Plant-wide modelling in wastewater treatment: showcasing experiences using the Biological Nutrient Removal Model

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ABSTRACT

Plant-wide modelling can be considered an appropriate approach to represent the current complexity in water resource recovery facilities, reproducing all known phenomena in the different process units. Nonetheless, novel processes and new treatment schemes are still being developed and need to be fully incorporated in these models. This work presents a short chronological overview of some of the most relevant plant-wide models for wastewater treatment, as well as the authors' experience in plant-wide modelling using the general model BNRM (Biological Nutrient Removal Model), illustrating the key role of general models (also known as supermodels) in the field of wastewater treatment, both for engineering and research.

Key words | chemical and biological processes, physico-chemical, plant-wide modelling, wastewater treatment, water resource recovery

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LIST OF ACRONYMS

AD	Anaerobic digestion
ADM	Anaerobic Digestion Model
AnMBR	Anaerobic membrane bioreactor
AOO	Ammonium oxidizing organisms
A/O	Anoxic/Aeration system
ASDM	Activated Sludge-Digestion Model
ASM	Activated Sludge Models
BNRM	Biological Nutrient Removal Model
BOD	Biological oxygen demand
BSM1	Benchmark Simulation Model
BVSS	Biodegradable volatile suspended solids
CAS	Conventional activated sludge
CBIM	Continuity-Based Model Interface Methodology
CFD	Computational fluid dynamics
COD	Chemical oxygen demand
COST	European Cooperation in Science and Technology
DESASS	Design and Simulation of Activated Sludge Systems
DO	Dissolved oxygen concentration
FISH	Fluorescence in-situ hybridization
GAO	Glycogen-accumulating organisms
GHG	Greenhouse gas
IWA	International Water Association
LCA	Life cycle assessment
MBR	Membrane bioreactor
NOO	Nitrite oxidizing organisms
OUR	Oxygen uptake rate
PAO	Polyphosphate-accumulating organisms
PCM	Plant-wide modelling
PC-PWM	Physico-chemical PCM
SBR	Sequencing batch reactor
SHARON	Single reactor system for High activity Ammonium Removal Over Nitrite
SRO	Sulphate reducing organisms
SRT	Sludge retention time
STP	Standard Temperature and Pressure
STR	Scientific and Technical Report

doi: 10.2166/wst.2020.056

TAN	Total ammonium nitrogen
VSS	Volatile suspended solids
WRRF	Water resource recovery facilities
WWTP	Wastewater treatment plant

INTRODUCTION

Wastewater treatment modelling

In the wastewater treatment field, mathematical models are useful tools for research and development, as well as for design and optimization of the different processes involved. Mathematical modelling efforts are highly stimulated by different social, economic and environmental factors, such as the more and more stringent legislation, the urgent need for water recycling and carbon footprint reduction and the importance of general cost savings and public profile issues, among others. These factors force a move towards a more sustainable wastewater treatment design, where wastewater must turn into a source of resources such as reclaimed water, bioenergy and bioproducts (i.e. nutrients, biosolids). This paradigm shift requires the integration of sustainable processes in future water resource recovery facilities (WRRFs) (Batstone *et al.* 2015; Robles *et al.* 2018). In this respect, mathematical modelling plays a key role in the incorporation of the circular economy principles in the wastewater treatment sector.

This work presents a short overview of some of the most relevant plant-wide models for wastewater treatment, as well as the authors' experience in plant-wide modelling using the general model BNRM (Biological Nutrient Removal Model). The paper aims to illustrate the key role of plant-wide models in the field of wastewater treatment, both for engineering and research.

Initially, wastewater treatment modelling focused on the biochemical processes taking place either on the water line or the sludge line. The Activated Sludge Models (ASM, Henze *et al.* 2000) and the Anaerobic Digestion Model (ADM1, Batstone *et al.* 2002) introduced the use of the Gujer or Petersen table (stoichiometric matrix) and are still today the most widely used tools for modelling activated sludge processes and anaerobic digestion (AD) processes, respectively. More recently, modelling efforts were focused on plant-wide modelling and aimed at simulating the whole plant, taking into account the effect of side-streams on mainstream. In this respect, a higher descriptive capacity of the whole wastewater treatment system can only be achieved if physico-chemical and chemical processes are also taken into account. For instance, a proper pH calculation has proven to be necessary since it affects the stoichiometry and kinetics of biological (nitrification/denitrification) and chemical processes (phosphorus precipitation, gas solubility, etc.). Gas transfer processes also determine the effectivity of aeration, which involves a significant energy consumption and affects the carbon footprint estimation of WRRFs.

Plant-wide models

Plant-wide models have been developed following two different approaches: the interfaces approach and the general approach (also known as supermodel approach). The *interfaces approach* consists of connecting existing standard models by means of an interface between units and their models. Copp *et al.* (2003) and Nopens *et al.* (2009) defined ASM1-ADM1 interfaces, whereas Vanrolleghem *et al.* (2005) developed the Continuity-Based Model Interface Methodology (CBIM) proposing a procedure to connect any standard model. Dedicated tools have also been developed and widely adapted, such as the COST/IWA Benchmark Simulation Model No.1 (BSM1) (Copp 2002; Jeppsson & Pons 2004), the BSM1_LT (Rosen *et al.* 2004), the BSM2 (Jeppsson *et al.* 2006; Nopens *et al.* 2010), the BSM2G (Flores-Alsina *et al.* 2011) and the BSM-MBR (Maere *et al.* 2011). They consist of a standardized simulation procedure for control strategies design in WWTP and their evaluation in terms of effluent quality and operational cost. The main advantage of using an interface-based approach with respect to other integrated methodologies such as general models is that the original model structure can be used, and there is thus no need for state variable representation in all process units with the resulting increased use of computational power, model complexity and adverse model stability characteristics (Grau *et al.* 2009).

On the other hand, the *general approach* makes use of a single model to describe key processes taking place in a WWTP. A single set of state variables is used, which includes the components of all processes involved. Therefore, different groups of microorganisms (e.g. aerobic, anaerobic and facultative) are considered in all treatment units and their growth will be determined by the environmental conditions. In this case, the user does not need to decide which model should be applied for each system. In general models, there is a common characterization of the state of the process and the explicit calculation of pH is required as well. With higher computational costs, general models have become more and more feasible due to advances in computer technology. There are significant and successful plant-wide models following the general approach in literature. For instance, the general Activated Sludge-Digestion models (ASDM) implemented in BioWin (EnviroSim Associates Ltd) (Jones & Takács 2004), the Biological Nutrient Removal Model (BNRM) (Seco et al. 2004; Barat et al. 2013; Durán et al. 2017), the plant-wide modelling methodology proposed by Grau et al. (2007), the plant-wide mass balance based steady-state WWTP model proposed by Ekama (2009) or the Sumo©, Mantis2 and Mantis3 models incorporated in the Sumo© and GPS-X software, respectively.

It has to be stressed that under both approaches (the interfaces approach and the general approach) continuity equations need to be fulfilled in every process so that mass and charges balances are met.

Current research on plant-wide models

As WRRFs increase in complexity, more complete and reliable plant-wide models are needed, able to reproduce the behaviour of the whole system. Novel processes are still being developed for water resource recovery (membrane-based processes, microalgae cultivation, etc.), but also mature and established technologies are being integrated in novel treatment schemes in order to achieve energy-positive WRRFs (Solon et al. 2019a). On the other hand, greater understanding of the hydrodynamics or the microbiological and biochemical fields have led to the development of the so-called computational fluid dynamics (CFD) models (Rehman et al. 2017) and metabolic models (Lopez-Vazquez et al. 2009), respectively.

Currently, plant-wide modelling efforts are focused on integrating different model extensions to better reproduce the phenomena occurring in wastewater treatment and incorporate the new concepts and technologies that are emerging under the umbrella of the circular economy. For instance, the last extensions of BSM2 are focused on modelling phosphorus plant-wide, a common goal within the scientific community mainly due to the issue of phosphate rock depletion. Flores-Alsina et al. (2015) proposed a plant-wide aqueous phase chemistry module describing pH variations and ion speciation/pairing in wastewater treatment process models whereas Kazadi Mbamba et al. (2016) developed a physico-chemistry framework. Afterward, Solon et al. (2017) integrated both extensions and also developed a new set of biological and physico-chemical process models to describe the required tri-phasic compound transformations and the close interlinks between phosphorus, sulphate and iron cycles. These extensions have been validated and then applied to optimize the chemical phosphorus removal in wastewater treatment systems (Kazadi Mbamba et al. 2019). On the other hand, the last extension of the general model proposed by Grau et al. (2007) incorporated a physico-chemical plant-wide framework (Lizarralde et al. 2015) which has been applied to optimize the phosphorus management strategies in Sur WWTP (Madrid, Spain) (Lizarralde et al. 2019) and to quantitatively assess the energy demand and resource recovery of different WRRF configurations (Fernández-Arévalo et al. 2017).

On the other hand, a plant-wide modelling approach which takes into account greenhouse gases (GHG) has become a common goal among researchers in the quest to reduce the carbon footprint of WRRFs (Mannina et al. 2016). Flores-Alsina et al. (2011) proposed a model called BSM2G which includes the estimation of the potential on-site and off-site sources of GHG emissions. This extension was then applied, for instance, to show the importance of adding GHG emissions as key performance evaluation criteria in WRRFs (Flores-Alsina et al. 2013). On the other hand, Mannina et al. (2019) proposed a plant-wide model for carbon and energy footprint which quantifies direct and indirect GHG emission related to biological and physical processes.

In summary, literature in the field shows an increasing and successful progress in plant-wide modelling, which can – and should – support the transition of WWTPs into WRRFs (Pretel et al. 2016b; Solon et al. 2019b), in order to facilitate water and nutrient recycling and carbon footprint reduction, but also general cost savings and compliance to new legislation. Table 1 shows a summary of the above presented plant-wide models, developed and applied during the last two decades. Due to the complexity of the models, their application is usually carried out by means of different software tools. Table 2 shows a summary of the simulation platforms commercially available (sometimes free of charge). These tools present a library of different models the user chooses from or implement their own models. At times, they include sewer networks or river quality models.

PLANT-WIDE MODELLING USING BNRM

Model description

The Biological Nutrient Removal Model No.1 (BNRM1) for dynamic simulation of WWTPs was described by Seco et al.

Table 1 | Overview of some plant-wide models for wastewater treatment

Plant-wide model	Reference	Type
BSM2	Jeppsson *et al.* (2006), Nopens *et al.* (2010)	Interfaces
BSM-MBR	Maere *et al.* (2011)	
BSM2G	Flores-Alsina *et al.* (2011)	
Extended BSM2 a plant-wide aqueous phase chemistry module describing pH variations and ion speciation/pairing	Flores-Alsina *et al.* (2015)	
Extended BSM2 a modular physicochemistry framework (PCF)	Kazadi Mbamba *et al.* (2016)	
Extended BSM2 from Flores-Alsina *et al.* (2015) and Kazadi Mbamba *et al.* (2016) and new set of biological and physico-chemical process models (P, Fe and S cycles)	Solon *et al.* (2017)	
Mantis2 and its extension Mantis3	Propietary model from Hydromantis, Environmental Software Solutions Inc.	General
Sumo© models	In-house developed at Dynamita	
The general Activated Sludge-Digestion Model ASDM	Propietary model from Envirosim	
Biological Nutrient Removal Model (No.1, No.2, No.2S)	Seco *et al.* (2004), Barat *et al.* (2013), Durán *et al.* (2017)	
Plant-wide mass balance based steady-state WWTP model	Ekama (2009)	
The plant-wide modelling methodology (PWM)	Grau *et al.* (2007)	
Physico-chemical plant-wide modelling (PC-PWM) methodology for incorporating physico-chemical transformations into multiphase wastewater treatment process models	Lizarralde *et al.* (2015)	
A plant-wide wastewater treatment plant model for carbon and energy footprint	Mannina *et al.* (2019)	

Table 2 | Overview of some computer platforms that implement models for wastewater treatment

Available software	Reference
DESASS	http://calagua.webs.upv.es/
BioWin ©	http://envirosim.com/products/biowin
AquaSim	http://www.eawag.ch/de/abteilung/siam/software/
West	https://www.mikepoweredbydhi.com/products/west
GPS-X™	http://www.hydromantis.com/
SIMBA # water	http://www.inctrl.ca/software/simba/
SUMO19	http://www.dynamita.com
EnviroPro Designer ®	https://www.intelligen.com/enviropro_overview.html
STOAT	http://www.wrcplc.co.uk/ps-stoat

(2004). The physical, chemical and biological processes included were, respectively, settling and clarification processes (flocculated settling, hindered settling and thickening), volatile fatty acids elutriation and gas–liquid transfer; acid–base processes (equilibrium conditions are assumed); organic matter, nitrogen and phosphorus removal, acidogenesis, acetogenesis and methanogenesis. One of the most important advantages of this model was that no additional analysis with respect to ASM2d was required for wastewater characterization. Thus, the usual physiochemical parameters determined in a WWTP were enough to determine the model components.

However, this model did not consider nitrite and failed to accurately simulate the AD because precipitation processes were not considered. Therefore, an extension was proposed and named Biological Nutrient Removal Model No.2 (BNRM2) (Barat *et al.* 2013). This extension comprised the components and processes required to simulate nitrogen removal via nitrite and the formation of the solids most likely to precipitate in anaerobic digesters (struvite, amorphous calcium phosphate, hidroxyapatite, newberite, vivianite, strengite, variscite, and calcium carbonate). Apart from nitrite oxidizing organisms (NOO), two groups of ammonium oxidizing organisms (AOO) were considered since different sets of kinetic parameters had been reported for the AOO present in activated sludge systems and SHARON (Single reactor system for High activity Ammonium Removal Over Nitrite) reactors.

The latest extension to the BNRM2, called BNRM2S, includes the activity of the sulphate reducing organisms (SRO) and was validated with a pilot-scale anaerobic membrane bioreactor under steady-state and dynamic conditions (Durán *et al.* 2017).

The collection model BNRM is implemented in the simulation software DESASS (Ferrer *et al.* 2008) for steady-state and dynamic modelling. DESASS is linked with the geochemical model MINTEQA2 for equilibrium speciation calculations (Allison *et al.* 1991; EPA 2006). The solution procedure implemented in the software consists of a sequential iteration among the differential equations for the kinetic governed processes and the algebraic equations for the equilibrium governed processes. The section below 'Full-scale model applications' shows a compilation of experiences where the modelling results were obtained with this software, illustrating the potential of plant-wide modelling in research and development as well as in design of new plants or optimization of existing ones.

Wastewater characterization

Although the BNRM considers key physical, chemical and biological processes taking place in WWTPs, the required wastewater characterization is similar to the one for Activated Sludge Model No. 2d (Henze *et al.* 2000). Thus, the needed analyses are the following: COD (total and soluble fraction), BOD_{lim} (total and soluble fraction), nitrogen (total and soluble fraction), ammonium, nitrite, nitrate, phosphorus (total and soluble fraction), orthophosphate, volatile fatty acids, pH, alkalinity and different ions such as sulphate, calcium, potassium and magnesium.

Model calibration

Accurate model predictions require a proper calibration of the model parameters. Model calibration can be carried out by fitting model predictions to dynamic experimental data (on-line calibration) or with laboratory experiments (off-line calibration). The IWA STR on Guidelines for using ASMs presents a procedure for on-line calibration (Rieger *et al.* 2012). The drawback of this kind of calibration for the BNRM is that, due to the high number of parameters included and given a set of experimental data, different sets of parameter values will be able to reproduce the dynamic system performance, although not all of them will necessarily be able to predict plant performance when operating conditions are changed. For this reason, we recommend identifying the high influence model parameters (a small variation in these parameters leads to significant variations in model predictions) and calibrating them with off-line laboratory experiments isolating the activity of each microorganism group. Values obtained with this method are more reliable since they are obtained with experiments carried out under different conditions (substrate, inhibitors or oxygen concentration). With this philosophy, Penya-Roja *et al.* (2002) developed an off-line calibration methodology for heterotrophic, autotrophic and polyphosphate accumulating organisms. The developed methodology consists in isolating specific processes for these bacterial groups and it is mainly based on oxygen uptake rate (OUR) measurements. The methodology was upgraded by Jimenez *et al.* (2011, 2012) to estimate the model parameters related to the two bacterial groups involved in the nitrification process (AOO and NOO).

These kinds of respirometric experiments provide information about the maximum bacterial activity under certain conditions, including biomass concentration of the different bacterial groups. In order to determine the maximum growth rate for each of these groups (in $time^{-1}$ units) it is important to determine their concentration. Borrás (2008) developed a methodology to estimate the concentrations of PAO, GAO, AOO, NOO, methanogens and SRO in an activated sludge sample. This methodology is based on determining the percentage of viable bacteria (obtained by means of the LIVE/DEAD® BacLightTM Bacterial Viability Kit) and the percentage of each specific group over the whole bacteria in terms of area using fluorescence in-situ hybridization (FISH), a molecular cytogenetic technique. Knowing the suspended COD concentration of the sample, the concentration (in COD units) of each specific bacterial group can be estimated from the results obtained with the FISH.

Other specific calibration methodologies can be found in literature, such as that proposed by Claros *et al.* (2011) for AOO r-strategists, since it is known that the growth rate of AOO in a SHARON reactor (r-strategists species) depends on free ammonia (FA) concentration whereas the growth rate of AOO in activated sludge systems (k-strategists species) depends on total ammonium nitrogen (TAN) concentration. It should be noted that in the case of off-line calibration it is still a challenge to reach consensus regarding the methodologies to be used.

Literature on off-line calibration procedures for anaerobic digestion processes is scarce. Durán (2013) developed an off-line procedure to calibrate the high influence parameters of other anaerobic microorganisms such as sulphate reducing bacteria. One of the reasons for the predominance of on-line procedures for model calibration could be that no equivalent parameter to the OUR measurement (reliable and easily obtained with cheap and robust sensors) can be used for off-line experiments. Another reason might be the difficulty in isolating the activity of different bacterial groups, which is a current challenge regarding model calibration.

Model validation

Model validation consists of verifying the ability of a calibrated model to reproduce the observed system under different operating conditions. Once the model has been validated, it can be used reliably for predicting plant performance. It is important that the model is successful under changing conditions with small variations in parameter values; that is, without the need to recalibrate too often when applied under changed conditions. If a parameter needs to be tuned and the new value is too different from the originally calibrated one, this is an indication of the existence of different considerations not included in the model (inhibition, interaction with other microorganisms, not enough specialization in the specification of the organisms' groups, etc.). A compromise needs to be met between the accuracy of the model (in the sense of detailed description of organisms and processes) and the stability of the parameters. In this sense, metabolic processes have a considerable amount of constant parameters, since all stoichiometry is calculated based on the metabolism of the organisms and kinetic parameters are practically constant. In this kind of model, the need for calibration is drastically reduced. Their difficulty comes from the complexity in defining the equations for processes that are at times complicated to describe, which remains a current challenge in model development. In metabolic models the trade-off is between parameter calibration and the complexity of the model. The benefit is a very robust model that, once validated, renders very trustworthy simulations.

Regarding the model under study, different examples of BNRM validation can be found in literature. Serralta *et al.* (2004) demonstrated the model's capability to predict the pH variations taking place in an A/O SBR system; Barat *et al.* (2011) showed the model's capability to predict the variations in potassium, magnesium and calcium concentrations in an A/O SBR jointly with precipitation and redissolution processes; Durán *et al.* (2017) showed that the model was able to reproduce the performance of an anaerobic membrane bioreactor (AnMBR) pilot plant (effluent composition, biomass wasted and biogas production) in different steady- and non-steady-state periods.

Full-scale model applications

WWTP design, upgrade and optimization are among the most important applications of mathematical models in wastewater treatment. Mathematical models allow comparing the results obtained for different treatment schemes, different operating conditions, variable influent wastewater composition, etc. and therefore selecting the best alternative. The application of the BNRM to different full-scale WWTPs is presented below. Examples are given of simulation results in quantitative (flows, concentrations, etc.) but also qualitative terms (development of strategies, schemes and decision support).

Design of a conventional WWTP

The WWTP in Sevilla (Spain) went out to public tender, in which some criteria for the characteristics of the plant were included. The treatment flow of this plant is 100,000 m^3/d. The BNRM was applied to design all the elements of the plant. Simulations rendered information on dimensions of the different treatment units, effluent quality, aeration needs, sludge production, $FeCl_3$ needs, biogas production, NaOH and $MgCl_2$ addition for struvite recovery, as well as operational parameters for the activated sludge reactor and anaerobic digestion. An alternative solution to the proposed design criteria was also developed (Figure 1). This alternative solution was based on reducing sludge retention time (SRT), enhancing biological phosphorus removal, rearranging the sludge line to reduce uncontrolled precipitation problems and recovering phosphorus as struvite. A struvite crystallization unit was designed in order to recover the phosphorus from the reject water in the form of a slow-release fertilizer. Simulation results show that around 50% of the influent phosphorus would be recovered and 4.8 t/d of struvite would be produced.

Design of an AnMBR-based WWTP

The WWTP in Santa Rosa (Spain) was upgraded in 2016 with an AnMBR in order to demonstrate this technology as a sustainable alternative for sewage treatment. The plant was designed for treating 18 m^3/d at ambient temperature: 15 °C in winter and 25 °C in the summer season and with ground-buried reactors. Modelling results under

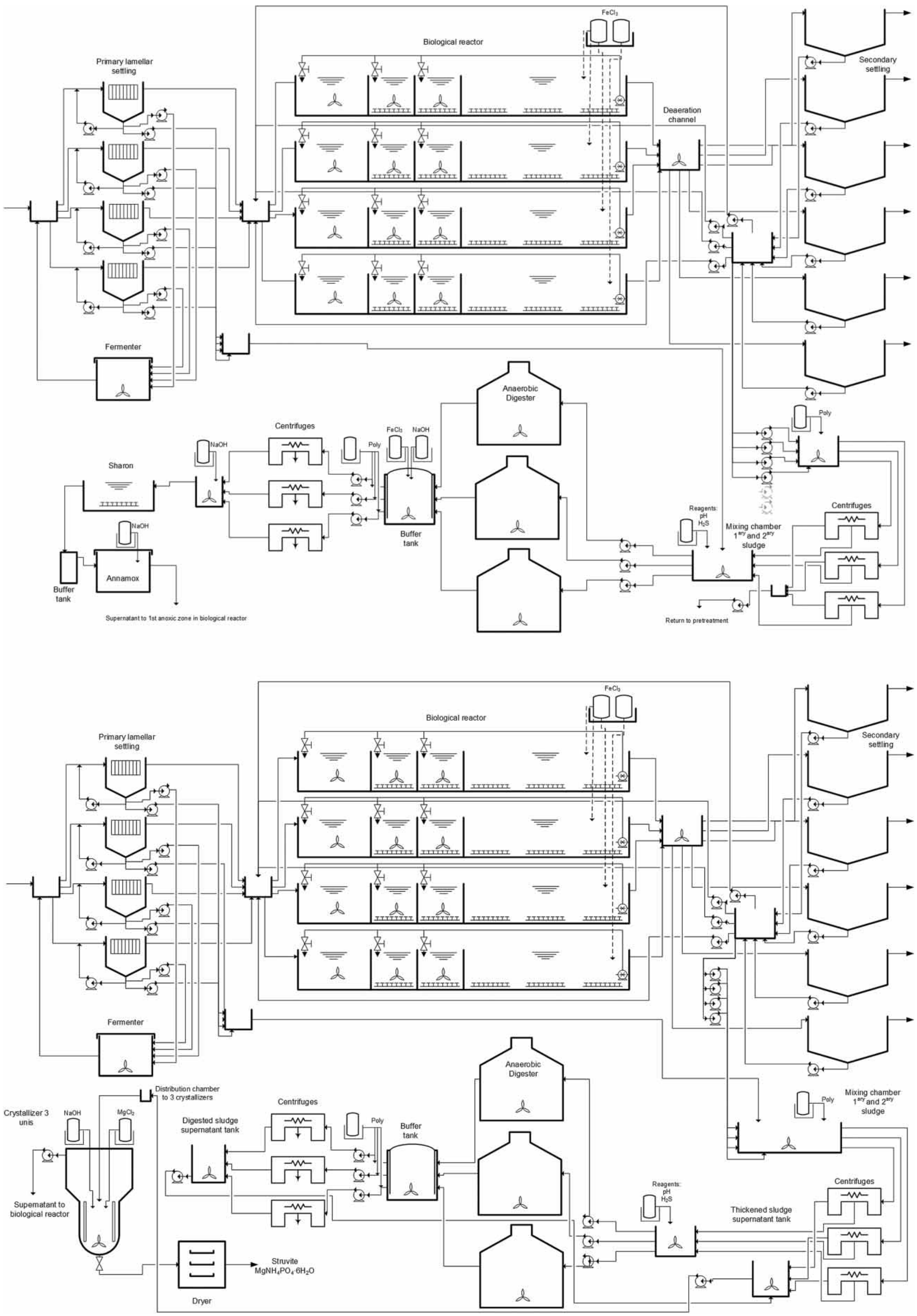


Figure 1 | Flow diagram of the base solution (above) and alternative solution (below).

different operating and environmental conditions lead to the recommendation of operating at an SRT of 60 days, for which a biogas production depending on temperature was estimated: 1.34 or 1.70 m^3/d (with a methane content around 74%) was expected when operating at 15 or 25 °C, respectively. Methane yield resulted in circa 160 and 200 STP L_{CH4}/kg COD being removed at 15 °C and 25 °C, respectively. It is important to point out that sulphur concentration in the influent oscillated around 65 mg S/L, affecting therefore methanization of organic matter due to the competition between SRO and methanogens, which could be reproduced by the model. The effluent quality parameters were also evaluated by simulation. The simulations revealed that the permeate could be used for fertigation purposes due to its ammonium and phosphate concentrations, while COD, BOD and SS were far below the discharge limits. Moreover, low amounts of waste sludge were achieved, this sludge already being stabilised. Specifically, 0.127 and 0.115 kg VSS (volatile suspended solids) per m^3 of treated water were produced with a biodegradable volatile suspended solids (BVSS) content of 32.3 and 21.5% when operating at 15 °C or 25 °C, respectively. The application of the plant-wide model also allowed prediction of the behaviour of the new plant in the event of polluting load increase or wastewater flow increase.

Revamp of a WWTP by including an AnMBR

Currently, the urban WWTP in Torrent (Spain) cannot treat all the incoming wastewater flow and therefore a new installation needs to be built to increase the treatment capacity from 6,000 to 18,000 m^3/d. Since agricultural activity in the area has a demand of 6,000 m^3/d of water for irrigation, an AnMBR system of this capacity was deemed appropriate and therefore designed. The modelling results revealed the production of a high quality effluent, which complies with solids and organic matter content discharge limits and presents nutrient concentrations for fertigation that allow for savings in the use of inorganic fertilizers. It will be possible to treat the effluent in the conventional activated sludge system in periods without agricultural need. The interconnection of the streams with a plant-wide model made it possible to simulate the whole new system proposed.

Upgrade of a conventional WWTP

The plant-wide model was used to simulate different options for upgrading the Denia WWTP (Spain). This WWTP treats around 18,000 m^3/d and was initially designed for organic matter removal and nitrification. The biological treatment consisted of a conventional activated sludge process where primary and excess sludge were aerobically digested (Figure 2). The decision to upgrade the WWTP was made in order to meet the European Commission requirements for total nitrogen and phosphorus in sensitive areas and solve the existing odour problems caused by insufficient stabilization of the excess sludge. Different scenarios were simulated and the results are to be used to support the decisions related to the WWTP upgrade. The modifications carried out in the treatment scheme consisted of operation under extended aeration conditions, converting the biological reactors and the aerobic digesters into one plug-flow biological reactor, converting the old primary settlers into anoxic reactors, and removing phosphorus by chemical precipitation. Moreover, simulations of significant ammonium and COD peak loads showed that increasing the anoxic zone would reduce sludge flotation problems. Therefore, an impeller was installed in the first part of the biological reactor to avoid suspended solids sedimentation when the air control valve was closed in order to increase the anoxic volume. The plant modifications proposed were successfully implemented (Seco et al. 2005).

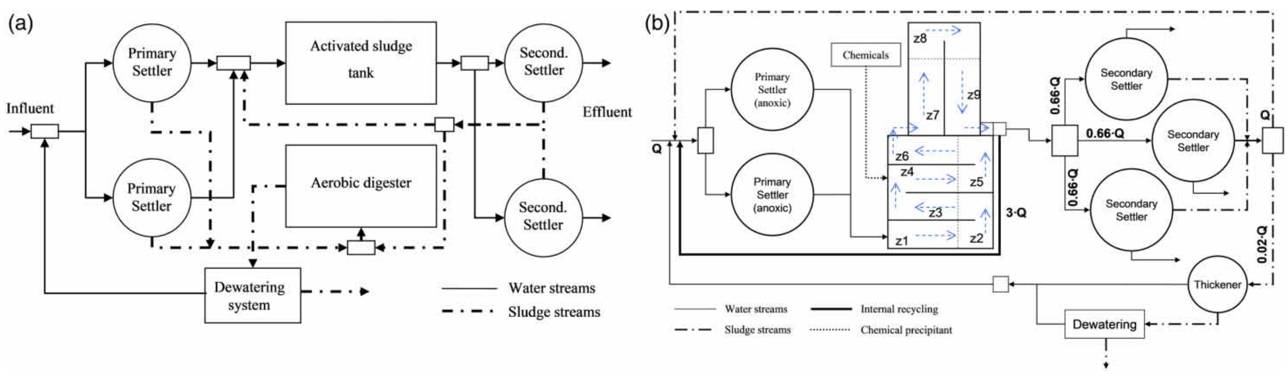


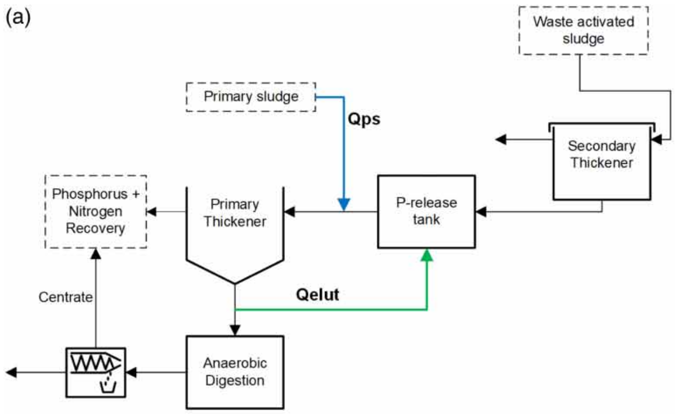
Figure 2 | Treatment scheme of Denia WWTP: (a) original, (b) upgraded.

Upgrade of a conventional WWTP for P recovery

In WWTP with biological P removal it becomes very interesting to enhance P recovery and minimize uncontrolled P precipitation. For this, a modification in the sludge line was proposed after a simulation study and tested in different full-scale applications (Tarragona, Calahorra and Murcia-Este WWTPs). The simulations evaluated the potential P recovery by mixing the thickened sludges in a mixing chamber before the anaerobic digestion and pumping the mix towards the primary thickener, therefore obtaining an overflow stream highly enriched in orthophosphate available for its recovery. Figure 3(a) shows the schematic description of the simulated sludge line configuration and Figure 3(b) shows the concentration of orthophosphate in the overflow stream, estimated at different operational conditions in Murcia-Este WWTP. The details of the simulation and optimization work in the Tarragona WWTP can be found in Ruano *et al.* (2012) while Martí *et al.* (2017) describe the case of Calahorra WWTP. This configuration allows recovery of up to 40% of the incoming phosphorus and considerably reduces the uncontrolled phosphorus precipitation in digesters, pipes, centrifuges and other equipment.

Optimization of an industrial WWTP

Plant-wide models can also be applied to simulate treatment processes of industrial wastewaters. In these cases, the steps of wastewater characterization and parameter calibration take a crucial role. Several complete analytical campaigns are required for wastewater characterization and values from literature cannot be adopted. Model parameter values should be obtained with off-line calibration methodologies to detect bacterial inhibitions. Table 3 shows, as an



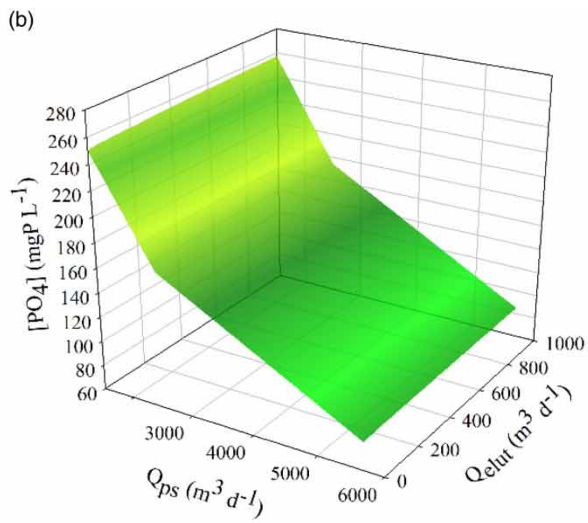


Figure 3 | (a) Schematic representation of the sludge line configuration simulated (b) concentration of phosphorus in the primary thickener overflow at different operational conditions: primary sludge flow (Q_{ps}) (blue line into the primary thickener) and elutriation flow (Q_{elut}) (green line from the primary thickener to the P-release tank). The full colour version of this figure is available in the online version of this paper, at http://dx.doi.org/10.2166/wst.2020.056.

Table 3 | Values of the main model parameters calibrated for the industrial wastewater and the reference ones for sewage proposed in BNRM1 (Seco *et al.* 2004)

	Model parameter	Calibrated	Default
Y_{OHO}	Yield for heterotrophic biomass	0.38	0.63
$\mu_{OHO,Max}$ (d^{-1})	Maximum heterotrophic growth rate	1.04	6
b_{OHO} (d^{-1})	Heterotrophic decay rate	0.18	0.4
$K_{F,OHO}$ (mg DQO·l^{-1})	Saturation coefficient for fermentable matter	17.19	4
$\eta_{\mu OHO,Ax3}$	Correction factor for anoxic conditions	0.05	0.43
$\mu_{AOO,Max}$ (d^{-1})	Maximum autotrophic growth rate	0.2	1
b_{AOO} (d^{-1})	Autotrophic decay rate	0.05	0.15
$K_{NH,AOO}$ (mg N·l^{-1})	Saturation coefficient for ammonium	0.38	1

example, the values obtained for the high influence model parameters in the WWTP of a petrochemical company, quite different from the typical values for urban WWTPs. This showed that wastewater characteristics influence the activity of microorganisms to a large degree.

Figure 4 shows the oxygen uptake rate values recorded at different substrate concentrations for heterotrophic and autotrophic bacteria. Very high substrate concentrations (higher than usual for urban WWTPs) are required for heterotrophic bacteria to reach their maximum activity. Maximum activity of autotrophic bacteria is relatively low but is reached at low ammonium concentrations.

Development of control strategies

Control system design, calibration and validation can be supported by plant-wide models, since it is possible to reproduce the response of the operational units to the performed actions. For instance, plant-wide models allow taking into account the effect of dewatering and supernatant streams recycling to the mainline, affecting the virtual nitrogen loading rate. For this, Ruano *et al.* (2017) used the simulation software DESASS (Ferrer *et al.* 2008), the IWA BSM1 (Alex *et al.* 2008) as a working scenario and the software LoDif Biocontrol® (Ferrer *et al.* 2011) in order to design, calibrate and validate control strategies for optimal nitrogen removal (minimized energy consumption) in activated sludge systems. Figure 5 shows a schematic representation of the development procedure for these controllers to be implemented in full-scale WWTPs.

An example of simulation results from one of the designs carried out in the study is shown in Figure 6. The dissolved oxygen concentration (DO) through a plug-flow reactor was controlled by changing the DO setpoints through time. When the aeration capacity was sufficient, the DO concentration oscillated near the established DO set points. The pattern of the DO set points showed similarities with the dynamics in ammonium concentration, mainly as a result of the information obtained from the pH sensors that were used to modify the DO set point. Suitable overall process performance was achieved, resulting in enhanced nitrogen removal efficiencies. Moreover,

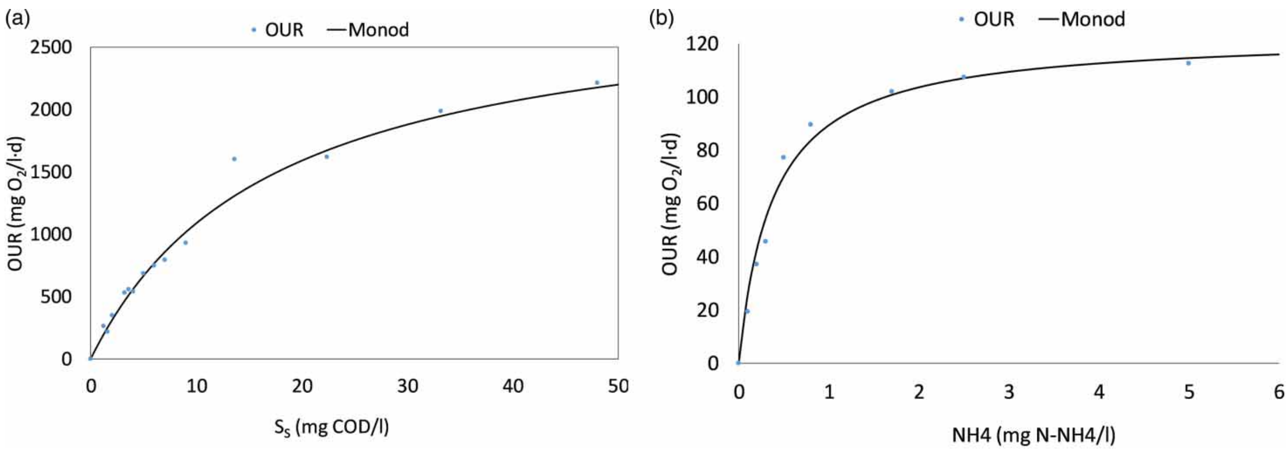


Figure 4 | OUR values obtained at different substrate concentrations for (a) heterotrophic bacteria, (b) autotrophic bacteria.

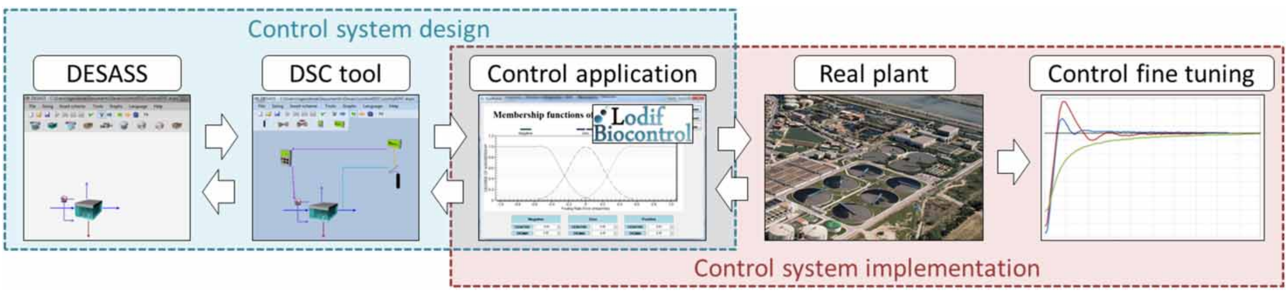


Figure 5 | Schematic representation of the development procedure for the controllers to be implemented in WWTPs.

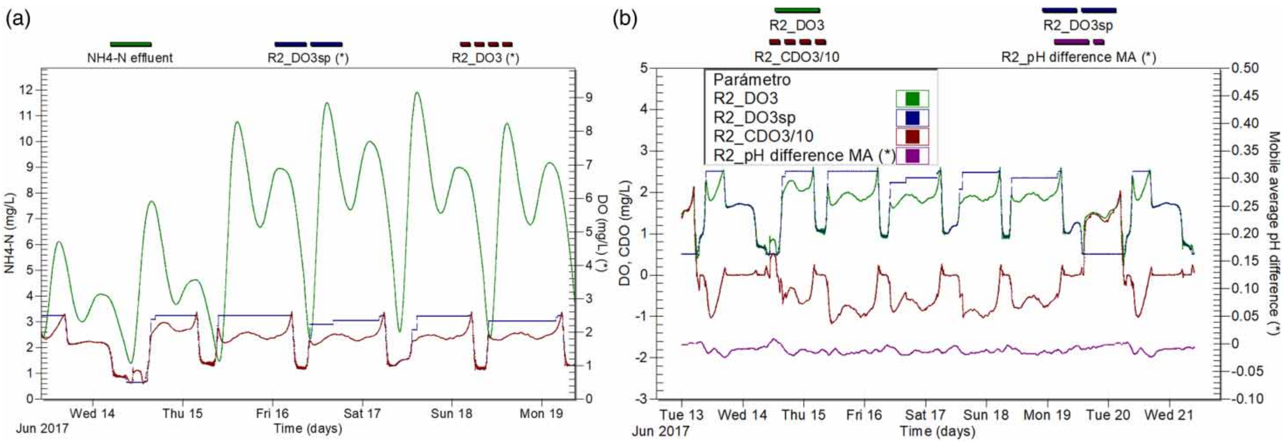


Figure 6 | Evolution of: (a) DO set point (R2_DO3sp) and ammonium concentration in the outlet of the aerobic reactor (NH4-N effluent). R2_DO3 is the measured DO concentration in the reactor lane 2; and (b) inputs to the controller (Moving Average of pH difference (R2_pH difference MA), cumulative DO error in the third aerated chamber over ten (R2_CDO3/10), DO (R2_DO3) and DO set point (R2_DO3sp) in last aerated chamber).

compared to the baseline scenario, the controller significantly reduced the energy demand. Specifically, power requirements were reduced from approximately 0.13–0.10 kWh per m^3 of treated water.

Other extensions for plant-wide modelling

A filtration model was also included in the collection model BNRM in order to allow simulation of a wider spectrum of processes. Specifically, a model was proposed for immersed MBRs taking into account the effect of biogas sparging and back-flushing on cake detachment, as well as the risk of forming irreversible fouling. This specific model was validated in an AnMBR system equipped with industrial-scale membranes in the short (Robles *et al.* 2013a) and the long term (Robles *et al.* 2013b) and used for control purposes, showing that it is possible to efficiently maintain low fouling rates by the application of an upper layer fuzzy-logic controller. In addition, this model was applied to optimise the performance of an AnMBR at pilot scale, obtaining energy savings of up to 25%. A model-based optimization method was also applied to improve the performance of AnMBRs (Robles *et al.* 2014, 2018).

Regarding integration of energy and environmental aspects on the modelling target, Pretel *et al.* (2016a) extended the collection model BNRM with a plant-wide energy model, which was validated in an AnMBR system treating sewage at steady- and unsteady-conditions. The results indicated that the model was capable of reproducing energy variations even when operating at dynamic conditions (i.e. variations in ambient temperature and/or inflow temperature). Pretel *et al.* (2016b) combined this model with life cycle assessment (LCA) for comparing different treatment technologies. In this case, the conclusion could be achieved that an AnMBR combined with a CAS-based post-treatment results in significant reductions in different environmental impact categories mainly due to reduced power requirements.

SUMMARY AND FUTURE PERSPECTIVES IN WASTEWATER TREATMENT MODELLING

After the development and wide spread of biochemical models to describe separately the most relevant processes in wastewater treatment, the field has evolved in the last decades in the direction of creating plant-wide models that are able to reproduce the increasing complexity of the plants as a whole. These models take cost into account, as well as a variety of processes such as chemical equilibria, oxygen transfer, greenhouse gas generation, etc. and they intend to be widely and easily applicable. They have a key role in process design, optimization and control. The viability of applying a plant-wide model increases with advances in computer technology and the development of simulation platforms. The major role of these plant-wide models has been shown in this work with a series of case studies where WWTP simulation studies were performed applying the BNRM model on the DESASS platform.

Remaining challenges in the field of plant-wide modelling are, on the one hand, related to the model itself:

(i) Further extensions: newly modelled processes remain to be added as extensions in plant-wide models. In some cases, new models have been developed according to the standardized notation, which facilitates their inclusion. Some studies already show examples of the possibility of this combination, with processes such as enhanced anammox (Dorofeev *et al.* 2017), granular sludge reactors (Dold *et al.* 2018), enhanced biofilm processes (Moretti *et al.* 2018; Ji *et al.* 2019), microalgae and cyanobacteria activity (Shoener *et al.* 2019), autotrophic denitrification using sulfur (Liu *et al.* 2016), membrane contactors and degassing membranes for component separation (Nagy *et al.* 2019), life cycle analysis (Ontiveros & Campanella 2013) or energy balance (Drewnowski *et al.* 2018). Some commercial models such as BioWin, SUMO or GPS-X already include some of the most used extensions.

(ii) New pollutants: especially in the case where new legal discharge limits are established (e.g. emerging pollutants or heavy metals). Including these components in a plant-wide model will constitute a great challenge, given the high number of pollutants that could possibly be considered and the often-complex routes of degradation and interaction amongst them and other wastewater components. A considerable effort will be needed to study the fate of pollutants in each treatment unit and therefore the formation of intermediate and final compounds, some of which are pollutants as well.

On the other hand, achieving a real wide spread of plant-wide models among operators of water resource recovery facilities is a current challenge for the scientific community involved in the development of such models. The full potential of plant-wide models for designing new sustainable WRRF, as well as for optimizing existing ones, can only be achieved when these models are transferred to real application.

Regarding model calibration and validation, a consensus is needed on calibration protocols in order to minimize the variability among model parameters obtained in different studies. As commented before, the IWA STR on Guidelines for using ASMs (Rieger *et al.* 2012) presented a protocol for on-line calibration in the water line. There is still a need for similar standardized calibration procedures for the sludge line, in the case of off-line calibration and for plant-wide models.

Exploring the considerable amount of information currently available on the performance of full-scale implemented processes should also gain importance as a modelling tool in the near future since authors consider that big data in WRRFs is widely underutilized (Newhart *et al.* 2019). Although the quality of this data might be in cases questionable, the wide spread of the use of probes, for instance, can provide interesting and useful data about some of the most usual processes in a WWRF. In this respect, coupling data-driven modelling methods for plant-wide process monitoring and control with mechanistic plant-wide models will boost plant-wide optimization (Ge 2017). Other kinds of useful data that could be obtained from WWTP operators are the observed oscillations in water flow and pollutant concentrations, which can be daily, seasonal, or event-dependent such as rain or other one-time events (sporting, cultural, etc). Plant-wide models can make use of this data to develop operational strategies (rules of action) for special cases, simulating different scenarios and the plant response to possible corrective measures. In addition, integrating computational fluid dynamics models (CFD) with plant-wide models for smarter operation and optimal design still remains a big challenge.

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First received 20 September 2019; accepted in revised form 28 January 2020. Available online 11 February 2020