a very low exergy stream and its application is limited to use in the plant itself or in WWTPs located near a residential area or near hot water demanding areas (IWA Resource Recovery Cluster, 2015). In spite of this, its high coefficient of performance (COP or the ratio of heating provided to work required), which is between 1.77 and 10.63, makes it a promising technology (Hepbasli et al., 2014).

Simulation results show that a considerable fraction of the mass energy content is released to the atmosphere or aqueous phase as biological heat (35–40%) due to the transformations that occur in the system. Among these transformations, nitrification reactions bring more specific energy to the system (21.61 kJ gN_{rem}^{-1}), followed by the COD oxidation reactions. Around 30% of the mass energy content is converted into biogas and goes to the CHP unit. In this specific case, for a mass flow of 7.7 t_{COD} d^{-1} (42.6 kg_{COD} m^{-3}) entering the anaerobic digester and a temperature of 13 °C, it is not possible to maintain the mesophilic temperature, and 3–5% of COD is addressed to the boiler, reducing the electrical energy production. Consequently, in this particular case, only 10% of the mass energy content in MWW is converted into electricity, losing the remaining energy by heat dissipation (4%), through the effluent (8% mass content and 37% thermal content), through the sludge (26%), and digester heating (15%). From the analysis of Fig. 5, it can be said that in a conventional plant, most of the influent energy potential is lost as heat (digester heating and oxidation reactions).

Points highlighted in sections 4.1 and 4.2, show that a rigorous energy and mass flow analysis is crucial for assessing the potentiality of the plant in terms of (1) energy use and recovery and (2) valuable recovered products production. According to this, section 4.3 will show as an example, a simulation-based analysis of the three plant layouts presented in section 3 and for different operating scenarios.

4.3. Comparative analysis of COD and nutrient (N/P) flux distributions in a conventional, upgraded and C/N/P decoupling WWTP

In order to analyse the potential of the wastewater mass energy content, a set of PWM simulations has been carried out. To that end, the distribution of COD, N and P flows throughout the plants was assessed in the traditional, upgraded and C/N/P decoupling plant under stationary conditions for a temperature of 18 °C. At this temperature all the biogas is converted into CHP in the three case-studies, which simplifies the comparison. The results obtained are shown in Figs. 6–8: Fig. 6 shows the total and biodegradable (in brackets) COD flux distributions throughout the plant for each configuration (6a-6c); Fig. 7 shows the total N and NH_4-N (in brackets) flux distributions along the plant (7a-7c); and finally, Fig. 8 shows the total P and ortho-P ($H_2PO_4^{-} + HPO_4^{=} + PO_4^{-3} + FePO_4$; in brackets) flux distributions along the plant (8a-8c).

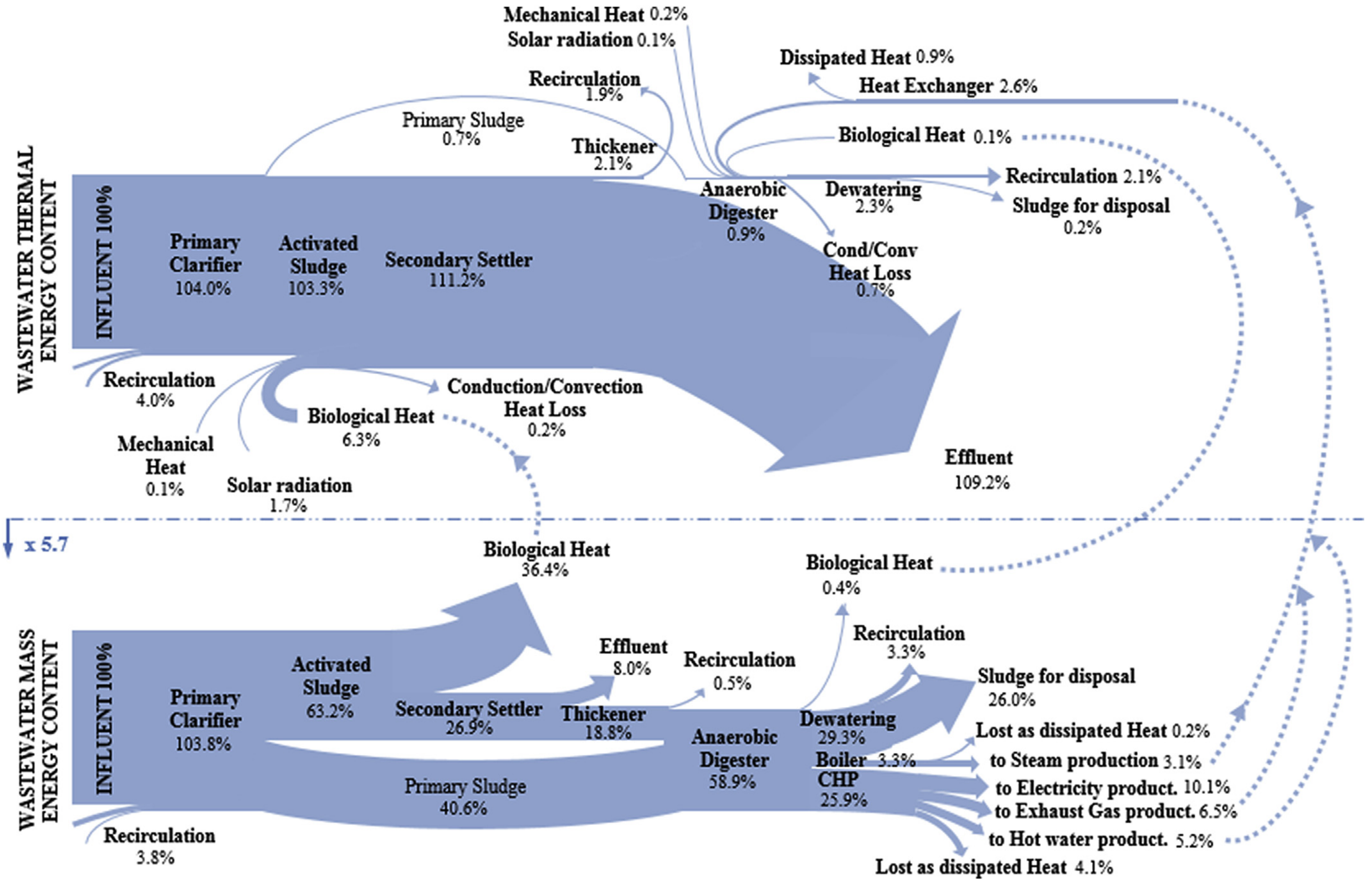

Fig. 5. Simulation of the wastewater mass and energy content distribution throughout the conventional WWTP.

4.3.1. Conventional WWTP

As discussed in the previous section, the way to use the maximum energy content of COD is to convert this organic matter into CH_4. Although in the conventional plant analysis (Figs. 6a, 7a and 8a), only 29% of the influent COD is transformed into biogas (Fig. 6a; Cogeneration flux), this value turns into 43% if the influent non-biodegradable organic matter (20% of the COD (S_I, X_I)) and the non-biodegradable fraction produced in the plant (12% (S_P, X_P)) are not considered. Given this, it is clear that maximising the biogas generation by (1) producing more primary and secondary sludge and (2) transforming part of the non-biodegradable organic matter into biodegradable, for example, by using mechanical (ultrasound treatments, high-pressure homogenisation), thermal (thermal hydrolysis), chemical (ozonation, Alkali treatments) or biological alternatives (Pérez-Elvira et al., 2006), could improve significantly the organic matter energetic potential.

Regarding the total N (TN) balance of this study, 58% of the N is denitrified (Fig. 7a; Gas Stripping flux), 17% and 25% are extracted from the effluent and dewatered sludge (Fig. 7a; Effluent and Sludge for disposal fluxes), respectively, and 25% of the N is recirculated back to the water line (Fig. 7a; Recycling flux) almost all as NH_X-N (96% of this flux is NH_x-N). The N percentage extracted from this dewatered sludge is not a fixed value and it is closely related to the degree of volatile solids (VS) removed in the anaerobic digestion process. The volatile solids removal efficiency is approximately proportional to the degree of NH_X-N released. In this case, for a VS removal of 51%, a formation of 51% NH_x-N with respect to the TN feed to the digester has been observed (see the NH_x-N increase between the Digestion and Dewatering flux).

Finally, as previously mentioned, P is a component that is extracted from the plant only in the effluent and sludge. Thus, the flow of total P (TP) in the dewatered sludge (80% in this case; see Fig. 8a, Sludge for disposal flux) depends on the P concentration in the influent and effluent. For a high P load influent (25 gP m^{-3}, Henze and Comeau, 2008) the percentage of TP extracted as solids can be 92–96%, while for a low P load influent (6 gP m^{-3}, Henze and Comeau, 2008) it can be about 60–80%, which is in accordance with our calculations.

4.3.2. Upgraded WWTP

In this case, incorporating the thermal hydrolysis technology, allows the secondary sludge biodegradability to be increased (by 40% in this particular study), thus converting the non-biodegradable matter, X_P, into biodegradable matter (X_{CH}, X_{PR}, X_{LI}) and consequently increasing biogas production (by 27% in this particular case study (estimated as the difference between the Cogeneration flux of Fig. 6a and b), and by 40% when only secondary sludge is digested). This production depends mainly on the proportions of primary and secondary sludge fed to the digester. The extra amount of COD transformed into methane is approximately the same as the amount by which COD decreased in the dewatered sludge, in this case the extracted COD was reduced by 19% (estimated as the difference between the Sludge for disposal flux of Fig. 6a and b), and the sludge produced by 12% (as a function of the VSS/TSS ratio). The degradation of this new fraction of biodegradable organic matter (part of X_P) will release 25% more NH_X-N and 23% more ortho-P in the digested sludge (difference between the Sludge for disposal flux of Fig. 7a and b, and Fig. 8a and b, respectively), thereby decreasing the content of TN and TP in dewatered sludge and increasing the content of NH_X-N and ortho-P

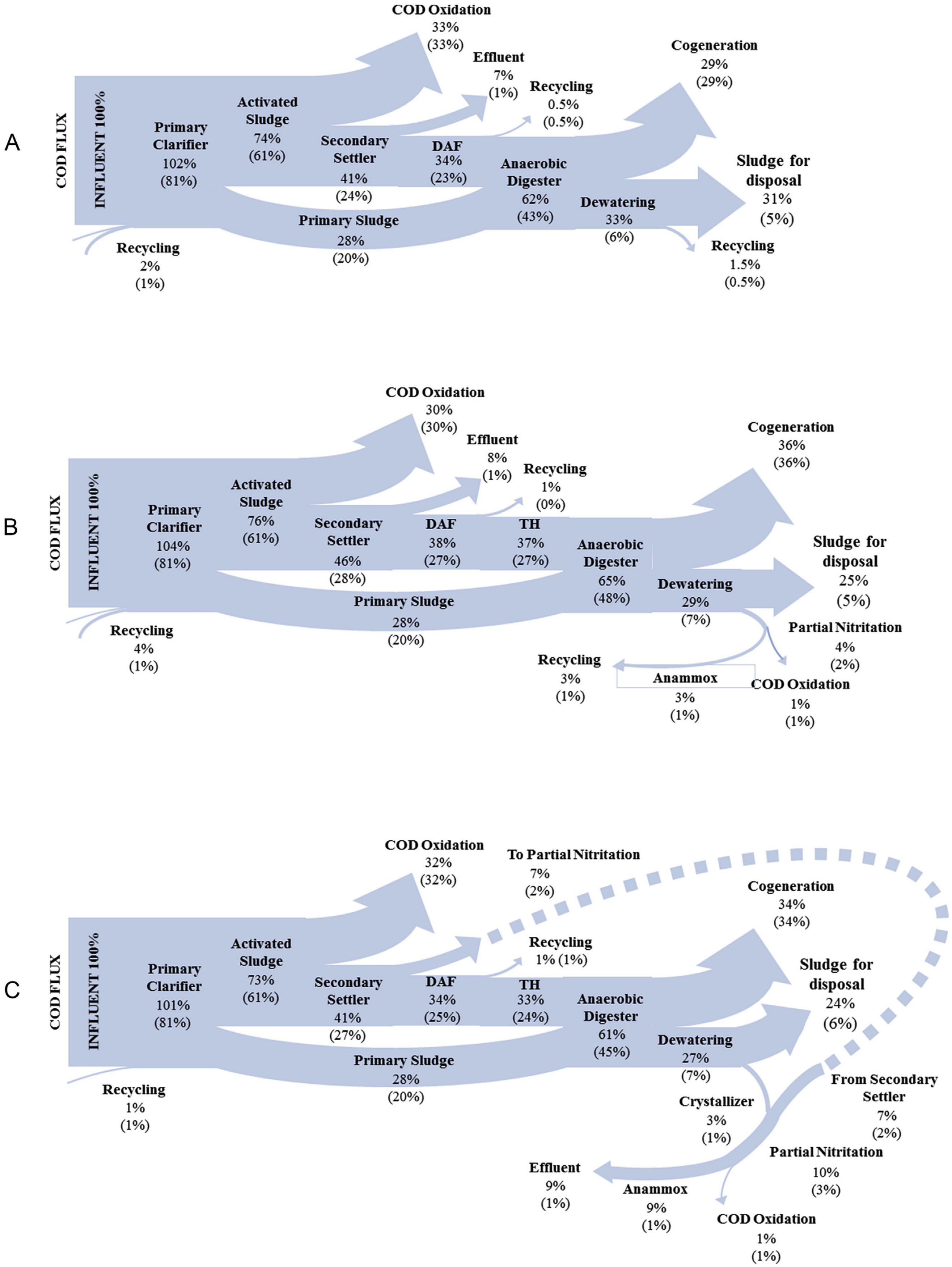

Fig. 6. Simulation of the total COD and (biodegradable COD) flux distributions throughout: (a) a conventional WWTP, (b) an upgraded WWTP, and (c) a C/N/P decoupling WWTP.

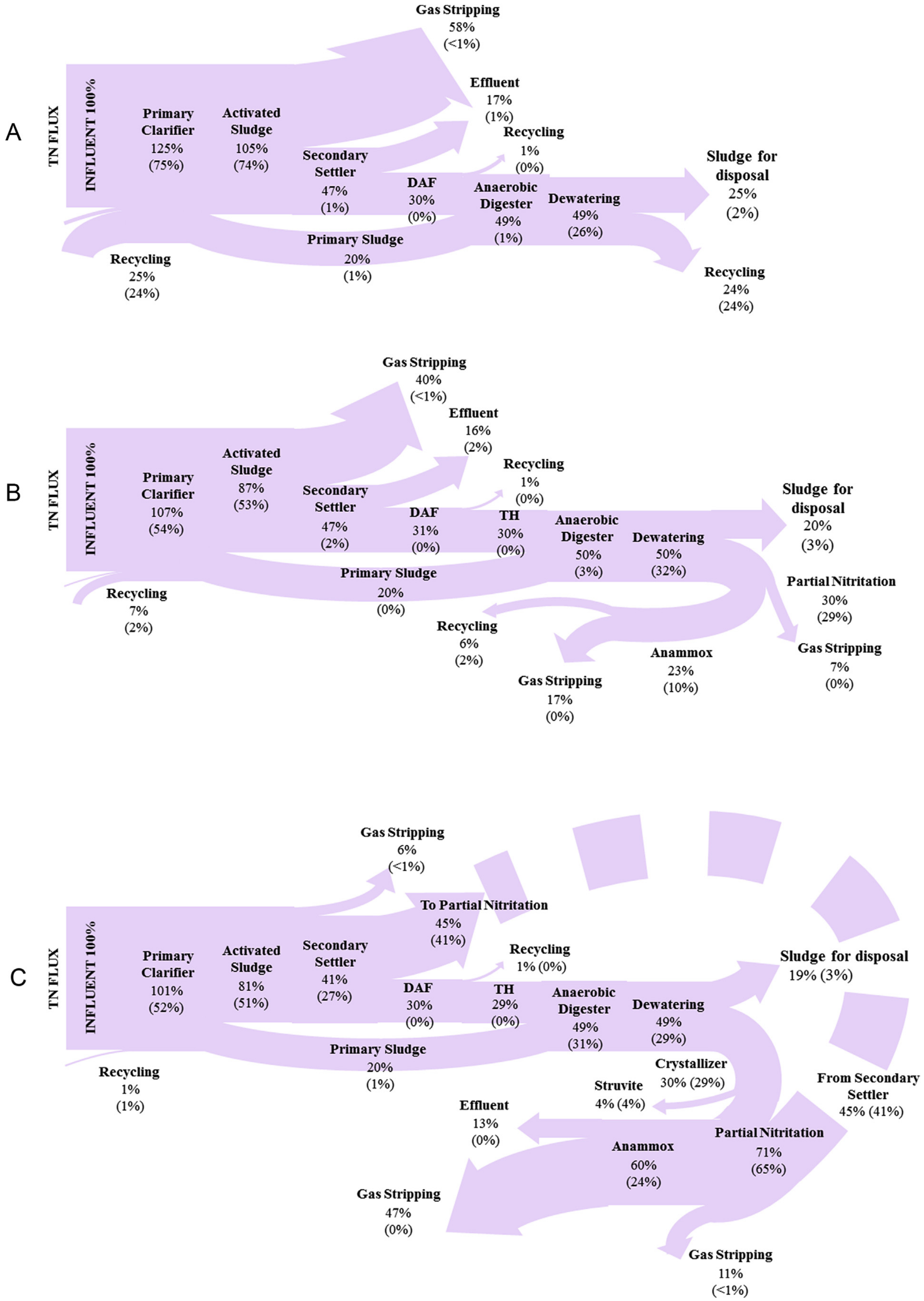

Fig. 7. Simulation of the TN and (NH_X-N) flux distributions throughout: (a) a conventional WWTP, (b) an upgraded WWTP, and (c) a C/N/P decoupling WWTP.

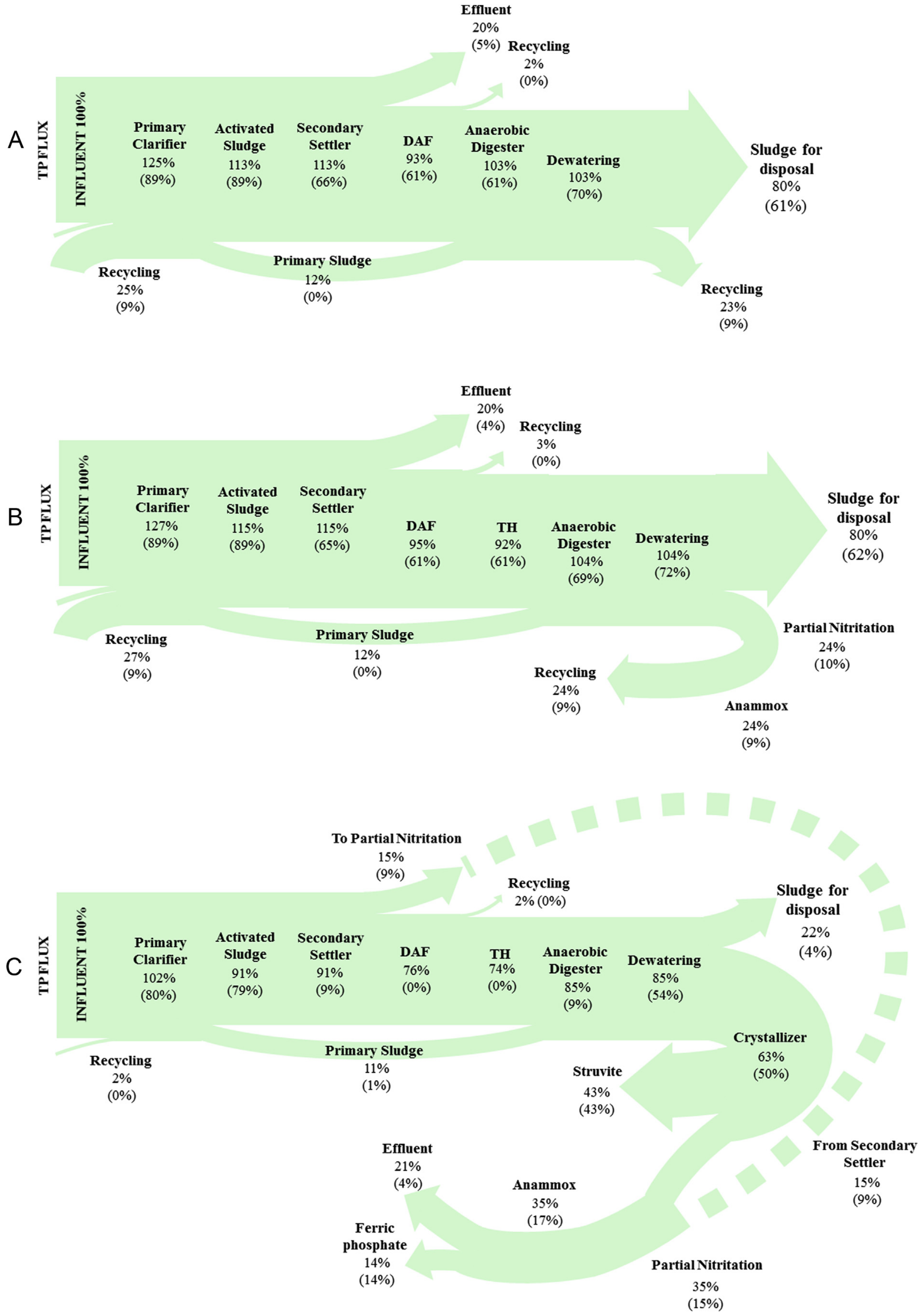

Fig. 8. Simulation of the TP and ortho-P flux distributions throughout: (a) a conventional WWTP, (b) an upgraded WWTP, and (c) a C/N/P decoupling WWTP.

slightly (by 25% and 23%, respectively). Thus, the resulting reject water will contribute to an increase in the N load to be treated in the AS process by up to 30%. This can be a problem if the biological plant does not have sufficient capacity to treat this additional nitrogen load. Thus, before incorporating any such technology, it is useful to analyse its repercussions and viability on the plant as a whole.

With the inclusion of the nitritation/Anammox process the total N flux in the reject water stream was reduced by 70% and the NH_X-N flux by 92% (differences between the Recycling fluxes of Fig. 7a and b), decreasing in turn the NH_X-N to be treated in the AS process by 28% (estimated with the Activated Sludge fluxes of Fig. 7a and b). By using either energy-efficient technologies (nitritation/Anammox) or conventional N removal technologies (denitrification-nitrification processes), the N gas released to the atmosphere is similar in both cases (58%). In this plant layout, due to the pre-treatment incorporated (TH), the plant has to treat more NH_X-N or more biodegradable nitrogen. This results in increased amounts of nitrogen lost by stripping (64%; Fig. 7b, sum of Gas Stripping fluxes).

The release of these extra nutrients can increase the probability of uncontrolled precipitation of salts (struvite, calcium, ortho-P, etc.), if the concentration of ions (Mg^{++}, Ca^{++}, etc.) is considerable and if the process conditions favour them. Thus, although the plant does not have biological P removal, the P released in the digestion can be enough to generate uncontrolled precipitation problems.

4.3.3. *New WRRF concept: C/N/P decoupling WWTP*

This new treatment concept consists of treating each compound (organic matter, N and P) in the most efficient way possible, promoting recovery and maximising energy use: organic matter is valorised as biogas, the P is recovered as struvite and the N is treated with energy-efficient technologies.

By working at a low solids retention time of 3 days (to avoid nitrification and an excessive accumulation of inerts), the production of non-biodegradable organic matter, due to decay processes, is lower (12% lower than in the conventional configuration) (Jimenez et al., 2015), but the same amount of CO_2 is produced due to acidogenesis, PAO growth and polyP storage reactions (Fig. 6a and c; Gas Stripping fluxes). This implies a similar oxidation of COD, which translates into a similar amount of biodegradable organic matter available to be digested in anaerobic digestion. Therefore, this plant layout should not be used with the goal of increasing biogas production. Once again, to increase the biodegradability of the sludge, a thermal hydrolysis unit was introduced to the plant configuration, obtaining in this case a 21% increase in biogas production (estimated as the difference between the Cogeneration flux of Fig. 6a and c). If the objective had been to only maximise the production of biogas, without paying attention to the removal and recovery of P, the configuration could have been modified to a high load fully aerated configuration (without anaerobic reactors to accumulate the P), and in that case, biogas production would have increased up to 40% (about 20 %–25% due to the thermal hydrolysis and another 15 %–20% due to the high-rate process).

In the anaerobic digestion process the ortho-P accumulated in PAO bacteria is released, along with the ortho-P previously released into the TH process. Unlike a configuration without biological P removal, in which the percentage of ortho-P ions ($H_2PO_4^- + HPO_4^= + PO_4^{-3}$) at the outlet of digestion is 9–11% of the TP influent, in a configuration with P accumulation this percentage can increase up to 54% (Fig. 8c; Dewatering flux). Thus, the dewatered sludge will contain 72% less P, but a greater amount of ortho-P ions. The recovery of this ortho-P can be accomplished by recovery in crystallization units. The percentage of P recovered depends on factors such as the influent P and ions (uncontrolled precipitation problems) composition, the required effluent quality, the P accumulation efficiency of AS processes, the need for chemical agents in the water line ($FeCl_3$) and the efficiency of VS removal in digestion, among other things, making it possible to recover 43% of P as struvite (Fig. 8c; Struvite flux).

Finally, a large proportion of the influent N (71%; Fig. 7c, Partial Nitritation flux) will be treated with efficient technologies, since N fluxes recovered as struvite and released by stripping into the AS process were minimal (in this particular case by 4% and 6%, respectively).

The mass flow analysis allows tracking of model components throughout the plant. In a WRRF concept, these components are associated with a source of valuable products (struvite, VFAs, etc.) and bioenergy (mainly COD components). So indirectly, it is an analysis of the plant recovery potential, and consequently an analysis of the plant efficiency. In this frame, the aim of the last section was the estimation of the treatment costs associated with these streams and the quantification of the energy produced or recovered.

4.4. *Analysis of the costs distributions in a conventional, upgraded and C/N/P decoupling WWTP for different influent COD/N/P ratios*

The most influential factors on WWTP operating costs are the plant layout and the composition of the MWW influent. In order to analyse the effect of these factors, a global economic analysis of each plant layout was carried out for different influent COD/TN ratios (Table 2), under stationary conditions and for a temperature of 18 °C. The ratio TN/TP has been maintained constant. Reactor volumes and operational set-points have been optimised for each particular plant layout and for each influent composition. Additional details about influent conditions can be found in Table A.1 in the Supplemental Information Section 2. In the overall cost balance, there are two costs that have not been considered: sludge disposal costs and costs of production/sale of struvite. Sludge disposal costs are very dependent on the area and type of treatment they receive. In the case of struvite, the sale price is very variable. For this study it has been considered that the production costs are equal to sale benefits.

Fig. 9 summarises the results obtained in all these optimizations. The operating cost distributions of each plant and for each influent are represented by the bars, the CHP electric energy recovery has been included as a negative cost, while the net cost is represented by blue dots. A first analysis of the cost distribution shows that positive operating costs are very similar for the conventional and upgraded WWTP, while the C/N/P decoupling WWTP reduces the expenses significantly. For all configurations, these operating costs are mainly associated with influent N concentration and show a low dependence to the variations of influent C load. In the upgraded and C/N/P decoupling plants, negative operational costs (energy recovery) are increased, due to a more efficient use of the influent COD. Contrarily to the positive costs, energy recovery is mainly associated with C load and exhibits a very low dependence with the N concentration in the influent (except for the critical case of very low C/N ratio in the conventional plant). Finally, total costs are clearly positive in a conventional plant, while the upgraded configurations could theoretically get a neutral cost balance only for high C/N load ratios. However, the C/N/P decoupling plant has a real potential for obtaining a negative cost balance for a broad range of influent characteristics (especially at high C/N ratios and at high concentrations of influent COD).

Fig. 10 shows the effect of influent concentrations on the most representative costs (aeration and dosage costs and electricity production) and on the plant self-sufficiency (%) for the three plant-

Table 2
C/N ratios considered for the influent characterization.

		Low C	Medium C	High C
		444 gCOD m^{-3}	592 gCOD m^{-3}	740 gCOD m^{-3}
Low TN (LN)	43 gN m^{-3}	COD/TN = 10.3	COD/TN = 13.8	COD/TN = 17.2
Medium TN (MN)	57 gN m^{-3}	COD/TN = 7.8	COD/TN = 10.4	COD/TN = 13.0
High TN (HN)	71 gN m^{-3}	COD/TN = 6.3	COD/TN = 8.3	COD/TN = 10.4

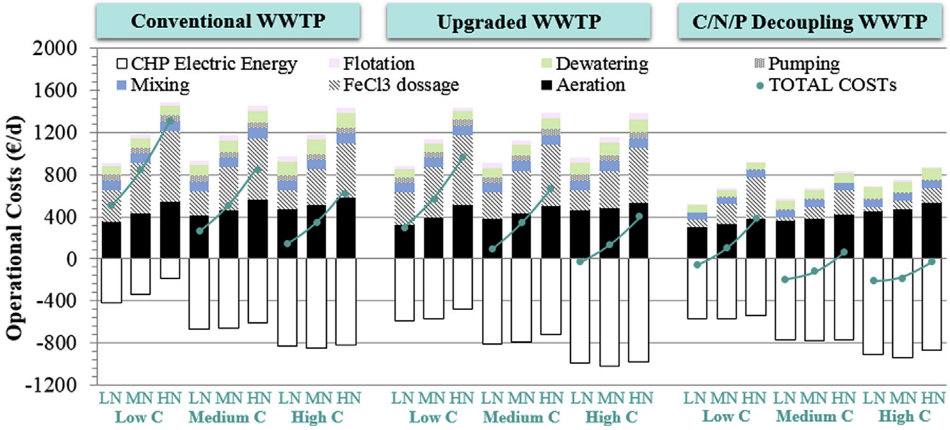

Fig. 9. Operating cost analysis in a conventional, upgraded and C/N/P decoupled WWTP for different COD/TN ratios: Cost distribution in columns and net operating costs represented by the blue dots (€/d). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

layouts under study.

The aeration costs exhibits a logical growing trend in the three configurations for increasing N and COD loads (Fig. 10a). It is also remarkable to see the very limited influence of N load to the aeration power in the C/N/P Decoupling WWTP, reflecting the high efficiency of this advanced configuration for the removal of N. The Upgraded plant has incorporated a Nitritation/Anammox process to treat rejected supernatants, reducing overall aeration costs around 6–15% without sludge pre-treatment processes, and somewhat lower, at around 3–11%, when a thermal hydrolysis is incorporated. For the C/N/P Decoupling plant layout, aeration savings of 16–29% are achieved for low-medium COD loads and savings of 4–8% for higher concentrations.

In $FeCl_3$ dosage costs, a similar trend has also been found in the three configurations. Ferric chloride dosage depends directly on the influent P content, but indirectly on the C/N ratio. In the first two configurations dosage costs are similar, since in both configurations ferric chloride is used to remove all the phosphorus. The third configuration in turn provides savings in chemical reagents, 78–80% for high C/N ratios and savings of 42–61% for low ratios. Phosphorus removal is performed through biological reactions, and chemical agents are only used to adjust the water line effluent and the rejected water (after recovering 84% of ortho-P as struvite) to effluent quality standards. In addition to the significant reduction in operating costs this configuration provides a value-added product such as the struvite. The analysis did not consider the costs of production of struvite, but neither the profit after its sale. It was considered a neutral balance. Still, using the Sankey diagrams such as those used in the previous section (Fig. 8c), a struvite maximum production of 1.9 $kg_{struvite}$ kgP_{inf}^{-1} (assuming an 84% efficiency in the crystallization unit) for virtually all influents was estimated. Thus, the third plant minimises operating costs by promoting the recovery of biological products and maximising the use of energy.

Analysing Fig. 10c, it can be seen, as expected, that the biogas production depends exclusively on the influent COD concentration. The incorporation of the TH process has led to increased biogas production by increasing the biodegradability of the sludge. For both configurations the increased production is close to 20%. The dependence of COD is clear, therefore it is possible to set a ratio to estimate the electrical energy generated in CHP per unit of COD fed to the plant: 0.46 kWh $kgCOD_{inf}^{-1}$ for the conventional plant, 0.55 kWh $kgCOD_{inf}^{-1}$ for the upgraded plant and 0.52 kWh $kgCOD_{inf}^{-1}$ for the C/N/P decoupling WWTP.

Finally, Fig. 10d shows a comparative picture of the self-sufficiency for the three plants. Conventional WWTPs were designed based on traditional biological treatments under a “removal philosophy”, being difficult to achieve the total energy self-sufficiency. As shown in Fig. 10d, the total self-sufficiency degree is closely linked to the C/N influent ratio and to the influent COD concentration, and this can vary in the conventional plant from 12% for very low COD/TN ratios, up to 85% for very high ratios. Consequently, the treatment plant layouts comparison with different influent ratios would not be entirely correct, nor ensuring that a configuration is always self-sufficient without mentioning the influent ratio of the analysed plant (Jenkins and Wanner, 2014). The philosophy of the second configuration is based primarily on increasing energy production in order to achieve a net overall balance closer to self-sufficiency, in this case between 33% and 103%. In this second configuration, it is possible to achieve the self-sufficiency but only with high COD/TN ratios (Fig. 10d). Finally, the main objective of the third configuration (C/N/P decoupling WWTP) is the operational costs minimization, by promoting the recovery of bio-products and maximising the use of energy. With this configuration, it is possible to achieve the plant self-sufficiency for almost all COD/TN influent ratios (58% for low COD/N ratios and up to 130% for high ratios), especially at high COD concentrations. Finally, it should be mentioned that the observed slope changes are due to the availability or not of the readily biodegradable COD to denitrify, an effect that will be more important in conventional plants where large amounts of nutrients are recycled.

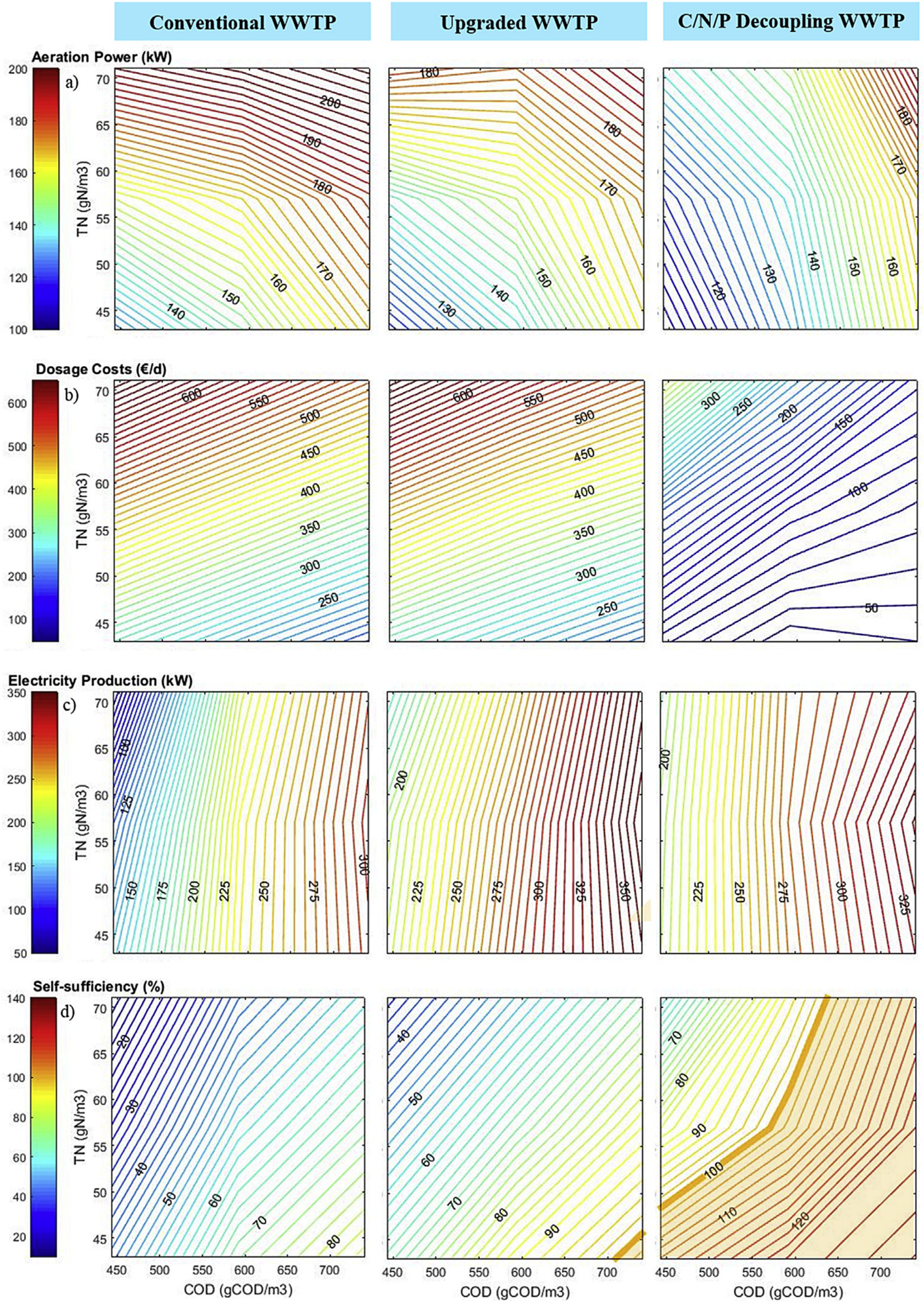

Fig. 10. (a) Aeration Power, (b) dosage costs, (c) electricity production, and (d) plant self-sufficiency in a conventional, upgraded and C/N/P decoupled WWTP for different COD/TN ratios.

5. Discussion and conclusions

Plant-wide simulations allows a thorough, comprehensive and refined analysis of different plant configurations from an energy and resource recovery perspective. To demonstrate the potential of the tool and the need for simulation analysis, this paper compared three different plants: (1) a conventional WWTP, (2) an upgraded or retrofitted WWTP, and (3) a new WRRF concept known as a C/N/P decoupling WWTP.

Analysing the layouts from a standpoint of resources and energy utilization, a low utilization of the energy content of the components could be observed in all configurations. The only resource that can be recovered efficiently as energy is the organic matter transmitted to the gas phase. The oxidation of the components in the aqueous medium (AS process and nitritation/Anammox technology) releases a large amount of energy as heat that is transmitted to the atmosphere or extracted by the effluent (in these simulations about 37%). This energy is difficult to recover or the recovered energy has a low exergy. Therefore, oxidations in the aqueous medium should be minimised and instead oxidations should be promoted in the gaseous phase. Another key to maximising the COD energy use is to incorporate technologies that increase sludge biodegradability ($X_P \rightarrow X_{CH}, X_{PR}, X_{LI}$), such as the TH process incorporated in the second and third layouts. In the conventional plant, the COD used to produce biogas was around 29%. The TH technology increased this to 36% in the upgraded plant and 34% in the C/N/P decoupling WWTP. In turn, the process reduced sludge production by 12% and by 22%, respectively, in these two plants.

Regarding resource recovery methods, N recovery techniques are really expensive (ion exchange methods or stripping processes), or as in the case of the technique that could compete with the removal processes, struvite precipitation, the N recovered is minimal (4% estimated by the C/N/P decoupling WWTP simulation, Fig. 7). In the case of P, the scarcity of natural P resources converts the recovery of P in the first alternative. The conventional and the upgraded plants removed P by $FeCl_3$ precipitation and only the third configuration attempted to recover the P. The maximum estimated struvite recovery was 43% (Fig. 8) and the estimated maximum struvite production was 3.7 $kg_{struvite}\ kgP_{inf}^{-1}$ for virtually all influents.

Analysing the costs obtained in the study, it can be seen that WWTP self-sufficiency is closely linked to the influent COD/TN/TP ratio and to the influent COD concentration. In all plants the trend was similar, the highest degree of self-sufficiency was obtained for the higher ratio values. Achieving self-sufficiency was not possible in the conventional plant, in the upgraded plant it depended on the influent ratio, and in the C/N/P decoupling WWTP layout self-sufficiency was feasible for almost all influents (58% for low COD/TN ratios and up to 130% for high ratios), especially at high COD concentrations. Simulations for different influents showed that, as expected, operating costs increased with the influent load. Assessing costs in detail, aeration was the most significant cost in all configurations (36–48% in the conventional and upgraded plants and 41–65% in the C/N/P decoupling WWTP) followed by the chemical dosage, especially in the first and second configurations (20–48% in the conventional and upgraded plants and 5–28% in the C/N/P decoupling WWTP). Regarding plant qualities, the differentiating factor of the upgraded WWTP layout was the increased biogas production. The thermal hydrolysis process increased the biodegradability of the secondary sludge by 40% and electricity production by 19–21% for medium/high COD concentrations and by 43–162% for low COD concentrations. The decrease in aeration costs was not significant in this second configuration (3–11%) due to the NH_X-N release in the TH process (25% more NH_X-N), although efficient nitritation/Anammox technologies were used to treat rejected water. The fundamental feature of the C/N/P decoupling WWTP was the increase in electricity production (savings of 10–20% for high COD/TN ratios and 39–198% for low ratios) and the decrease in $FeCl_3$ requirements (78–80% for high COD/TN ratios and 42–61% for low ratios) and aeration costs (16–29% for high COD/TN ratios and 4–8% for low ratios), three qualities that enable the plant self-sufficiency.

Through simulation it has been found that each resource has its optimal way of being treated, and thus the key to maximising the recovery of resources and energy is the independent treatment of nutrients and COD, valorising the organic matter, and recovering or treating the nutrients.

Note that the results shown in this paper rely on specific model parameters and slight changes in model parameters could lead to different solutions. Regarding parameters to obtain mass and energy fluxes, these models have been widely used and studied for years, since the uncertainty in these balances is reduced. The greatest uncertainty would be in the thermal hydrolysis process, since this process depends very closely on the type of sludge and its characteristics. In this paper, an increase in biogas production of 40% has been considered. To extrapolate these results to a real plant, an experimental analysis of the biodegradability of the sludge should be performed to corroborate these results. In the absence of experimental data, this study can be used as an appropriate starting point in the comparison of configurations. On the other hand, parameters to calculate economic costs have greater uncertainty than previous. In this case, to minimise the uncertainty, costs have been assigned to each manipulated variable which reduces uncertainty compared to empirical or black-box models.

As a general conclusion, it can be seen that PWM constitutes a very suitable tool for rigorously and globally assessing the incorporation of new leading-edge technologies in conventional plant layouts, or for the analysis of new configurations. The plant layouts proposed in this paper are just a sample of the possibilities for upgrading or designing innovative plants, but they have enabled an analysis of the current needs and challenges that need to be addressed. Even so, the methodology presented here is generic and can be used for any other plant. The use of plant-wide models is, in this context, very useful to ensure that complex plants featuring different technologies can be analysed reliably and that the model faithfully reproduces the plant behaviour, also in terms of energy and chemical consumption.

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Appendix A. Supplementary data

Supplementary data related to this article can be found at http://dx.doi.org/10.1016/j.watres.2017.04.001.

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