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Plant-wide modelling for assessment and optimization of upgraded full-scale wastewater treatment plant performance

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Abstract

This paper presents the design of a plant-wide CNP (carbon-nitrogen-phosphorus) simulation model of a full-scale wastewater treatment plant, which will be upgraded for tertiary treatment to achieve compliance with effluent total nitrogen (TN) and total phosphorus (TP) limit values. The plant-wide model of the existing plant was first designed and extensively validated under long-term dynamic operation. The most crucial step was a precise characterization of input wastewater that was performed by extending the plant performance indicators both to a water line and sludge line and systematically estimating identifiable wastewater characterization parameters from plant-wide performance indicators, i.e. effluent concentrations, biogas and sludge production, and sludge composition. The thus constructed simulation model with standard activated sludge model (ASM2d) and anaerobic digestion model (MantisAD) overpredicted ortho-P and ammonia-N on the sludge line, indicating a need to integrate state-of-the-art physico-chemical minerals precipitation models to simulate plant-wide interactions more precisely. The upgraded plant with multimode anaerobic/anoxic/oxic configuration shows limited denitrification potential. Therefore, additional reject water treatment was evaluated to improve effluent TN and TP performance.

Key words: biological wastewater treatment, full-scale, model validation, plant upgrading, plant-wide model, wastewater characterization

INTRODUCTION

In the past two decades, the mathematical models of wastewater treatment processes, simulation software tools, and model building procedures have matured so that the use of models has become a common way to analyse and predict the behaviour of wastewater treatment plants (WWTPs). A family of activated sludge models (ASMs) (Henze *et al.* 2000) and an anaerobic digestion model (ADM1) (Batstone *et al.* 2002) are considered as standard models of biological processes in WWTPs. In recent years a shift has been seen towards Plant-Wide Modelling (PWM), i.e. integrating water line and sludge line models to achieve optimal solutions for the design, operation, and control at the level of the whole plant. Such an integrated view is also needed to meet emerging challenges in WWTP operation that require plant-wide consideration, such as energy minimization, resource recovery, and environmental impact assessment.

To support plant-wide consideration, different modelling and simulation tools have been designed. For example, a Benchmark Simulation Model No. 2 (BSM2) includes water line and sludge line processes and enables long-term plant-wide evaluation, supervisory control and optimization (Jeppsson *et al.* 2007; Solon *et al.* 2017). In addition, a PWM library proposed by Fernandez-Arevalo *et al.* (2017) presents a comprehensive tool for mass and energy flux distribution analysis of different plant configurations. Commercial WWTP software tools are also supporting PWM. However, despite

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this development, the evaluation of plant-wide models against full-scale data is still very rare. As Kazadi Mbamba *et al.* (2016) comments, 'there has been little systematic research validating standard models such as the ASM series and ADM1 in a plant-wide context and using real full-scale plant data'.

An example of a full-scale plant-wide dynamic optimization with respect to energy consumption and effluent nitrogen components was presented in Puchongkawarin *et al.* (2015). Zaborowska *et al.* (2017) presented a model-based evaluation of technological upgrades for achieving energy neutrality, thereby using plant-wide CNP (carbon-nitrogen-phosphorus) model simulations at steady-state conditions after validating the model on full-scale four-day dynamic measurements. Recently, of particular interest has been the upgrading of CNP models with the physico-chemical framework (PCF) to describe mineral precipitation and thus more reliably describe phosphorus simulation and the plant-wide cycling of phosphorus (Flores-Alsina *et al.* 2016; Kazadi Mbamba *et al.* 2016).

This paper presents a full-scale design and long-term application of a plant-wide dynamic CNP model. The modelling and simulation study was performed in simulation software GPS-X^{TM} (Hydromantis, Hamilton, ON, Canada). The model was designed to predict the real plant performance after introducing technological changes for improved nitrogen (N) and phosphorus (P) removal. In the presented model application, wastewater characterization was the most extensive and demanding part of the modelling study. A new systematic wastewater characterization procedure based on sensitivity analysis is proposed, gaining advantages from plant-wide model consideration and evaluating plant performance both on the water line and sludge line. The study also shows some shortcomings of available standard models to properly model nutrients in the sludge line. While in our case the nutrient modelling on the sludge line was improved by adjusting the anaerobic digestion model stoichiometric parameters, a more sophisticated model with a PCF modelling framework might be needed for future model development.

MATERIALS AND METHODS

WWTP case study

The plant considered in the study is operated at 435,000 population equivalent (PE). The plant efficiently removes carbon and achieves nitrification, but lacks denitrification and phosphorus removal. The existing treatment facilities consist of mechanical treatment (screens, grit and grease chamber), a biological stage with a suspended biomass activated sludge process (three parallel plug-flow aerobic reactors and four parallel secondary clarifiers) and sludge treatment (sludge thickening, anaerobic digestion, dewatering and sludge drying).

The plant will be upgraded to enhance complete N and P removal. The preliminary design defined suitable technological solutions for the plant upgrade. The outcome of the preliminary design, i.e. the plant units, their volumes and operating conditions were used in simulations for evaluating the upgraded plant performance under dynamic conditions. The main changes are presented below.

Increased input load

The input load is expected to increase to 555,000 PE.

Primary clarifier

Primary clarifier will be introduced after the mechanical stage to remove the total suspended solids (TSS) from the water line to the sludge line and enhance the biogas production from sewage sludge in anaerobic digestion.

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Biological stage

The biological stage of the upgraded plant is designed as a multimode anaerobic/anoxic/aerobic process to achieve denitrification and biological P removal. For that purpose, each of the existing plug-flow aeration tanks in the three parallel lines will be transformed into four consecutive tanks. To achieve the necessary biological activity within the existing plant volumes, the biological stage is planned to operate at increased mixed liquor suspended solids (MLSS) concentrations.

Sludge treatment

Primary sludge and waste sludge will be treated in the separate thickener and dewatering units before processed in anaerobic digesters.

Plant-wide model

The model was designed in CNP library in GPS-X (Hydromantis 2016) to simulate the removal of carbon, N and P components. The unit processes, their physical parameters, and selected models are presented in Table 1. The biological reactors were modelled with the ASM2d model (Henze *et al.* 2000), while anaerobic digesters were modelled with the MantisAD model (Copp *et al.* 2005).

Table 1 | Unit processes and models with physical parameters for existing and upgraded plant configuration

Process unit	GPS-X unit process	Existing plant simulation	Upgraded plant simulation	GPS-X model	Physical parameter
Grit and grease chamber	Grit Chamber	x	x	empiric	
Primary clarifier	Rectangular Primary Clarifier		x	simple1d	9,999 m^3
Biological reactors	Plug-Flow Tank with four tanks	x	x	asm2d	39,000 m^3
Secondary clarifiers	Rectangular Secondary Clarifier	x	x	simple1d	24,000 m^3
Primary sludge thickener	Thickener		x	simple1d	1,850 m^3
Primary sludge centrifuge	Dewatering		x	empiric	
Waste sludge thickener	Thickener	x	x	simple1d	1,850 m^3
Waste sludge centrifuge	Dewatering	x	x	empiric	
Anaerobic digester	Anaerobic Digestion	x	x	mantisad	14,130 m^3
Secondary thickener	Pumping Station	x	x	noreact	1,850 m^3
Dewatering (centrifuge)	Dewatering	x	x	simple	
Sludge drying	Dewatering	x	x	empiric	

The upgraded plant simulation layout is shown in Figure 1. It includes three additional units, i.e. a primary clarifier, a primary sludge thickener, and a primary sludge centrifuge.

The biological reactors model was also changed. As seen in Figure 2, each biological plug-flow reactor will be transformed into four consecutive tanks with 25%, 19%, 34% and 22% of the total volume, respectively. The plant will operate in two configurations: AAO – anaerobic/anoxic/aerobic, or AO – anoxic/aerobic, depending on the wastewater temperature. AAO configuration is operated at high temperatures and enables biological P removal, nitrification, and denitrification. The AO configuration is operated at low temperatures and enables only nitrification and denitrification. In both cases the remaining P after the biological stage is removed by chemical precipitation. The upgraded plant operation and control conditions are described below.

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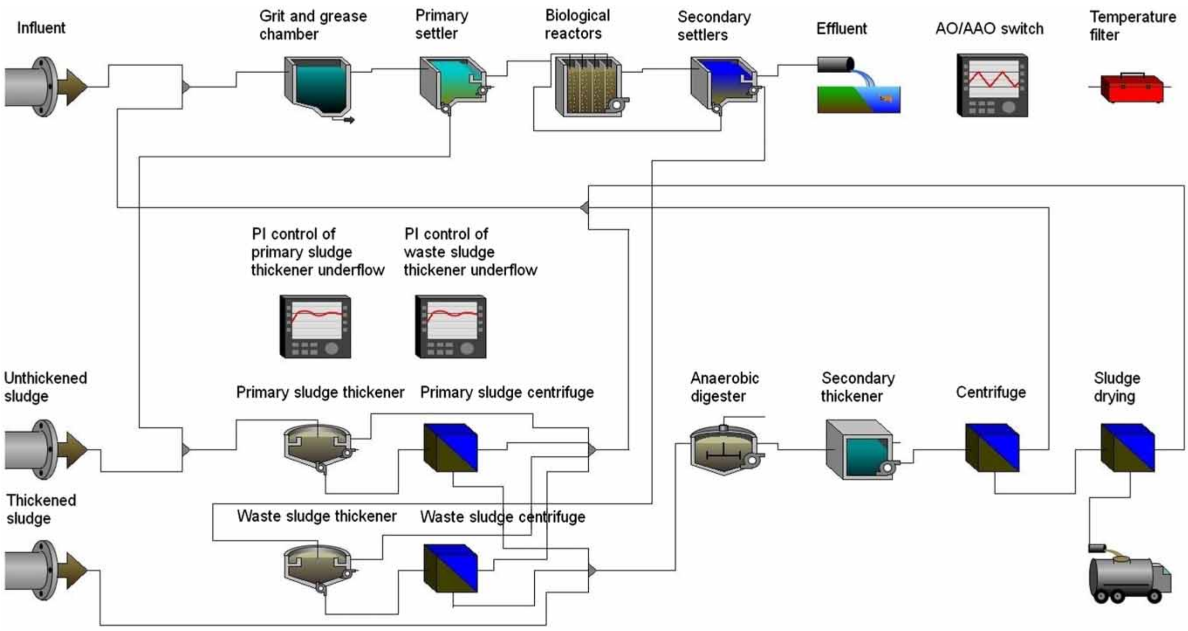

Figure 1 | Simulated plant layout of the upgraded plant configuration.

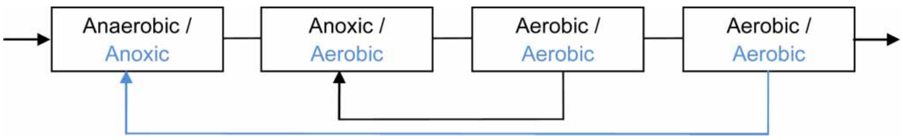

Figure 2 | Biological stage of the upgraded plant with four tanks and flexible configuration: AAO (anaerobic/anoxic/aerobic, indicated with black) or AO (anoxic/aerobic, indicated with blue).

AO/AAO configuration control

Switching between configurations is performed based on filtered wastewater temperature. Switching to AAO is performed at $T \geq 19$°C, and switching to AO at $T \leq 18.5$°C.

Dissolved oxygen (DO) control

DO in aerobic tanks is controlled at 1.5 mg/L.

Internal recycle flow control

Internal recycle flow is determined as four times the influent flow.

External recycle (return sludge) control

External recycle flow is simulated as 1.6 times the influent flow.

MLSS control

The upgraded plant is simulated at the increased MLSS concentration of 4,500 mg/L in the biological stage by adjusting the waste sludge flow by a PI controller. The MLSS controller parameters are: sampling time $t_s = 15$ min, proportional gain $K_p = 2\ m^6/(d\ g)$, integral time $T_i = 8$ days.

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Primary sludge control

The flow of primary sludge is determined by PI controller controlling the underflow TSS concentration at 20,000 mg/L. The primary sludge controller parameters are: $t_s = 15$ min, $K_p = 0.05\ m^6/(d\ g)$, $T_i = 4$ days.

Dry solids content control in the sludge line

The operation of the sludge line is determined by setting the dry solids concentration of different units to the values as defined in the preliminary design. The dry solids content of primary sludge and waste sludge after pre-thickener is 3.5% and 3%, respectively, after the primary and waste sludge centrifuge 6%, after the final centrifuge 25%, and in the final sludge 92%. To achieve the predicted dry solids content after pre-thickener, the underflow from thickener to centrifuge is both for primary sludge and waste sludge determined by a PI controller. The parameters of the controllers are: $t_s = 15$ min, $K_p = 0.05\ m^6/(h\ g)$, $T_i = 4$ days (primary sludge) and 8 days (waste sludge). In the empiric models of primary sludge centrifuge, waste sludge centrifuge, and sludge drying, the solids removal is specified by setting the desired underflow solids concentrations. For the final centrifuge, the dry solids concentration is resulting from setting the solids capture parameter (0.96) and polymer dosage parameter (0.28 kg/m^3). The centrifuge sludge treatability parameter was kept at the default value of 0.7.

Operation periods of centrifuge and sludge drying units

Dewatering and sludge drying units are operated depending on the sludge height in the secondary thickener, with low and high volumes of 250 and 1,200 m^3. During operation, the pumped flow from the secondary thickener to centrifuge is 28 m^3/h.

Wastewater characterization

The use of models in full-scale applications requires a detailed input wastewater characterization and calibration of model parameters (Petersen *et al.* 2002; Mannina *et al.* 2011). Wastewater characteristics determination, in particular chemical oxygen demand (COD) fractionation with regard to biodegradability (readily, slowly and inert) and physical aggregation state (soluble, particulate), is considered as the most important aspect of modelling WWTPs to properly predict transformation of different components within the plant (Muserere *et al.* 2014). The composition of the influent wastewater is also one of the most influential factors influencing WWTP operating costs (Fernandez-Arevalo *et al.* 2017).

Generally, wastewater characterization can be performed using two different approaches (Fenu *et al.* 2010): (i) experimental measurements with chemical/physical/biological methods (Tran *et al.* 2015) and (ii) 'trial-and-error' procedures that aim to fit experimental observations with model simulation by tuning the different wastewater characterization parameters.

As elaborated by Ekama (2010), the better the effluent quality required by the activated sludge system to perform biological nutrient removal, the more the wastewater's characteristics need to be accurately known. In the cases of biological N removal (nitrification and denitrification) and biological P removal, the wastewater N load (total Kjeldahl nitrogen (TKN) and ammonia-N) and P load (total P and ortho-P) need to be known. In addition, the influent's readily biodegradable COD also needs to be known, since it is important for the nitrate denitrified in the anoxic reactor, and it establishes the extent of biological P removal that can be achieved (readily biodegradable COD includes short chain fatty acids that are important for P removal).

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Wastewater characterization requires the determination of the following:

- five input COD fractions ($f_{rsi}, f_{rsf}, f_{rslf}, f_{rxi}, f_{rxs}$) that define inert soluble organic material (S_I), fermentable readily biodegradable organic substrates (S_F), volatile fatty acids VFA (S_{LF}), inert particulate organic material (X_I) and slowly biodegradable substrates (X_S) within measured COD. They also define the soluble COD (sCOD) and particulate COD (xCOD) as follows

$$\mathrm{COD} = \mathrm{sCOD} + \mathrm{xCOD} = S_I + S_F + S_{LF} + X_I + X_S = (f_{rsi} + f_{rsf} + f_{rslf} + f_{rxi} + f_{rxs})\mathrm{COD} \tag{1}$$

- f_{bod} parameter, which relates biological oxygen demand in the five-day period ($\mathrm{BOD_5}$) and BOD ultimate for the total biochemical degradation ($\mathrm{BOD_u}$)

$$f_{bod} = \frac{\mathrm{BOD_5}}{\mathrm{BOD_u}} \tag{2}$$

- i_{vt} and i_{cv} ratios, which are related to total suspended solids concentration (TSS), volatile suspended solids (VSS) and xCOD

$$i_{vt} = \frac{\mathrm{VSS}}{\mathrm{TSS}} \tag{3}$$

$$i_{cv} = \frac{\mathrm{xCOD}}{\mathrm{VSS}} \tag{4}$$

Within the wastewater characterization above, eight parameters need to be determined. By measuring input COD, $\mathrm{BOD_5}$ and TSS and taking into account their interrelations

$$\mathrm{COD} = S_I + S_F + S_{LF} + X_I + X_S \tag{5}$$

$$\mathrm{BOD_5} = f_{bod}\mathrm{BOD_u} = f_{bod}(S_F + S_{LF} + X_S) \tag{6}$$

$$\mathrm{TSS} = \frac{\mathrm{VSS}}{i_{vt}} = \frac{\mathrm{xCOD}}{i_{vt}i_{cv}} = \frac{X_I + X_S}{i_{vt}i_{cv}} \tag{7}$$

five parameters could be adjusted arbitrary, while the other three are determined from (5)-(7).

Estimation of wastewater characterization parameters is performed with the following procedure using long-term influent average values of COD, $\mathrm{BOD_5}$ and TSS measurements ($\overline{\mathrm{COD}}$, $\overline{\mathrm{BOD_5}}$ and $\overline{\mathrm{TSS}}$):

1) $f_{rsi}, f_{rsf}, f_{rslf}, f_{bod}$ and i_{vt} are determined from plant-wide sensitivity analysis as explained below
2) f_{rxs} is determined from interrelation between COD and $\mathrm{BOD_5}$ (6)

$$f_{rxs} = \frac{\overline{\mathrm{BOD_5}}}{f_{bod}\overline{\mathrm{COD}}} - (f_{rsf} + f_{rslf}) \tag{8}$$

3) f_{rxi} is determined from COD (5)

$$f_{rxi} = 1 - f_{rsi} - f_{rsf} - f_{rslf} - f_{rxs} \tag{9}$$

4) i_{cv} is determined from COD and TSS measurements (7)

$$i_{cv} = \frac{(f_{rxi} + f_{rxs})\overline{\mathrm{COD}}}{i_{vt}\overline{\mathrm{TSS}}} \tag{10}$$

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The choice of arbitrarily chosen parameters is performed with the sensitivity based tuning procedure that takes into account relations between influent wastewater characterization parameters and some key plant performance indicators, i.e. effluent COD, effluent TN, effluent TP, biogas production, dried sludge production, and the content of organic dry solids in dried sludge. The input-output mapping between wastewater characterization parameters and plant performance indicators is shown in Figure 3 and summarized in Table 2. Note that the performance indicators above do not include only the water line performance, but are also extended to the sludge line.

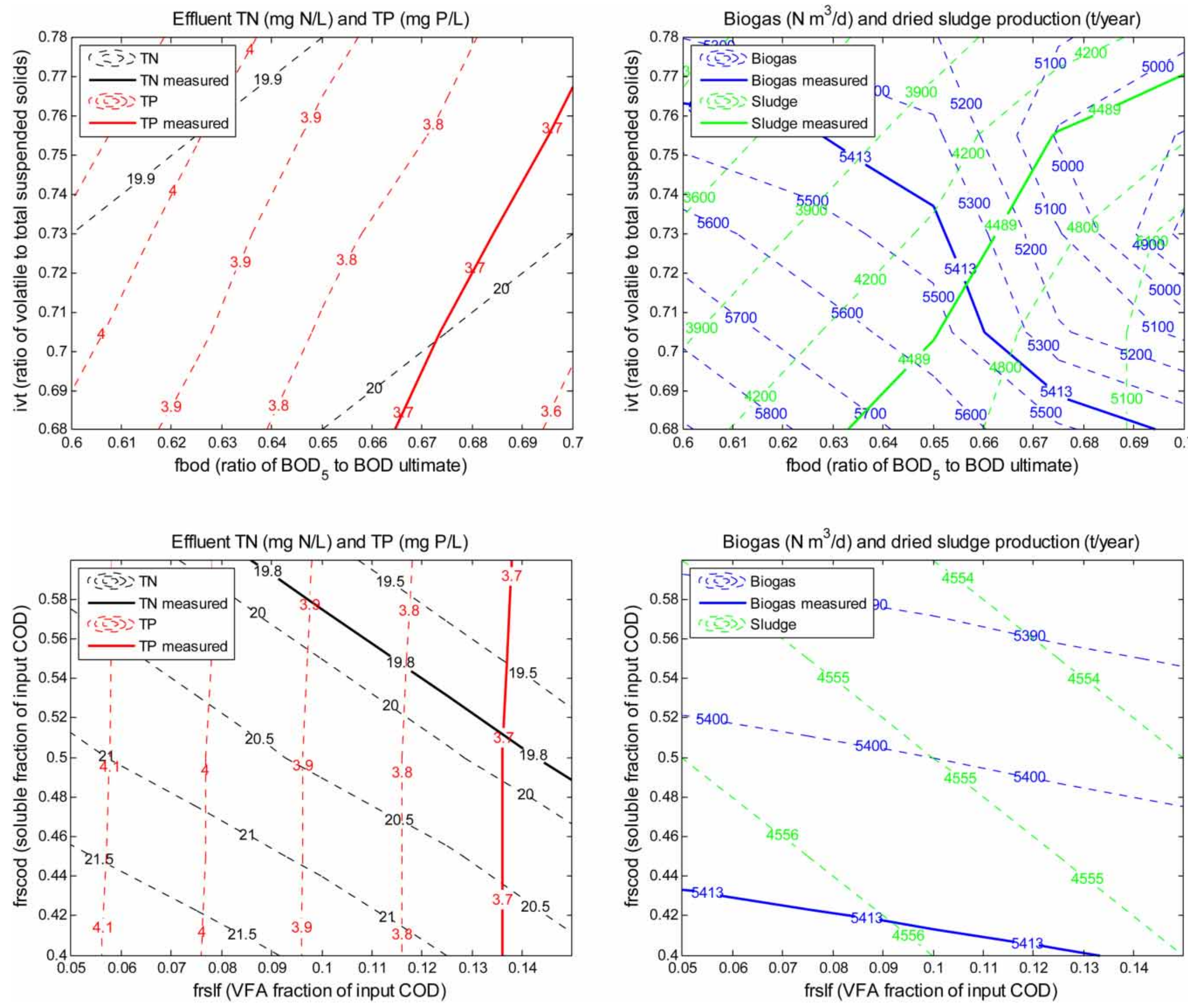

Figure 3 | Sensitivity analysis of plant performance on wastewater characterization parameters with indicated lines of full-scale long-term average performance.

Following relations in Table 2, the arbitrarily chosen parameters are determined as follows:

1) f_{rsi} is adjusted to match measured effluent COD.
2) f_{bod} and i_{vt} are adjusted to tune measured biogas production, dried sludge production and measured i_{vt} along the sludge line. As shown in Figure 3 (top right diagram), the adjustment is performed by taking into account the following relations:
   a) Increasing f_{bod} results in lowering the influent biodegradable part of COD and increasing the inert fraction of total COD. As a result, the amount of biomass in the sludge is decreased and the inert fraction is increased. Consequently, the biogas production from the biomass sludge in the anaerobic digester is decreased, while the sludge production is increased.

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Table 2 | Results of sensitivity analysis with the indicated influence of wastewater characterization parameters on plant performance

Influent wastewater characterization parameters		Plant performance indicators				
Influent parameter	**Symbol**	**Effluent COD**	**Effluent TN**	**Effluent TP**	**Biogas production**	**Sludge production**
Soluble inert fraction of input COD	f_{rsi}	+				
Fermentable biodegradable fraction of input COD	f_{rsf}		–			
VFA fraction of input COD	f_{rslf}		–	–		
Ratio of BOD_5 to BOD_u	f_{bod}			–	–	+
Ratio of volatile to total suspended solids	i_{vt}			+	–	–

   b) Increasing i_{vt} means reducing the influent inert inorganic matter and thus also reducing the final sludge production. The amount of inorganic matter in the biological stage is also reduced. Therefore, to keep the measured MLSS in the reactor, the plant has to operate at larger SRT, which results in smaller biogas production.

3) After setting f_{bod}, parameter f_{rslf} is adjusted to match effluent TP (Figure 3, bottom left diagram).
4) Finally, f_{rsf} (as a part of soluble COD fraction f_{rscod}) is adjusted to match effluent TN (Figure 3, bottom left diagram).

The final set of parameter values compared to their default values is presented in Table 3.

Table 3 | Influent wastewater characterization parameters with default and adjusted values

Parameter	Unit	Symbol	Default value	Adjusted value
Soluble fraction of total COD	–	f_{rscod}	0.25	0.5
Soluble inert fraction of total COD	–	f_{rsi}	0.05	0.059
Fermentable biodegradable fraction of total COD	–	f_{rsf}	0.2	0.311
VFA fraction of total COD	–	f_{rslf}	0	0.13
Particulate inert fraction of total COD	–	f_{rxi}	0.13	0.129
Slowly biodegradable fraction of total COD	–	f_{rxs}	0.62	0.371
xCOD/VSS ratio	gCOD/gVSS	i_{cv}	1.8	1.222
BOD_5/BOD_u ratio	–	f_{bod}	0.66	0.655
VSS/TSS ratio	gVSS/gTSS	i_{vt}	0.75	0.72

Adjustment of model parameters

According to several references (van Veldhuizen *et al.* 1999; Ekama 2010; Puchongkawarin *et al.* 2015), no major adjustments of kinetic and stoichiometric parameters in ASM and ADM models are required in practical applications, if wastewater characterization is performed satisfactorily. In a given case-study we have adjusted one kinetic parameter and two stoichiometric parameters.

Autotrophic maximum specific growth rate μ_{max} in ASM2d model was set to 0.96 d^{-1} (default value is 1 d^{-1}) to better match effluent TN, ammonia nitrogen (NH_4-N) and NO_3-N concentrations. Two stoichiometric parameters in the MantisAD anaerobic digestion model were also changed. The MantisAD model with default parameter values predicted well the TN and TP concentrations in digestate, but overpredicted NH_4-N and ortho phosphate (PO_4-P) concentrations. Overprediction of anaerobic digestion nutrient concentrations is also reported in other full-scale plant-wide model applications when using standard anaerobic digestion models. For example, Kazadi Mbamba *et al.* (2016) reported a 75% overestimation of phosphate release in anaerobic digesters when using the ADM1 model.

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Therefore, an improvement of model and inclusion of PCF for modelling minerals precipitation (Kazadi Mbamba *et al.* 2015) might be necessary for future work.

Conceptually similar as in PCF modelling, we assumed that a part of soluble inorganic N and P as modelled in MantisAD is captured by inorganic material (magnesium, calcium and potassium) and kept in the sludge. Therefore, two stoichiometric parameters in the MantisAD model were changed, i.e. the fraction of hydrolysed nitrogen becoming particulate inert nitrogen was set to 0.18 gN/gN (default value is 0) and the fraction of hydrolysed phosphorus becoming particulate inert phosphorus was set to 0.177 gP/gP (default value is 0). With this adjustment, we were able to better predict the N and P load in digestate and reject water, and thus obtain good N and P prediction after the mechanical stage in the water line.

RESULTS AND DISCUSSIONS

Plant measurements and evaluation criteria

Plant-wide simulations were performed for 426 days of full-scale plant operation. In the water line, plant measurements included daily average concentrations of regular laboratory and on-line measurements at the plant influent, after the mechanical treatment, in the mixed liquor after the biological reactors, and in the effluent. Dynamic inputs to the water line were measured wastewater temperature, inflow, COD, TKN, NH_4-N, TP and PO_4-P (estimated as 32% of TP). All the other data was used for model validation.

In the sludge line, the data included information on biogas production, sludge flow, mass, and solids concentrations at different locations. Monthly average values were available.

The mass flow returning from sludge line to water line was estimated from occasional plant measurements.

The goodness of fit between the simulated and measured data for the dynamic operation was evaluated with the following quantitative criteria:

i) Percentage of data where the error e_i between the measured value $y_{m,i}$ and simulated value $y_{s,i}$ lies within $\pm$ 20% of the measured value

$$|e_i| = |y_{m,i} - y_{s,i}| \leq 0.2 y_{m,i} \tag{11}$$

ii) Mean square relative error MRSE

$$\mathrm{MRSE} = \frac{1}{n}\sum_i \left(\frac{y_{m,i} - y_{s,i}}{y_{m,i}}\right)^2 \tag{12}$$

iii) Statistical coefficient of determination R^2 computed from the sum of squares of residuals SS_{res} and the total sum of squares SS_{tot} with regard to the mean of the observed data $\bar{y}$

$$R^2 = 1 - \frac{SS_{res}}{SS_{tot}} = 1 - \frac{\sum_i (y_{m,i} - y_{s,i})^2}{\sum_i (y_{m,i} - \bar{y})^2} \tag{13}$$

Existing plant simulation

Average values of plant measurements for the water line and their comparison with simulated data are presented in Table 4. Quantitative criteria for the influent and after mechanical treatment show good

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Table 4 | Measured and simulated data along the water line calculated from average daily values in the period of model simulation

Plant location	Process variable	Unit	Number of measured data points	Measured mean and standard deviation	Simulated mean and standard deviation	% of simulated data within ± 20% of measured value	MRSE	R^2
Influent	Flow[a]	m^3/d	426	82,561 ± 25,359	–	–	–	–
	TSS	mg/L	265	296 ± 98.6	311 ± 90.2	78.1	6.5	0.714
	COD[a]	mg COD/L	394	521 ± 165	–	–	–	–
	BOD_5	mg O_2/L	365	277 ± 98.5	275 ± 88.4	88.8	2.2	0.893
	TKN[a]	mg N/L	360	38.9 ± 11.0	–	–	–	–
	TP[a]	mg P/L	357	8.24 ± 2.45	–	–	–	–
	NH_4-N[a]	mg N/L	383	26.9 ± 8.0	–	–	–	–
After mechanical treatment	TN	mg N/L	344	47.2 ± 15.6	44.3 ± 13.3	74.4	5.0	0.583
	NH_4-N	mg N/L	366	31.0 ± 11.4	30.6 ± 10.5	79.2	4.8	0.820
	PO_4-P	mg P/L	372	3.18 ± 1.21	3.06 ± 0.93	69.9	52.9	0.589
After the biological reactors	TSS	mg/L	418	2,979 ± 352	3,011 ± 399	98.3	0.6	0.614
	NH_4-N	mg N/L	373	1.17 ± 1.31	0.65 ± 0.90	15.3	185	−0.198
Effluent	TSS	mg/L	278	8.9 ± 2.7	8.5 ± 1.8	42.1	27.7	−0.157
	COD	mg COD/L	402	39.4 ± 9.6	39.9 ± 7.2	66.7	7.2	0.150
	BOD_5	mg O_2/L	384	7.0 ± 2.7	3.7 ± 1.0	14.1	33.5	−1.610
	TN	mg N/L	398	19.8 ± 5.4	20.3 ± 6.4	71.4	5.7	0.442
	TP	mg P/L	355	3.70 ± 1.32	3.80 ± 1.0	64.2	11.6	0.556
	NH_4-N	mg N/L	373	1.43 ± 1.08	0.60 ± 0.86	5.9	51.1	−0.479
	NO_3-N	mg N/L	372	17.1 ± 5.3	18.6 ± 6.4	62.4	12.8	0.269
	PO_4-P	mg P/L	412	2.66 ± 1.06	3.59 ± 1.08	26.0	8,273	−0.218

[a]used as model input.

agreement for all evaluation criteria (i.e. similar mean and standard deviation of measured and simulated data, high % of simulated data is close to the measured data, low MRSE, R^2 close to 1), indicating good characterization of influent wastewater components.

Effluent data are also presented in Figures 4 and 5 as time plots as well as scatter plots of modelled versus measured data. The figures show that effluent TSS, COD, TN, TP and NO_3-N are well predicted by simulation. Note that good TN and NO_3-N performance was achieved by adjusting the μ_{max} parameter, as well as by lowering dissolved oxygen (DO) in the first tank of the plug-flow reactor to 0.5 mg/L to obtain partial denitrification. The performance of some other process variables was less satisfactory. The discrepancy is noticed for the following effluent variables:

- BOD_5, where the average of simulated data is lower than the measurements.
- NH_4-N, where the discrepancy is noticed both from quantitative criteria and signal plots. Simulated NH_4-N increases in winter conditions (days 230 to 350) because of lower temperatures, which could be also seen from the measurements. However, individual NH_4-N peaks could not be reached completely. The reason is that NH_4-N peaks very often appear also because of the short-term operational changes that are not recorded in daily operation and are thus not simulated (e.g. insufficient oxygen supply, increased nutrients load in reject water, unequal biomass and flow distribution between the parallel lines, etc.).
- PO_4-P, where the difference of 1 mg/L between measured effluent TP and PO_4-P is noticed but could not be reached in simulations as most of simulated effluent TP is in a form of PO_4-P.

Based on the results above it was concluded that the designed model presents the performance of the existing water line sufficiently well for the purpose of the plant upgrade, where particularly effluent TN and TP need to be well predicted to assess the performance after the plant upgrade.

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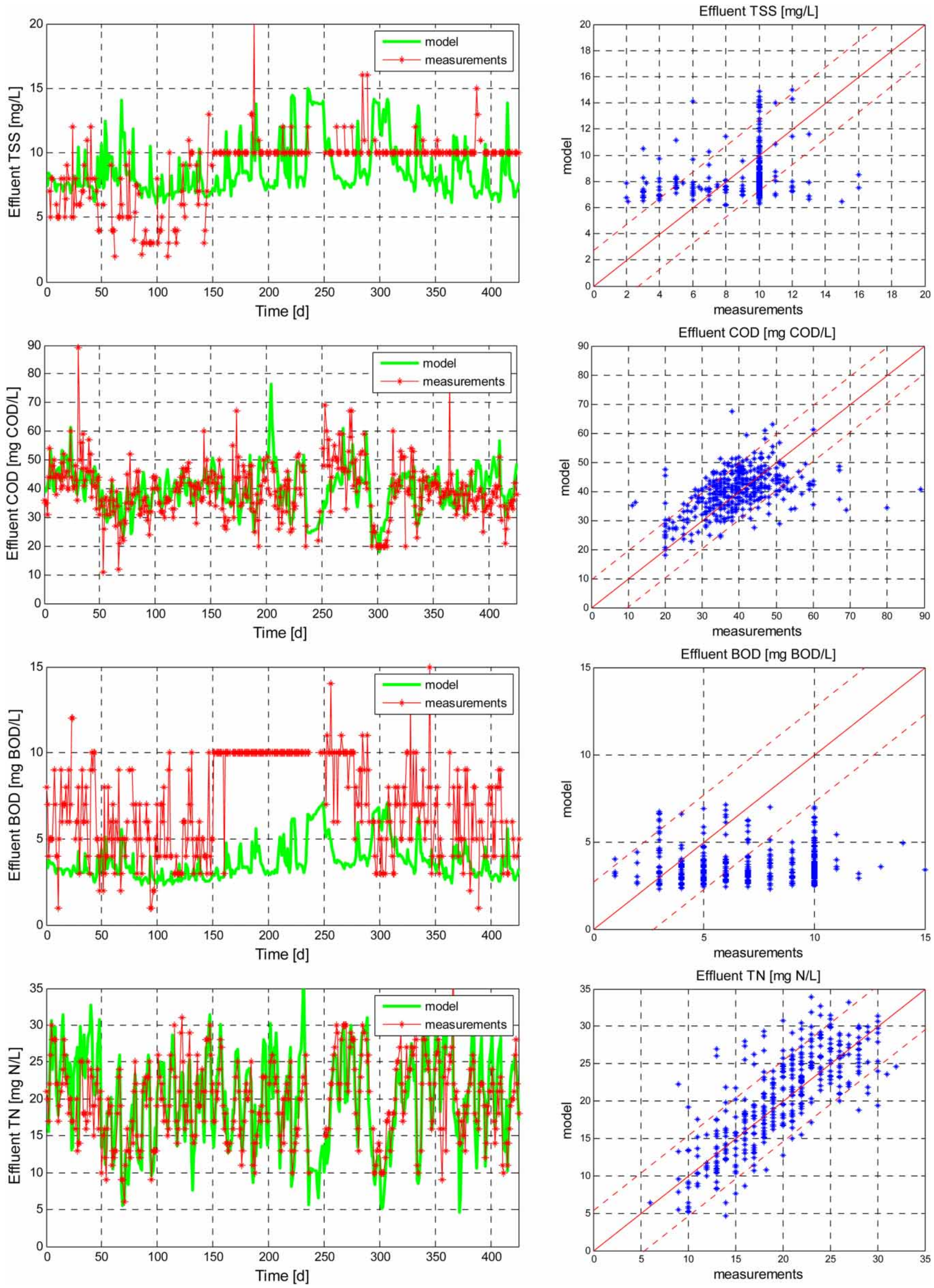

Figure 4 | Effluent TSS, COD, BOD_5 and TN in long-term model simulation compared with measurements (left diagram – time plot, right diagram – scatter plot of modelled data versus measurements with indicated straight lines of the standard deviation of measured values).

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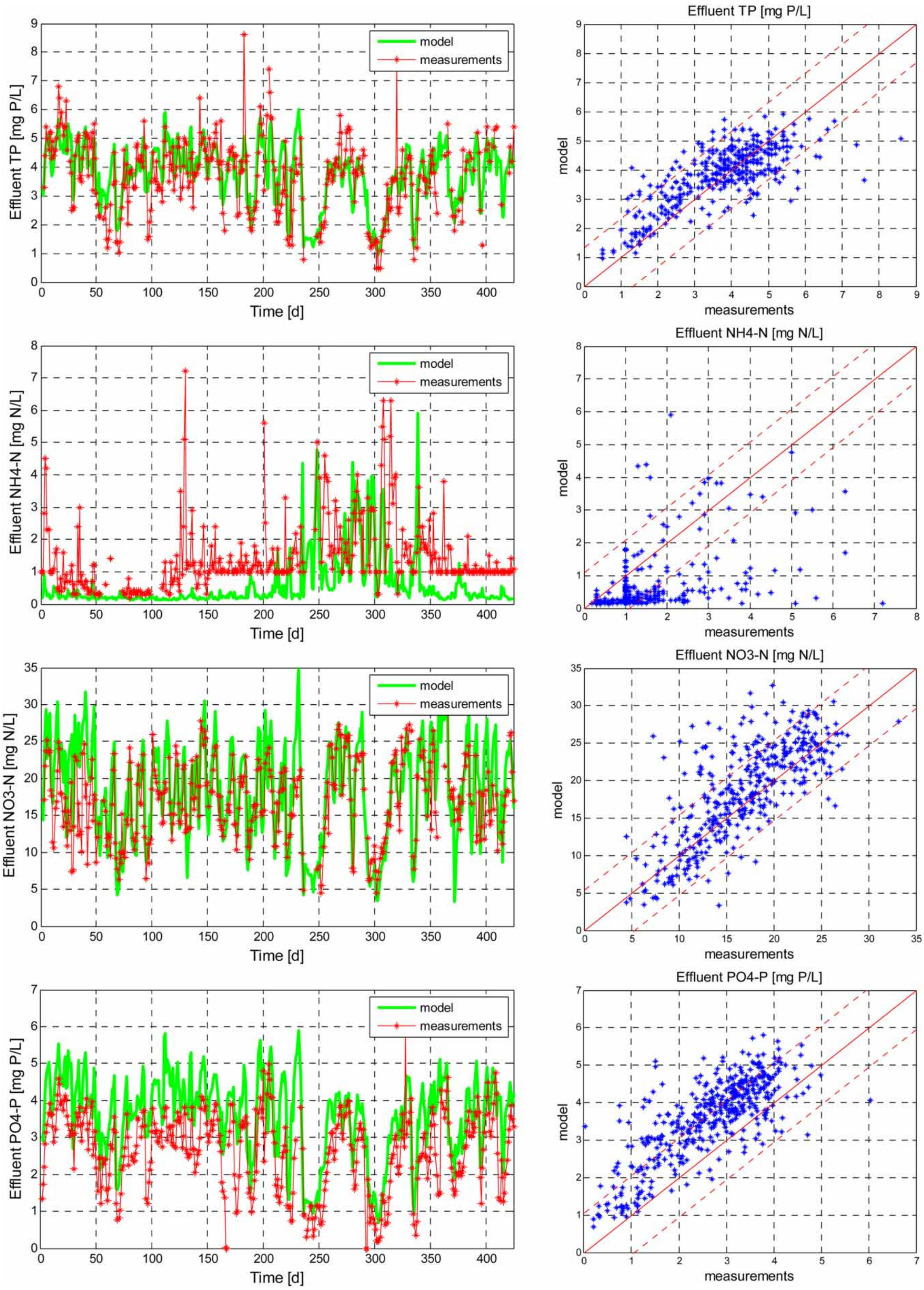

Figure 5 | Effluent TP, NH_4-N, NO_3-N and PO_4-P in long-term model simulation compared with measurements (left diagram – time plot, right diagram – scatter plot of modelled data versus measurements with indicated straight lines of the standard deviation of measured values).

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A comparison between average measured and simulated data of sludge production along the sludge line is presented in Table 5. It can be seen that the simulated values of flow, TSS, and VSS/TSS ratio are well in accordance with the measured values. For the dry matter, the discrepancies are larger, but the measured values are inconsistent and express large variations, e.g. significantly different calculated values of dry matter in waste sludge, sludge after pre-thickening and after waste sludge centrifuge.

Table 5 | Measured and simulated process variables along the sludge line calculated from average monthly values in the period of model simulation

Plant location	Process variable	Unit	Measured average	Simulated average
Waste sludge	Flow	m^3/d	~2,400	2,938
	TSS	g/m^3	~8,000	5,739
	VSS/TSS	–	~0.71	0.725
	Dry matter	t/year	6,688	6,164
Sludge after pre-thickening	Flow[a]	m^3/h	47.72	49.30
	TSS	g/m^3	14,140	13,946
	VSS/TSS	–	0.724	0.725
	Dry matter	t/year	5,895	6,075
Sludge after waste sludge centrifuge	Flow[a]	m^3/h	12,97	12.01
	TSS	g/m^3	64,509	56,063
	VSS/TSS	–	–	0.725
	Dry matter	t/year	7,327	5,892
Digestate after anaerobic digestion	Flow	m^3/h	12,30	12.83
	TSS	g/m^3	37,669	38,165
	VSS/TSS	–	–	0.561
	Dry matter	t/year	4,057	4,271
Sludge after the centrifuge	Flow[b]	m^3/h	3.26	3.27
	TSS	g/m^3	226,819	225,000
	VSS/TSS	–	–	0.561
	Dry matter	t/year	–	4,129
Dried sludge	Flow[b]	m^3/h	0.88	0.79
	TSS[a]	g/m^3	914,901	920,000
	VSS/TSS	–	0.589	0.561
	Dry matter	t/year	4,106	4,097

[a]used as model input.
[b]in the periods of sludge dewatering and drying in operation.

Simulations also confirmed a significant contribution of reject water to input load. During the periods of centrifuge and sludge drying operation, around 30% of TN and 15% of TP input load comes as a contribution of reject water from the sludge line because of high NH_4-N and PO_4-P concentrations in the centrate. In the periods when dewatering is not in operation this contribution is small (Table 6).

Upgraded plant simulation

The requirement for the upgraded plant is to achieve effluent concentrations below the limit values, i.e. TSS $\leq$ 35 mg/L, $BOD_5 \leq 20$ mg O_2/L, COD $\leq$ 100 mg COD/L, TP $\leq$ 1 mg P/L, TN $\leq$ 10 mg N/L and NH_4-N $\leq$ 5 mg N/L.

The upgraded plant was simulated for two different scenarios, i.e. (i) plant operated in the AAO configuration, (ii) plant operated by switching between the AAO and AO configurations, depending on the wastewater temperature. Long-term dynamic simulations were performed with increased input, which was simulated by increasing the inflow for 30%, while wastewater characterization and influent concentrations were the same as in the existing plant simulations.

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Table 6 | Mass flow returning from the sludge line to the water line (estimated values from occasional plant measurements and average values of long-term simulation) compared with plant influent

Plant location	Mass flow	Unit	Estimated from occasional measurements	Simulated
Return water without centrate	TN	kg N/d	73	93
	TP	kg P/d	19	21
	NH_4-N	kg N/d	8	1
	PO_4-P	kg P/d	8	9
Return water during centrifuge and sludge drying operation	TN	kg N/d	881	849
	TP	kg P/d	104	92
	NH_4-N	kg N/d	786	716
	PO_4-P	kg P/d	73	63
Influent	TN	kg N/d	2,950	2,945
	TP	kg P/d	628	624
	NH_4-N	kg N/d	2,020	2,014
	PO_4-P	kg P/d	–	200

Simulations of the upgraded plant have shown that effluent COD, BOD_5, and TSS were in both scenarios almost the same and below the limit values. Effluent TN and TP depend on the simulated configuration as shown in Figure 6. Operating the plant only in the AAO configuration gives low effluent TP, but during winter time the nitrification capacity is not sufficient, therefore effluent TN and NH_4-N limits could not be reached. By switching to AO during this period, the plant performance regarding N is satisfactory, but the P removal performance deteriorates. In this case, the surplus TP needs to be eliminated by chemical precipitation. Simulations have shown a slightly higher temperature for switching between the configurations (around 18°C) compared to expected 15°C in the preliminary design. According to annual temperature variation, the plant could operate with biological P removal approximately 45% of the time in a year.

Simulations shown in Figure 6 also revealed potential problems in reaching effluent TN below 10 mg/L in the AAO configuration. As seen in the first diagram in Figure 6, effluent TN in AAO (days 25–175) is higher than in AO (days 175 to 390) and is very close to the limit.

To improve the performance, additional reject water treatment, e.g. by deammonification, was evaluated. As already presented, returning water from the sludge line to the water line represents a significant N and P load to the water line. In the upgraded plant, this load will even increase because of higher sludge production and P accumulation in sludge in biological P removal. Therefore, a separate return water treatment could be an option to decrease the additional N load to the water line. Return water treatment was simulated by converting 90% of NH_4-N in return water to N_2 gas and 10% to NO_3-N (Schmidt *et al.* 2003; Capodaglio *et al.* 2016). Evaluation of this measure in comparison with reference upgraded plant simulation is presented in Table 7. It can be seen that the contribution of deammonification is significant, reducing both effluent TN and TP in the entire simulation period.

CONCLUSIONS

The study shows the design and full-scale validation of a CNP plant-wide simulation model, which was used to assess the performance of the plant after introducing changes in the water line and sludge line to comply with stricter effluent N and P standards.

Plant-wide consideration and extension of plant performance indicators also to sludge line (biogas production, dried sludge production, sludge composition) enabled a more precise wastewater

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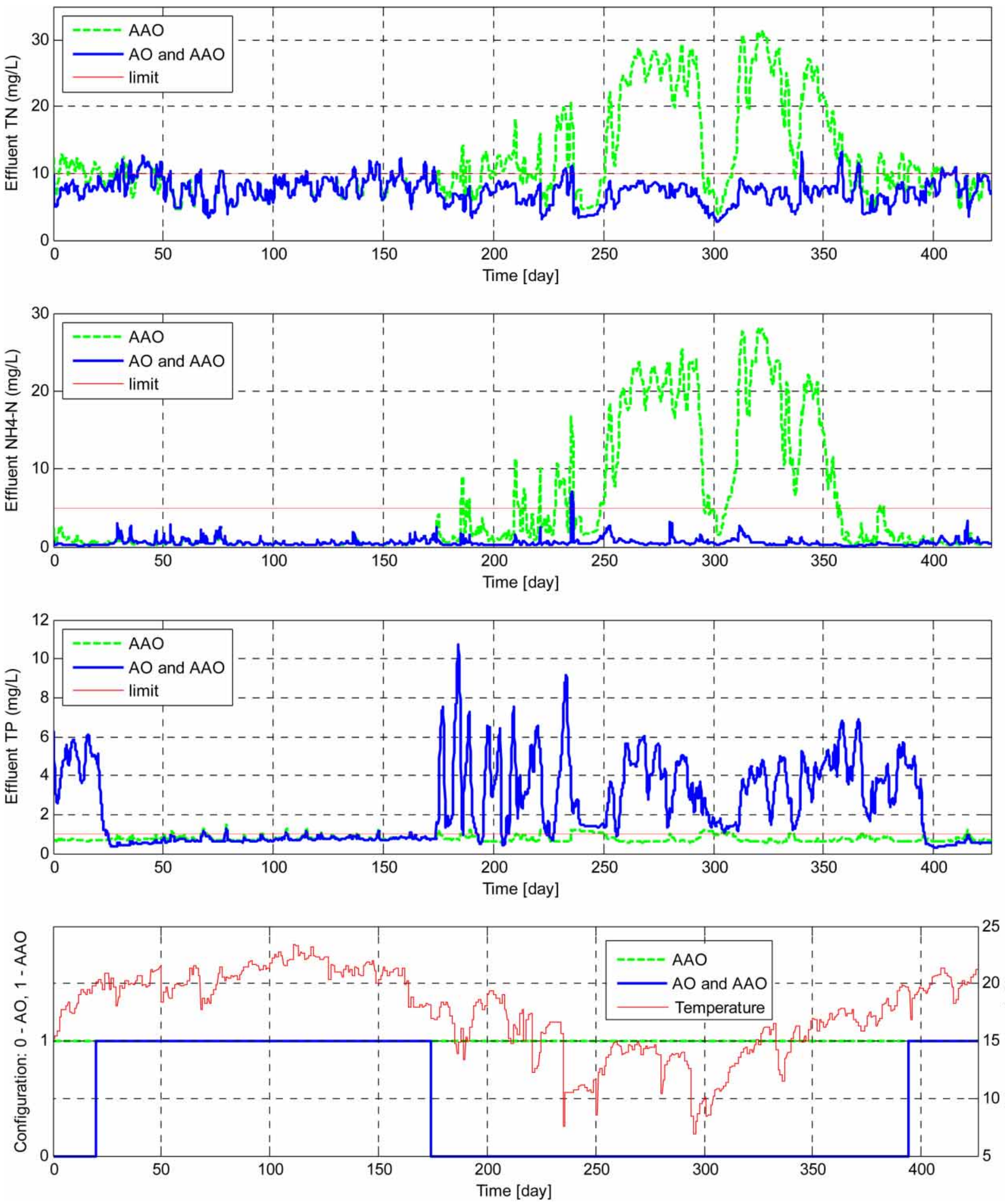

Figure 6 | Upgraded plant performance with respect to effluent N and P requirements for two scenarios, AAO configuration, switching between AO and AAO.

Table 7 | The values of the 85th percentile of effluent TN and TP concentrations for different operation scenarios

Simulation scenario	TN in AO mg N/L	TN in AAO mg N/L	Overall TN mg N/L	Overall TP mg P/L
Upgraded plant	8.23	9.90	9.18	4.73
Upgraded plant with deammonification	6.60	7.80	7.17	2.87

characterization, which is needed when effluent requirements increase. Within the proposed plant-wide wastewater characterization procedure a sensitivity analysis was applied to evaluate identifiable wastewater characterization parameters from available data.

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In the plant-wide simulation, the anaerobic digestion model overpredicted ammonia-N and ortho-P components in digestate, therefore two stoichiometric parameters of MantisAD model were adjusted to simulate partial capture of N and P by inorganic material and thus represent the reject water from the sludge line to the water line sufficiently well. Future work might need to include more complex physico-chemical models as recently presented in the literature (Kazadi Mbamba *et al.* 2015; Solon *et al.* 2017).

For the given case study the simulations show that the most challenging aspect is to achieve TN concentration below the limit value during biological P removal. In this case, the plant has a lower denitrification potential. These operating conditions could be enhanced by the inclusion of additional processes (e.g. deammonification) to reduce the reject water nutrient load from sludge treatment. The designed model will be further used for improved operation and control of the upgraded plant.

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