Data scarcity in modelling and simulation of a large-scale WWTP: Stop sign or a challenge

Data Scarcity in Modelling and Simulation of a Large-scale WWTP: Stop sign or a Challenge

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Abstract

Data scarcity can be considered as the main limitation for a more widespread utilization of mathematical models in the design, optimization and control of biological nutrient removal activated sludge systems (BNRAS). High cost and demanding workload related to experimental data and sufficient sampling campaigns make the data collection process an unpleasant necessity for managing stakeholders in modelling projects. Complicated use of online-sensors leading to frequent erroneous readings and dynamic nature of wastewater treatment processes can intensify the data scarcity problems. This paper investigates the influence of data scarcity on the development and calibration of wastewater treatment plant (WWTP) models. A straightforward methodology is proposed to address the challenges associated with data quality and quantity problems in modelling of a BNRAS in the largest Italian WWTP located in Castiglione, Italy. The plant operational modes, weather condition and sensor performance during the sampling campaigns were the main sources of the data scarcity. Influent, biokinetic, aeration, hydraulic and transport, clarifier, energy consumption and effluent sub-models were calibrated by use of the proposed extensive step-wise calibration process. The Monte Carlo analysis was performed to quantify the uncertainty of the modelling results. The proposed methodology could be implemented in engineering practice to develop and calibrate the WWTP models while it increases the awareness about modelling robustness and its characterized uncertainty to avoid bad modelling practice.

Keywords: Wastewater treatment; Activated sludge models; data scarcity; uncertainty assessment

1. Introduction:

The required effluent limits for wastewater treatment plants (WWTP) proposed in the EU Directive 91/271/EEC were surely the substantial motive for more implementations of the biological process in wastewater treatment industries. From the inauguration of these stringent effluent criteria, the application of biological nutrient removal activated sludge (BNRAS) systems has gained great popularity in Europe. Recently, considering the high capital and operational costs of these systems (Liu et al., 2011), control and optimization of these processes have become necessities. However, the complex, nonlinear and dynamic nature of biological and biochemical processes which take place in these systems, make controlling of their performance a challenging and not straightforward task. Mathematical models provide a valuable evaluation and decision-making tool for wastewater engineers to move forward towards the controlling and optimization of various wastewater treatment processes including BNRAS. The by far mostly used mechanistic models to mimic complex interactions in BNRAS systems are Activated Sludge Models (ASM) developed by the task group of International Association on Water Pollution Research and Control (IAWPRC) and summarized in Henze et al. (2000). The successful applications of these models in learning, design or process optimization and control have been reported in several studies (e.g. Ferrer et al., 2004; Balku and Berber, 2006; Beraud, 2009).

The large number and complicated nature of the simulated processes which are described by numerous state variables as well as kinetic and stoichiometric parameters result in high model complexity which is the main limitations for more frequent use of ASMs (Rieger et al., 2010a). To study the identifiability of model parameters and to translate the common quality measurements (e.g. TSS, BOD_5) into the ASM family parameters, several calibration guidelines have been developed: BIOMATH (Vanrolleghem et al., 2003), STOWA (Hulsbeek et al., 2002), HSG (Langergraber et al., 2004), WERF (Melcer, 2004). The high workload and financial resources required for specialized experimental studies proposed in these guidelines to obtain model parameters, are not usually accepted and welcomed by stakeholders and wastewater treatment companies. Erroneous on-line measurements due to irregular and deficient sensors maintenance and cleaning can cause a reduction of the amount of valid data. Consequently, data scarcity is the prevailing problem in WWTP modelling projects which has been discussed in several studies (e.g. Sochacki et al., 2009; Rieger et al., 2010b; Martin and Vanrolleghem, 2014; Borzooei et al., 2016).

Each WWTP is somehow unique, considering its service region, influent quality, industrial discharges, age of instruments, implemented treatment methods, maintenance program, the effluent standards should be followed, availability of online monitoring systems; their calibration and maintenance schedule, environmental conditions such as temperature and rainfall in catchment areas etc. (Bott and Parker, 2011; Schilperoort, 2011). As a result, implementing the calibration protocols cannot address all the issues and practical problems which may be encountered during a specific modelling project. Therefore, the pathway through which a WWTP is being modelled is also unique, challenging, and worth investigating.

This study proposes a stepwise approach for model development and calibration of the BNRAS system of Castiglione Torinese WWTP in Italy, taking into account the limited available operational data and a few measuring and sampling campaigns could be conducted. The main objective of this study was model-based optimization and upgrading of the existing plant to meet the effluent criteria and reduce the energy consumption which will be discussed in an accompanying study (Borzooei et al., in preparation) to keep this study focused on the framing of the model development and calibration. This paper adds to the existing knowledge in the field of WWTP modelling and simulation by presenting an additional real-world case study with its practical specifications and challenges. This research addresses the practical obstacles and difficulties, authors encountered due to data scarcity, dynamic nature and large-scale of the processes and finally proposes a multi-step methodology for modelling and calibration of the WWTP.

2. Materials and methods

2.1 Process description of the Castiglione Torinese WWTP

The centralized Castiglione Torinese plant is the largest Italian WWTP located in about 11 km Northeast of Turin, capital of Piedmont, Northwest of Italy. The plant was designed for treatment of about 590,000 m^3/d of combined municipal and industrial wastewater, corresponding to an organic load of 2.1 million of equivalent inhabitants. The influent wastewater after the pre-treatment (coarse and fine screens and grit, sand and grease removal) is unevenly introduced to 4 wastewater treatment modules, each consisting of 2 primary clarifiers (volume $V_{PC} = 8070$ m^3) and 2 anoxic tanks ($V_{AN} = 13500$ m^3), 6 aeration basins (volume $V_{AR} = 8736$ m^3) with fine bubble membrane diffusers and 6 secondary clarifiers (volume $V_{SC} = 8020$ m^3). This resembles a typical Modified Ludzack-Ettinger (MLE) activated sludge system with primary clarifiers. The mixed liquor recirculation (MLR) pipes connect the aerobic to the anoxic zones to bring the nitrate to be denitrified in the anoxic units. The underflow from 6 secondary clarifiers flows back to the anoxic tanks through a return activated sludge (RAS) recycle channel by three Archimedes screws in each module. A part of activated sludge also is continuously extracted from the system and sent to the sludge treatment units as the waste activated sludge (WAS) to ensure the biological balance in the system. The final effluent of the secondary clarifiers flows to the final filtration units where it is divided between 27 multilayers sand and coal filtrations. Reject water from sludge treatment units (RWS) and reject water from final filtration units (RWF) are entered to the main wastewater stream after pre-treatment units. The plant was designed to remove organic matter and nitrogen. In addition, chemical phosphorous removal (CPR) is achieved by adding a ferric chloride solution ($Fecl_3$) into the RAS stream. Currently, the plant efficiently removes carbon and achieves nitrification and P-removal but lacks denitrification.

2.2 Collection of existing data

Several visits to the WWTP and frequent meetings with operators and management staff were carried out to thoroughly understand the plant configuration and identify the current process schemes. Various implemented operational modes, number and locations of the online measuring instruments and their cleaning and maintenance periods in addition to number and locations of the automatic samplers used for regular sampling of the plant, were identified. Further, all the existing information including routinely collected data based on 24 h time proportional composite samples (available from 2009 to 2016), physical characteristics of treatment units (e.g. tanks configurations, detail information about aerators and mixers, capacity and control scheme of pumps etc.) and operational data (e.g. flow splits, aeration control parameters, recycle streams etc.) were collected and studied.

2.3 Additional measurement campaigns

Due to a large scale of the WWTP, practical challenges in monitoring and controlling of some operational parameters during the short period of sampling time and financial limitations of the project, a restricted modelling boundary was determined. In place of modelling of the whole plant, half of the single wastewater treatment module was investigated. Based on the availability of sensors and accessibility of measurement points, measurement campaigns were carried out to estimate MLR (Q_{MLR}) and RAS (Q_{RAS}) flow rates. MLR tubes were lain down underground with low accessibility and to protect them against corrosion action of the wet soil, they have been coated by the thick layer of the coal-tar pitch which makes the applicability of the ultrasonic flowmeter, impossible. Instead, Q_{MLR} was estimated based on the maximum capacity of the recirculation pumps. Q_{RAS} was measured by the combination of the float method (in the access channel) and velocity estimation by ultrasonic velocity meter. The obtained value was validated with the maximum capacity of the Archimedes screws pumping the RAS to the anoxic units.

2.4 Wastewater characterization

One of the most important factors in WWTP modelling is the characterisation of the influent wastewater. The initial influent characterization was performed according to the protocol developed by the Dutch foundation for applied water research (STOWA: Hulsbeek et al., (2002)); however, some minor modifications were made. For identification of COD fractions, 24 h composite samples with 1.5-hour intervals were collected in duplicates on 07/03/2016 to 14/03/2016 (4 working days) from influent and effluent of the studied module. The time between sampling and experimental analyses was kept as short as possible, and samples preserved in temperature less than 4°C to prevent any biological activities before laboratory tests. A physico-chemical method based on the combination of flocculation with $Zn(OH)_2$ and filtration with 0.2 μm nylon filters was implemented for estimation of the readily biodegradable (S_s) and inert soluble (S_I) COD fractions. The slowly biodegradable COD (X_s) fraction was estimated by a BOD monitoring procedure. For inhibition of nitrification 20 mg/l Allylthiourea (ATU) was added. Each sample was tested by 2 BOD-flasks for validating the results. The summary of all implemented methods for COD fractionation is tabulated in Table 1.

Table 1. Procedure, method and results of COD fractionation based on measurements carried out at Castiglione Torinese WWTP

Measured parameters					COD fractions				
Definition	Sym	Unit	Average value	Method	Definition	Sym	Unit	Equation	Average value
Influent total COD	COD_{inf}	g $COD.m^{-3}$	557	LTC[a]	Inert soluble COD	S_I	g $COD.m^{-3}$	$0.9\ COD_{s,eff} - 1.5\ BOD_{5,eff}$	6.5(±1.6)
Influent soluble COD	$COD_{s,inf}$	g $COD.m^{-3}$	57	FL[b] and LTC[a]	Readily biodegradable COD	S_s	g $COD.m^{-3}$	$COD_{s,inf} - S_I$	50.1(±6.3)
Effluent soluble COD	$COD_{s,eff}$	g $COD.m^{-3}$	16	FL[b] and LTC[a]	Slowly biodegradable COD	X_s	g $COD.m^{-3}$	$BCOD - S_S$	241.3(±9.1)
Influent BOD_5	$BOD_{5,\ inf}$	g $BOD_5.m^{-3}$	198.7	LTB[c]	Inert particulate COD	X_I	g $COD.m^{-3}$	$COD_{inf} - (S_I + S_S + X_S)$	258.5(±15.5)
Influent BOD ultimate	$BOD_{u,\ inf}$	g $BOD.m^{-3}$	248	CF[d] of $BOD_u = \frac{1}{1-e^{K_{BOD}t}} BOD_t$					
Rate constant of the BOD vs. time	K_{BOD}	-	0.34	CF[d] of $BOD_u = \frac{1}{1-e^{K_{BOD}t}} BOD_t$					
Influent biodegradable COD	BCOD	g $COD.m^{-3}$	291.5	Calculation from $BCOD = \frac{1}{1-f_{BOD}} BOD_u$ Assumption: f_{BOD}= 0.15					
Effluent BOD_5	$BOD_{5,\ eff}$	g $BOD_5.m^{-3}$	5	LTB[c]					

[a] Laboratory COD tests (LCK314- COD Cuvette setup)

[b] Filtration and flocculation

[c] Laboratory BOD tests (OXITOP control Measuring System (OC-110) (Weilheim, Germany))

[d] Curve fitting method with Trust-Region or Levenberg-Marquardt algorithms

2.5 Additional sampling campaigns

An intensive 20-day sampling campaign was carried out on working days from 26 September to 21 October 2016. The sampling plan including sampling type, location and frequency as well as sufficient instructions about handling, storage and laboratory analytical tests, were well-prepared and communicated to the responsible staff. The grab samples were collected from influent and effluent of each treatment unit (P_1 to P_5 in Fig. 1) and from the RAS channel (P_6). Between samples collected from one and a subsequent point, a lag time was set according to the average hydraulic retention time (HRT) of the corresponding unit. For the sludge line, samples were collected from the RAS on 3:00 pm of each sampling day.

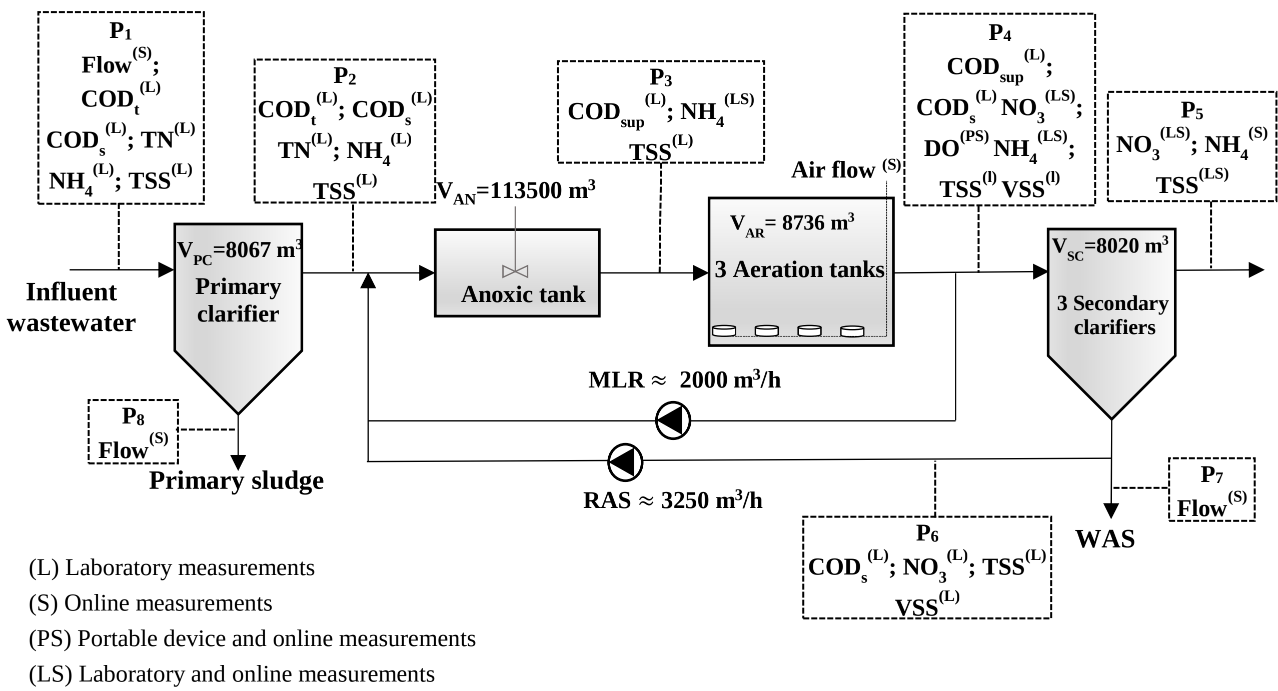

Fig. 1. The scheme of studied half wastewater treatment module in Castiglione Torinese WWTP with locations and types of measurements

Following wastewater characteristics of each grab sample were analysed according to IRSA methodology (Blundo et al., 1994): total COD (COD_t), soluble COD (COD_s), supernatant COD (COD_{sup}), total suspended solids (TSS), total nitrogen (TN), ammonium (NH_4), nitrate (NO_3). For measurement of COD_{sup} the supernatant samples were taken from the surface of grab samples after 2-3 min of decantation.

All the soluble parameters were measured after filtration with 0.45μm filters following by flocculation. Starting the sampling point from before primary clarifier, the impact of both reject water streams (RWS and RWF) was considered. All online measurements (parameters with (S) superscript) were recorded from the Supervisory Control and Data Acquisition (SCADA) system. To validate some of the online-measured parameters, laboratory analyses of grab samples (parameters with (LS) superscript) and/or real-time measurement with the portable device (parameter with (PS) superscript) were carried out. Additionally, a 2-day composite sampling campaign was carried out from influent and effluent of the studied module on 02/11/2016 and 06/11/2016 to understand the dynamic patterns of influent and effluent concentrations on weekend and weekday. The sampling was conducted from 9:00 am to 6:00 pm. Using two autosamplers, 8 composite samples were collected by 2 h interval and further analyzed in the laboratory to measure COD_t, COD_s, $N\text{-}NH_4$, $N\text{-}NO_3$, and TSS.

2.6 Model development

In this study, wastewater treatment process simulator, GPS-X ver.6.5.1 (Hydromantis, 2016) was used to mimic various treatment procedures, run the simulations as well as perform parameter estimation and uncertainty analysis. Since no tracer test was performed during the operation of the WWTP, the hydraulic characteristics of bioreactors were approximated by a “tanks-in-series” approach. In this approach for the flow regimes which are between the ideal plug-flow and completely mixed hydraulic flow patterns, a series of complete-mix reactors are used. The flow condition in aeration units was further evaluated using an empirical formula. Murphy and Boyko (1970) proposed the Eq. 1 based on the investigating the results of the dispersed plug flow model in the full-scale aeration reactors with various depth ratio from 0.87 to 2.04.

$$\frac{E_L}{W^2} = 3.118.(q_A)^{0.346} \qquad (1)$$

where E_L is the longitudinal dispersion coefficient, m^2h^{-1}, q_A the air flow rate per unit volume of the tank (T^{-1}) and W is the reactor width (L). The Eq.1 was also recommended in US EPA (1993) for both fine and coarse bubble diffused air systems. For each aeration unit, the average value of E_L was calculated in the sampling campaign period. The corresponding value of the dispersion number was calculated as (E_L/uL), where u is the average longitudinal velocity and L is the length of the aeration tank. Aeration units with a dispersion number lower than 0.2 and higher than 4 are classified as plug flow and completely mixed systems respectively (Zima et al., 2008). The average dispersion numbers calculated from Eq. 1 for three aeration units were between 1.8 and 2. These results suggested that considering continuous stirred-tank reactor (CSTR) for each aeration unit was a good approximation. Further, assuming the completely mixed condition in the anoxic unit, it was simulated with a single CSTR. The biochemical activities occurring in the aeration and anoxic reactors were simulated by the ASM1 model (Henze et al., 2000). Since due to the data scarcity in this project CPR process was not modelled, ASM1 was the best choice to mimic carbon and nitrogen removal processes (Gernaey et al., 2004).

Considering the available data about clarifiers, an ideal primary clarifier model (removal efficiency model) and pre-compiled one-dimensional secondary clarifier model proposed by Takács et al. (1991) were implemented. The non-reactive flux-based model considers 10 horizontal layers, of which the 5^{th} (from top) is the feed layer. Since the information regarding the settling parameters was not available, the correlational model (Hydromantis, 2016) was implemented in which settling parameters are correlated to the sludge volume index (SVI) and clarification factor (c_f). For simplification, assuming an equal hydraulic load of 3 secondary clarifiers they were modelled as a single flat bottom circular clarifier with accumulated volume. The endogenous denitrification process due to the presence of biologically active solids in the secondary clarifiers (see section 3.1) was modelled by placing a virtual anoxic CSTR after the clarifier unit in the RAS stream with the volume of the sludge blanket. As a conservative estimation by operators, this volume was equal to 50% of V_{SC}. The biochemical processes in this virtual reactor were described by ASM1.

Available physical and operational parameters were adjusted for each modelling unit. The depth and volume of the basins, as well as the specification of diffusers (height and number) for each aeration unit were entered. This information was elaborated for calculation of the standard oxygen transfer efficiency (SOTE) according to correlation method reported in Hydromantis (2016). To model the aeration system, initially, SOTE was measured by entering the air flowrates collected during the sampling campaign. Further, a linear proportional–integral (PI) controller was used to regulate the airflow pumped to each basin based on dissolved oxygen (DO) measurements.

The energy consumption (EC) of each modelling unit was estimated by implementing the operating cost models in the GPS-X platform. The aeration energy was estimated based on the air flow rate and the efficiencies of the blowers and motors. The required blower energy was evaluated from the adiabatic compression equation (Mueller et al., 2002). Pumping energy was linked with pumping flowrate as well as head losses. Mixing energy was estimated by considering the power per unit volume of the mixing (PPUV) parameter. The sub-models used for each process are summarized in Table 2.

Table 2. Sub-models of the Castiglione Torinese WWTP

Unit process	Physical model	Process model
Influent model	1 Influent unit	COD states influent [a]
Primary settling	1 circular unit	Ideal clarifier [a]
Pre-denitrification	1 CSTR	ASM1[b]
Aeration system	3 CSTRs	ASM1[b]
Secondary clarification	1 circular unit	Simple 1-D[c]
Denitrification in secondary clarifiers	1 virtual CSTR	ASM1[b]
Energy consumption	All units	Operating cost [a]

[a] (Hydromantis, 2016); [b] (Henze et al., 2000) ; [c] (Takács et al.1991)

2.7 Model Calibration

Model calibration is an iterative procedure for adjusting model parameters (physical, operational, kinetic) to improve the fit to observed set of data. The definition does not include additional measurements and model structural modification. As a general step-wise calibration procedure in this study, the following steps were undertaken:

Step 1) The first steady-state simulation of the model was conducted with the reference parameters for a period equivalent to at least three times the average SRT of the system. and Modelling results were qualitatively (visual and graphical) compared with available measured data.

Step 2) The most sensitive parameters of each sub-model were detected based on experience and common sense, engineering judgment, BIOMATH (Vanrolleghem et al., 2003) and STOWA (Hulsbeek et al., 2002) calibration protocols. In a few cases, full-scale observations and sensitivity analysis using one-variable-at-a-time approach (Makinia et al., 2005) also contributed in the selection of these parameters.

Step 3) To compensate for the correlational impact of adjusted parameters, first the influent model was calibrated followed by primary and secondary clarifiers to achieve the solids mass balance in the system. Further, aeration followed by biokinetic models were calibrated. It should be emphasized that the calibration of each sub-model is not independent as the modelled processes are coupled together. As a result, several iterations with loops to the earlier steps were required. Selected parameters in each sub-model were estimated by a Nelder-Mead simplex (polyhedron) algorithm available in GPS-X. The methodology is a multi-dimensional method not relying on gradient information for minimization of the objective function (Press, 2007). The maximum likelihood objective function as well as default values of reflection, expansion, shrink and contraction constants presented in Hydromantis (2016) were used for parameter estimation. Proper lower and upper bounds were introduced for each parameter according to literature (e.g. Jeppson, 1996; Henze et al., 2000; Afonso and da Conceição Cunha, 2002) or by experience. It should be stressed that in case of encountering identifiability problem in which more than one combination of model parameters could result in a good fit to the observed set of data, the realistic parameter combinations were identified according to objective of the project and real practical and theoretical data about the involved process in the plant (Kristensen et al., 1998).

Step 4) The obtained parameters and concentrations from steady state runs in step 3 were used as the initial conditions for dynamic simulations and the dynamic calibration was performed iterating the procedure in step 3.

For calibration of the aeration process, initially, α factors (ratio of process water to clean water mass transfer coefficients) were adjusted to improve the fit to observed set of DO, NH_4 and NO_3 concentrations measured in the effluent of each aeration unit. Further, the implemented PI controllers were tuned with adjustment of the DO setpoint (see section 3.1), proportional gain (K_c) and integral time (T_i) tuning constants.

The calibration of the EC models was performed considering the specific electricity consumption values reported in Panepinto et al. (2016) for some of the electro-mechanic devices in the Castiglione Torinese WWTP. These values were acquired from the tele-control system and some direct measurements to evaluate overall energy features of the plant. Two calibrating parameters namely pressure drop in piping and diffuser downstream of blower (PD) and combined blower and motor efficiency (BME) were adjusted, for calibration of the aeration energy model. The pumping energy models were calibrated by adjustment of pump efficiency (PE) and pipe friction loss (PFL), assuming constant static system head. Mixing energy models were calibrated by adjusting power per unit volume (PPUV) parameters. The calibrated parameters and data used for calibration are presented in Table 3.

Table 3. Calibrated and target parameters

Modelling unit	Calibrated model Parameter	Data used for calibration	Target measured parameter
Influent input	S_s, S_I	L	Influent COD_s
	i_{vt}, i_{cv}	L	Influent TSS
Primary clarifier	Re_p	L	TSS and COD in P_2
Secondary clarifier	FPB, C_c	S	TSS in P_5
	SVI	S	TSS in P_6
Aeration units	α	S	Air flow rate and DO in P_4
PI controllers	DO_{set}, K_c, T_i	S	Air flow rate and DO in P_4
Biokinetic units	K_{OA}, μ_A, b_A	S and L	NH_4 in P_4 and P_5
Pumping units	P_e, PFL	Energy audit monitoring	Energy consumption data
Mixing units	PPUV	Energy audit monitoring	Energy consumption data
Aeration units	BME, PD	Energy audit monitoring	Energy consumption data

2.8 Evaluation of the results

The calibrated model was validated to assess the quality of the simulation results by quantifying the deviations between the model outputs and observations. To this end, the root mean squared error (RMSE) and the mean absolute percentage error (MAPE) were used as quantitative measures of the model prediction accuracy with respect to effluent TSS, NH_4 and NO_3 observations. These statistical criteria were calculated from Eq. 2 and Eq. 3.

$$MAPE = \frac{100}{n} \sum_{t=1}^{n} \left| \frac{P_t - m_t}{P_t} \right| \qquad (2)$$

$$RMSE = \sqrt{\frac{\sum_{t=1}^{n} (m_t - P_t)^2}{n}} \qquad (3)$$

where P_t is model predicted output, m_t is measured value at the t^{th} time instance and n is the total number of observations.

2.9 Uncertainty analysis

To assess the input (subjective) uncertainty of the developed model, the Monte Carlo Analysis (MCA) was performed. MCA provides a probabilistic shell around the deterministic models and quantifies the uncertainty of the model predictions by expanding the small size sample with the use of probability distribution functions assigned to input parameters and running several simulations with randomly selected model inputs (Bixio et al., 2002). Fig. 2 demonstrates the stepwise approach implemented in MCA.

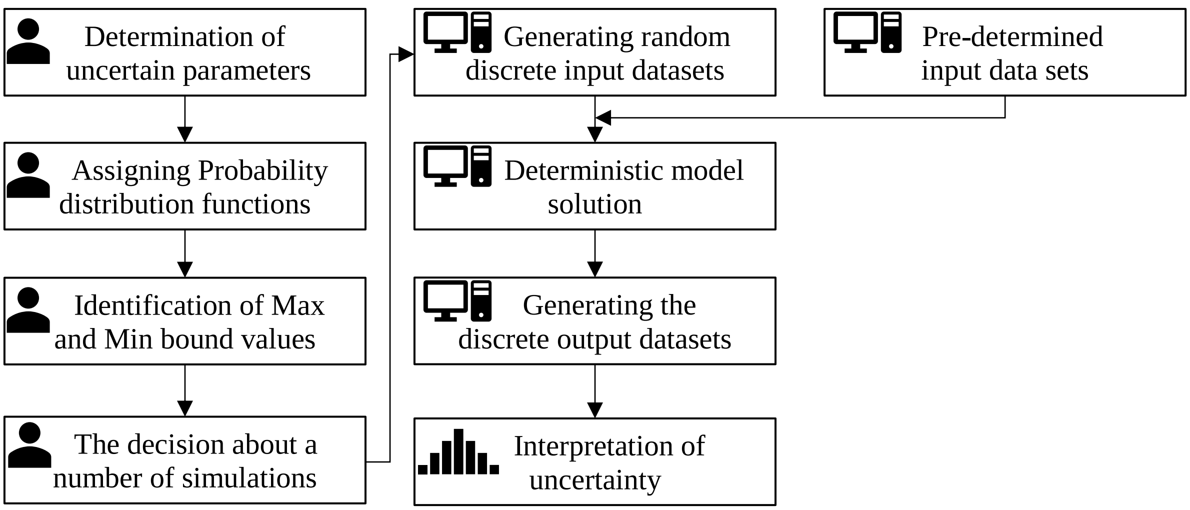

Fig. 2. Step-wise Monte Carlo analysis

In this study, 13 calibrated parameters (see Table 4) including 7 kinetic and stoichiometric parameters, α values of aeration basins and 3 operational parameters related to clarifiers were considered as uncertain input parameters.

Table 4. Uncertain parameters and their distribution functions in MCA

Category	Parameter	Unit	Distribution
C_1	μ_A	day^{-1}	Log-normal
C_1	K_{OA}	gO_2/m^3	Log-normal
C_1	b_{AUT}	d^{-1}	Log-normal
C_2	i_{cv}	gCOD/gVSS	Normal
C_2	i_{vt}	gVSS/gTSS	Normal
C_2	Re_p	-	Normal
C_2	α_1	-	Normal
C_2	α_2	-	Normal
C_2	α_3	-	Normal
C_2	C_C	-	Normal
C_2	SVI	ml/g	Normal
C_3	S_s	-	Normal
C_3	S_I	-	Normal

These parameters were categorized in 3 uncertainty classes depending on their level of uncertainty and the extent of available knowledge about them. The first class (C_1) corresponded to the numerically calibrated kinetic parameters. For the parameters in C_1 the universal parameter distributions proposed by Cox (2004) as well as uniform distribution functions were considered. Upper and lower bounds around their calibrated values were determined according to ranges proposed in the literature (Jeppson, 1996; Henze et al., 2000; Afonso and da Conceição Cunha, 2002). For the parameters in the second class (C_2), normal distribution functions were assigned with 25% upper and lower bounds around their calibrated values. The third class (C_3) corresponded to 2 influent COD fractions which were obtained by the calibration process. Parameters in this class were considered as highly uncertain parameters because of their nature (diurnal, monthly and seasonal variations) and identifiability problems occurred during their calibration process. For parameters in C_3, normal distribution functions were assigned with 50% upper and lower bounds around their calibrated values. It should be stressed that for the simplicity, parameters were assumed to be independent and their possible correlations were neglected.

Latin hypercube sampling (LHS) method was implemented for the sampling of the input uncertainty. To identify the sufficient number of replications in MCA, steady-state simulations were conducted with a various number of runs (from 100 to 10000) and input probability distribution graphs were developed accordingly. Graphs were further qualitatively (visual and graphical) analysed and the minimum number of replications which made the best agreement between assigned distribution function to input variables and the developed graph, was chosen as the sufficient number of runs. This simplifying method was chosen considering the available computational power and time of the project. Finally, the results were represented by mean, 5th and 95th percentiles and cumulative distribution functions (CDF).

3. Results and discussions

3.1 Data collection and practical challenges

Because of the sampling type (daily composite) and location in the plant routine data collection, the impact of RWS and RWF and wet-weather events could not be captured which makes the historical data not thoroughly representative of the real condition of the plant. However, modular and temporal trends of influent flowrate and concentrations in addition to observed ranges for mixed liquor suspended solids (MLSS) in aeration units and SVI in secondary clarifiers were identified from routinely collected data which were further elaborated in modelling and calibration (see section 3.3). Since no flow measurements could be conducted from the effluent of the treatment units, data accuracy evaluation (e.g. mass balance) could not be scrutinised in both routine data collection and the sampling campaign.

During the additional sampling campaign, mixing deficiency in the anoxic units due to mixer clogging was frequently observed. Several dead zones and floating sludge areas caused by diffusers fouling and bulk air emission due to relocated, broken or deformed diffusers bases were noticed in 3 studied aeration tanks.

In the sampling period, managing staff was advised to keep operational conditions of the studied module possibly unchanged. However, irregular discharge of RWS to the studied module as well as two extreme wet-weather events occurred during this period. Since both issues were found very important in the influent characteristics, recorded results were partitioned into two main categories: the 11-day normal operational condition in dry weather (NC-D) and the 9-day high load operational condition in wet weather (HC-W) in which discharge of RWS and heavy rain event occurred. During the 2-day dynamic sampling campaign the discharge of RWS was recorded in dry weather condition (HC-D). Table 5 shows the average influent concentrations of the studied module in each operational mode.

Table 5. Average of the influent concentration in different operational modes observed in sampling campaign period (26.10-21.11.2016)

Operational mode	Average and standard deviation of measured values [mg/l]					
	COD_t	COD_s	TN	NH_4	TP	TSS
NC-D	238(±45.5)	40.1(±7.3)	26.5(±3.3)	25.2(±0.05)	3.7(±2.7)	134.7(±37.9)
HC-W	407(±110.2)	41.9(±4.2)	34.6(±4.6)	29.3(±0.1)	7(±3.7)	274.1(±95.1)
HC-D	734(±135.7)	73.2(±13.2)	44.5(±4.2)	38.4(±2.2)	9(±1.8)	442(±95.1)

Partitioned results highlight the impact of RWS on influent characteristics since concentrations recorded in NC-D were found almost doubled or tripled in HC-D operational mode. Moreover, the dilution effect of a wet weather event on influent concentrations can be clearly detected, comparing the results recorded in HC-D and HC-W modes. Considering the high deviation of influent concentrations in various operational modes, it was decided to use collected data in NC-D mode for model calibration. The data collected in HC-D and HC-W modes were further elaborated in model-based optimization and scenario planning in an accompanying study (Borzooei et al., in preparation) to keep this study focused on the framing of the model development and calibration.

The collected data was further analysed to investigate the performance of treatment units. Comparing the COD_s, NH_4 concentrations recorded in P_2 and P_3 (see Fig. 1), the reactive nature of the primary clarifier was revealed with 270 and 110 kg/d increasing of the NH_4 and COD_s loads respectively. Comprehensive investigation of the reactive primary clarifier was performed in Borzooei et al. (2017). Likewise, observing the removal of NO_3 concentrations in 3 secondary clarifiers for almost 2 mg/l on average, the occurrence of denitrification during the studied period was confirmed. A tentative study based on decision tree proposed in Comas et al. (2008) was performed to evaluate the risk of rising sludge. The results confirmed the high risk of sludge rising in denitrifying clarifiers as a result of their high residence time and the influent nitrate level above the critical value (Henze et al., 1993). However, to certainly link the sludge rising phenomena, which were frequently observed in the plant, to the denitrification process, further investigation was proposed.

A high discrepancy was observed between online measurements of NH_4 and lab analyses of grab samples collected from the effluent of aeration units (P_4). These discrepancies resulted from the occurrence of several types of sensors failure including a long period with sensor fault (constant value) as well as periodic faults (incorrect scaling and/or out of normal range values) during the campaign (see Fig A. 2). Therefore, lab results were used for calibration process. Considering the performance of NH_4 sensor and investigating the DO concentrations and airflow rate recorded in the sampling period, it was induced that ammonium-based supervisory control system was not really implemented in controlling of the aeration systems, rather they were controlled manually.

3.2 Wastewater and biomass characterization

The initial fractionation of organic matter in influent wastewater was carried out according to methods proposed by standard Dutch guidelines (Roeleveld and Van Loosdrecht, 2002). Obtained results are presented in Table 1. The average contribution of individual ASM1 components to total COD was found as follows: S_I = 1.1%, S_s = 9.1%, X_s = 44 %, X_I = 45.8 %. The estimated S_s fraction corresponds to a low value but still within the reported range in several studies (e.g. Henze, 1992; Chachuat et al., 2005; Marquot et al., 2006; Pasztor et al., 2009) in which S_s constituted 3-35% and 14-57% of total COD in raw municipal and settled wastewater respectively. However, the estimated S_I fraction was found to be out of the suggested range which is 2-15% and 3-14.3% for raw and settled municipal wastewater (Pasztor et al., 2009). To solve the identifiability problem in the calibration of the influent model (see Table 3), S_I value was numerically calibrated while S_s was kept unchanged. The adjusted S_I value remained in the suggested range. The estimated X_I/total COD ratio (45.8%) was higher than the reported range (8-39%) (Henze, 1992; Roeleveld and Van Loosdrecht, 2002). The high X_I value can be linked to two factors: long hydraulic residence time in sewage pipelines and share of industrial wastewater in the. As proposed in several studies (e.g. Szaja et al., 2015; Pasztor et al., 2009; Quevauviller et al., 2007), for the large WWTPs like Castiglione Torinese which have more complex sewer collection system with a longer retention time of wastewater, the biological degradation of substrate fraction occur at bigger scale in sewer system which results the increase of inert particulate components. The higher inert COD fraction can be also linked with a presence of industrial wastewater (Mhlanga and Brouckaert, 2013). In the case of this study, Castiglione Torinese is the municipal WWTPs with a dominant contribution of non-industrial discharges in the wastewater influent.

The first estimated X_s/X_I ratio was revised based on calibration of the influent model. The X_s fraction was reduced from 44% to 37%. After this adjustment, X_s fraction remained within the typical range of 28-68% (Kappeler and Gujer, 1992; Roeleveld and Van Loosdrecht, 2002). Although the $S_s/(S_s+X_s)$ ratio was improved with the adjustment but it is still out of the typical range of 0.3-0.5 reported in Makinia et al. (2006). It should be emphasized that autotrophic (X_{BA}) and heterotrophic (X_{BH}) biomass concentrations were assumed equal to 0.1-1 and 0 mg/l respectively because these two fractions are included in particulate COD fractions.

3.3 Model calibration

The model was calibrated under a dynamic condition with the data originating from both laboratory and sensor readings on NC-D operational mode in the sampling period (26.10-21.11.2016) following the approach presented before. The final set of adjusted parameters and their original values are tabulated in Table 6. After the adjustment of two COD fractions (S_I and S_S) according to COD_s measurements, the influent model was calibrated by increasing i_{cv} to 1.85 gCOD. $(gVSS)^{-1}$ which was assumed based on the measurement of the COD_t and MLVSS in the aeration tanks while keeping i_{vt} constant.

In the calibration of the secondary clarifier model, clarification coefficient (C_c) was decreased to 0.42 to improve the final effluent TSS model prediction. The SVI was decreased from 150 to 130 ml/ to calibrate the sludge thickening process in the secondary clarifier and improve the fit to observed TSS values in RAS. The adjusted SVI value remained in obtained range (85-148 ml/g) from routine data collection (see section 2.2).

The calibrated α values for 3 aeration basins indicated higher aeration efficiency of one of the tanks in comparison to others. Since fouling factor (F_f) equal to 1 was assumed for all three tanks, the differences between α values can be the impact of diffusers fouling in real condition.

Table 6. Original and adjusted parameters in the calibration process

Parameter definition	Symbol	unit	Original value [a]	Adjusted value
Influent model				
Readily biodegradable COD fraction	S_s	%	20	9.1
Inert soluble COD fraction	S_I	%	5	8.5
XCOD to VSS ratio	i_{cv}	gCOD. $(gVSS)^{-1}$	1.8	1.86
VSS to TSS ratio	i_{vt}	gVSS. $(gTSS)^{-1}$	0.75	0.75
Clarifiers model				
Removal efficiency of primary clarifier	Re_p	-	0.5	0.44
Feed point from bottom depth of secondary clarifier	FPB	m	1	1.46
Clarification coefficient in secondary clarifier	C_c	-	0.5	0.42
Sludge volume index in secondary clarifier	SVI	ml/g	150	130
Aeration model				
Ratio of process- to clean- water mass transfer for aeration tank 1	α	-	0.6	0.49
Ratio of process- to clean- water mass transfer for aeration tank 2	α	-	0.6	0.59
Ratio of process- to clean- water mass transfer for aeration tank 3	α	-	0.6	0.48
Biokinetic model				
Maximum specific growth rate for autotrophic biomass	μ_A	day^{-1}	0.8	0.76
Oxygen half-saturation coefficient for autotrophic biomass	K_{OA}	gO_2/m^3	0.4	0.52
Autotrophic decay rate	b_{AUT}	d^{-1}	0.04	0.06
Pumping energy				
Pump efficiency primary clarifier	PE_P	-	0.7	0.12
Pipe friction loss primary clarifier	PFL_P	m	5	25
Pump efficiency of MLR	PE_{MLR}	-	0.7	0.65
Pipe friction loss of MLR	PFL_{MLR}	m	5	6
Pump efficiency of WAS	PE_{WAS}	-	0.7	0.2
Pipe friction loss of WAS	PFL_{WAS}	m	5	10
Pump efficiency of RAS	PE_{RAS}	-	0.7	0.4
Pipe friction loss of RAS	PFL_{RAS}	m	5	2.5
Mixing energy				
Power per unit volume for aeration tanks	$PPUV_{Ar}$	W/m^3	10	0.01
Power per unit volume for the anoxic tank	$PPUV_{An}$	W/m^3	10	2.5
Aeration energy				
Pressure drop in piping and diffuser Downstream of blower for 3 aeration units	PD	atm	0.069	0.08
Combined blower and motor efficiency	BME	-	0.7	0.25

[a] *(Hydromantis, 2016)*

The nitrification process was initially calibrated by decreasing the maximum specific growth rate for autotrophic biomass (μ_A) from 0.8 to 0.76 (d^{-1}) to improve the modelling results fit to the observed set of the ammonia level at the effluent of aeration tanks. It should be also mentioned that the nitrate concentration in aeration tanks was slightly decreased by adjusting the μ_A. This value corresponds to the reported range (0.2-1.2 d^{-1}) (Henze et al., 2000; Afonso and da Conceição Cunha, 2002). The ammonia and nitrate fits were further improved by increasing the autotrophic decay rate (b_A) from 0.04 to 0.06 (d^{-1}) and oxygen half-saturation index for autotrophic biomass (K_{OA}) from 0.4 to 0.52 gO_2/m^3. A higher estimated b_A value can be the result of the long oxic-SRT of the system (average 30 days) (Liwarska-Bizukojc et al., 2011). As stated in Arnaldos et al. (2015), several factors influence half saturation index including factors involved in transport in the bulk medium, into the floc, through the cell membrane, in the periplasm and enzymatic binding/release of a substrate. However, among all the influencing factors, the bulk mixing condition is logically the first factor to be investigated since its impact may overwhelm the contributions of other factors especially in case of non-uniform mixing condition. Since actual dead zones were observed in aeration tanks in the Castiglione Torinese plant during the sampling campaign; the advection limitation can be the explanation for the need to increase the K_{OA}. Both adjusted parameters (b_A and K_{OA}) corresponded well within the reported ranges (Henze et al., 2000; Jeppson, 1996). In the calibration of the pumping EC models, since no practical information was available about real PE and PFL values, one of their obtained combinations in the parameter estimation process was used. However, for calibration of the aeration EC model, based on the sensitivity analysis results, initially, the PD parameter was adjusted followed by BME.

3.3 Evaluation of modelling results

The results of the dynamic simulations for 3 effluent concentrations (TSS, NH_4 and NO_3) are presented in Fig. 3. Good prediction accuracy with respect to the short-term behavior of the effluent TSS was observed

(Fig. 3a) and expressed by the low values of the MAPE = 19 % and RMSE = 0.33 mg/l. It should be noted that a short period of sensor failure (constant value) in the first two days of the sampling affected the model evaluation results.

For both the description of the effluent NO_3 and NH_4, even though the differences between online data and model prediction were relatively higher (MAPE = 11-34 % and RMSE= 0.14-1.5 mg/l respectively), the model predictions reasonably follow the trend of the actual data (Fig. 3 b and c). However, the model frequently overpredicted the NO_3 level in the afternoon (from 14:00 pm) on each simulating day where real data showed drops and lower values. A possible reason could be the increased residence time (lower flow rate in afternoons) in the aeration tanks through which simultaneous denitrification can take place, especially in the dead zones in presence of enough readily biodegradable COD which is not captured by the way the mixing is currently modelled. Besides, in the ASM1 the same oxygen half saturation coefficient for heterotrophs (K_{OH}) is considered for modelling both the aerobic and anoxic growth of heterotrophic biomass. Hence, in the modelling approach, if aerobic growth of heterotrophs decreases, the capacity for anoxic growth will increase. This emphasizes the importance of K_{OH} in calibration process which was kept constant in this study due to data scarcity. Moreover, considering the occurrence of the denitrification in secondary clarifiers during the sampling campaign, a lower flow rate can result in the higher sludge residence time in the clarifier and consequently intensify the denitrification.

Since the calibration process was conducted based on the results of composite samples, logically the events with fast dynamics could not be well-captured by the developed model; however, the data with abrupt changes, disturbance and fluctuations in plant record data brought additional difficulties in the calibration process and parameter estimation. The removal efficiencies for effluent parameters were calculated based on actual measurement and dynamically simulated average values. The results proved that the model can predict 85-95% of the actual removal.

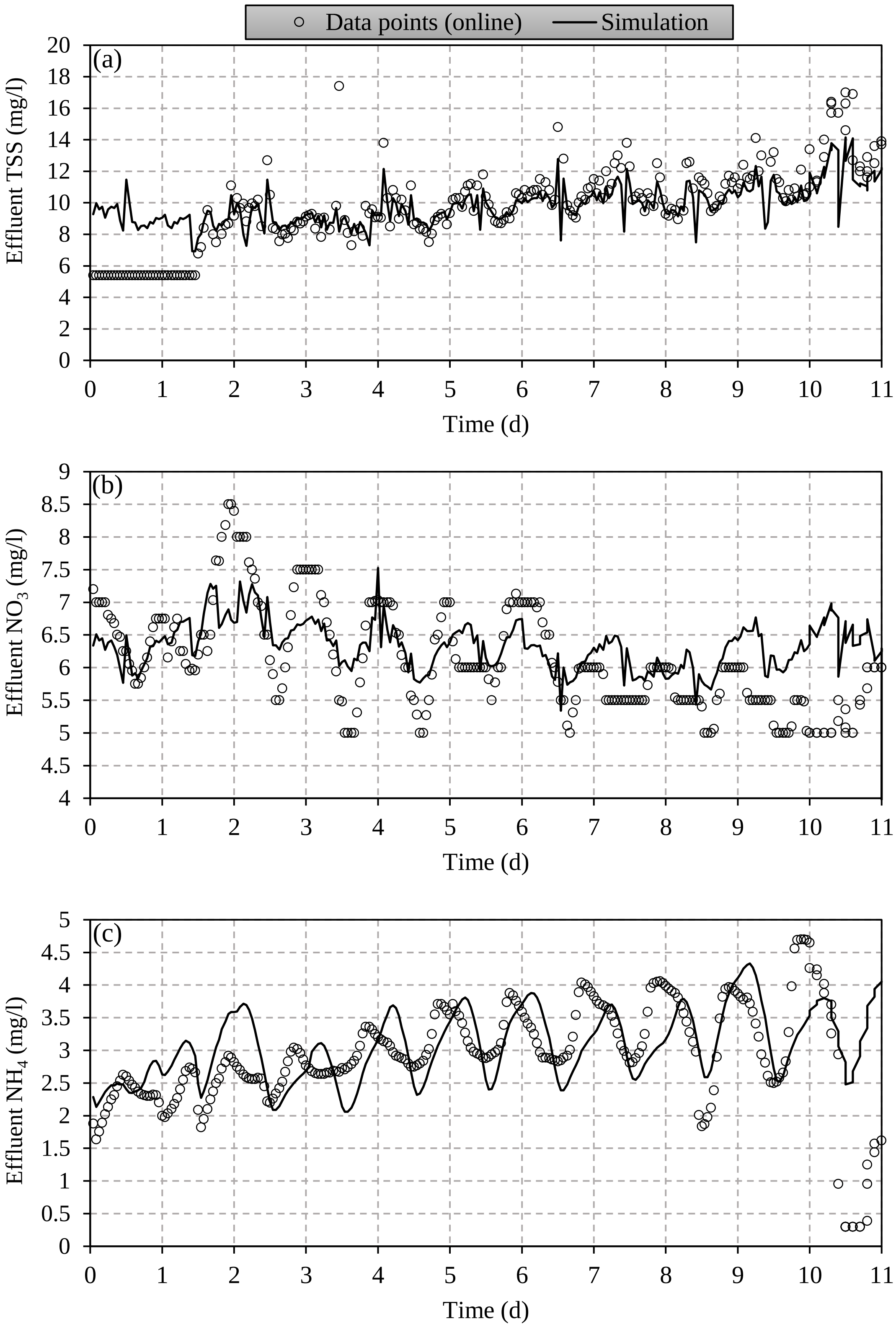

Fig. 3. Measurements vs. model predictions of effluent TSS (a), N-NO_3 (b), N-NH_4 (c) within the sampling campaign period (26.10-21.11.2016)

EC modelling results confirmed that aeration and pumping systems are the biggest energy consumers with 70-78% and 20-26 % of the total energy consumption of the studied module respectively. Measured and simulated daily averaged EC of treatment units were calculated (Fig. 4). The results presented in Fig. 4 proved that the model predictions are in relatively good agreement with energy audit data.

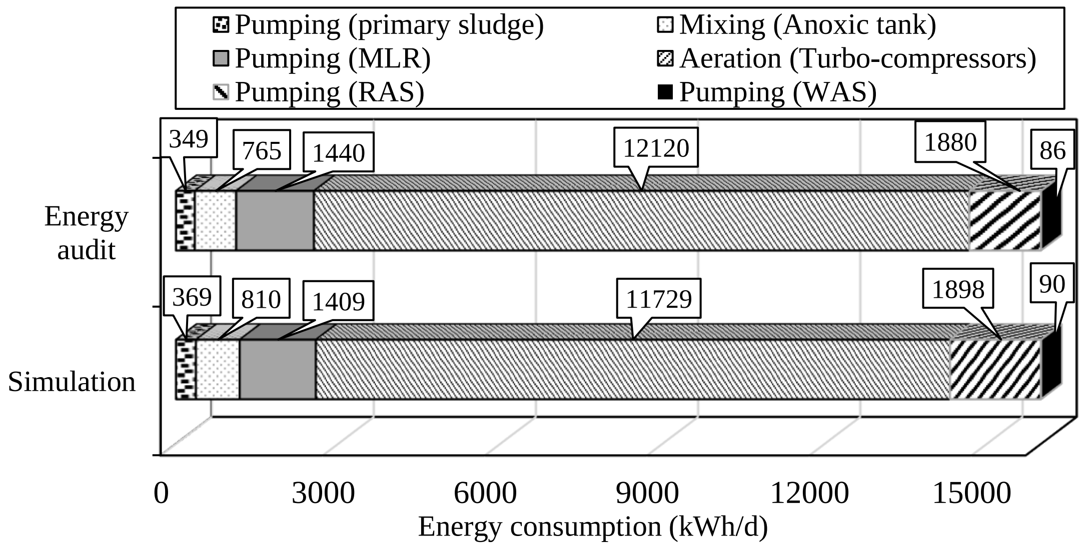

Fig. 4. Comparison of the measured and simulated daily averaged energy consumption of the studied module

3.4 Uncertainty assessment and improving proposals

To evaluate the uncertainty analysis results, CDFs of aggregated measure of averaged effluent TSS, COD_t, NO_3 and NH_4 concentrations were developed (Fig. 5). Comparing the results of the base-case simulation (Fig. 4) and the results presented in Fig. 5, one observes that there is considerable uncertainty concerning all effluent parameters. These results proved that uncertainty of the kinetic, stoichiometric, influent fractions and operational parameters cause significant variance in the predicted effluent concentrations. As regards the CDF of the effluent TSS (Fig. 5a) it can be noted that the spread of uncertainty is very broad. This can be due to two main reasons: (i) No MLSS controller was implemented in the model to counteract the uncertainty in the input parameters and as a result maintaining relatively stable MLSS level (ii) uncertainty of the operational input parameters regarding secondary and primary clarifiers.

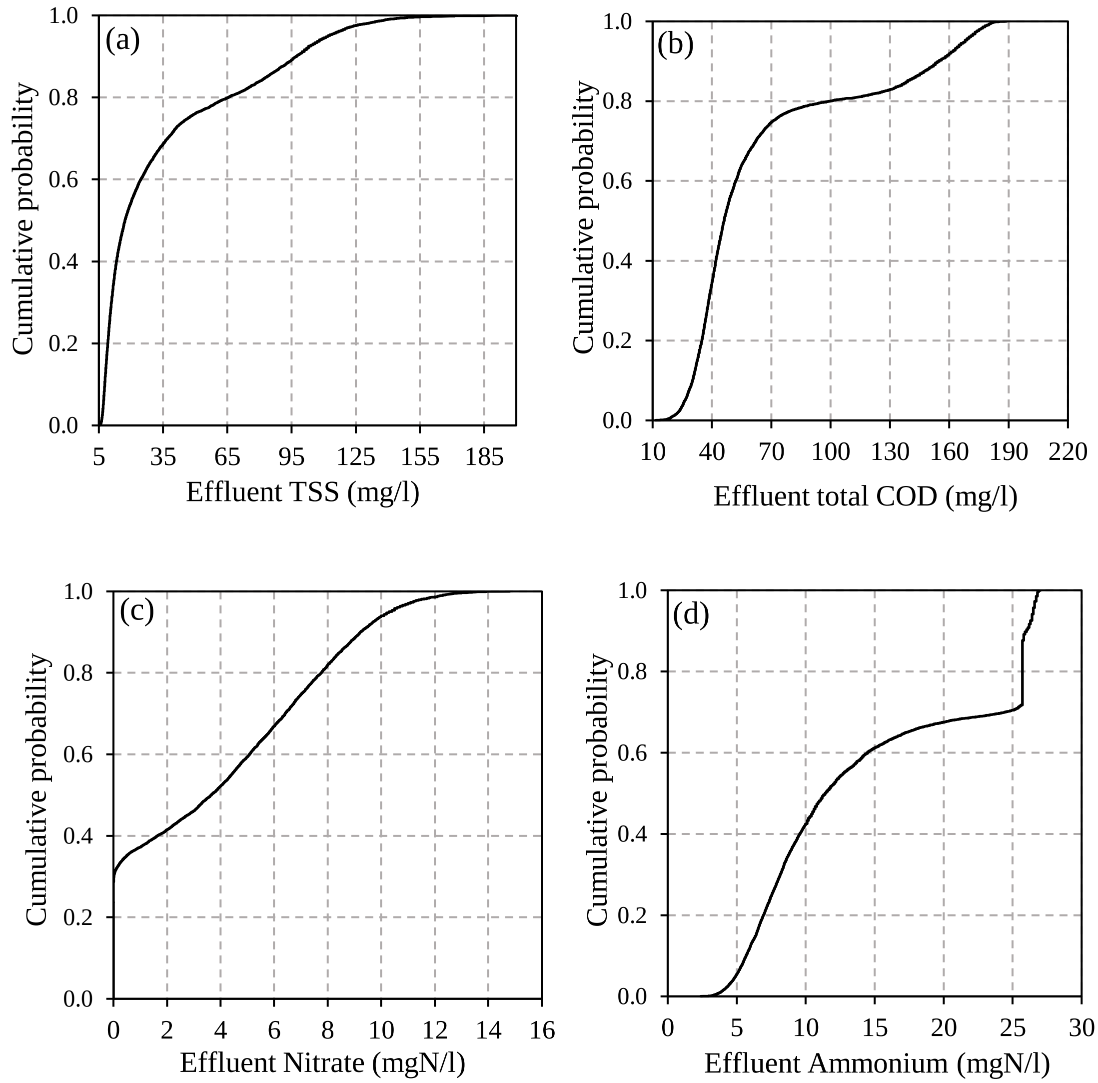

Fig. 5. Representations of uncertainty in four effluent parameters by the cumulative distribution function (CDF)

Conducting settling tests as well as representative COD fractionation and measuring campaigns associated with each operational mode and the tracer test to set-up an accurate hydraulic model for clarifiers were proposed to reduce the uncertainty the modelling results. Likewise, a wide range of uncertainty was observed in predicted effluent COD and nitrogen concentrations which can be linked to all sources of the uncertainty although the impact of operational parameters of clarifiers and mass transfer related parameters may be overwhelmed (Sin et al., 2009). Beside above-mentioned additional tests, application of the DO, NO_3, NH_4, TSS in-situ probes and actual implemented airflow controlling system in aeration units and conducting series of experimental batch tests to measure the kinetics parameters were proposed to improve the certainty of the modelling results.

5. Conclusions

This study proposes a novel methodology to address the impact of data quality and quantity problems on modelling and calibration of WWTPs. Historical data of the large-scale Castiglione Torinese WWTP, from January 2009 to December 2016, in addition to data collected in a few sampling and measurement campaigns, were utilized for model development and calibration. Unprecedented changes in weather condition, sensor performance and discharge of reject water from sludge treatment units during the sampling campaign were found intensifying sources of data scarcity in this project. The practical information presented in this study, stresses the role of a well-designed data collection process for both performance investigation and troubleshooting of treatment units which is usually overlooked, or its importance underestimated. The reactive nature of the primary clarifier and denitrification in the secondary clarifier were identified based on sampling campaign results. The developed model comprises biokinetic, aeration, hydraulic and transport, clarifier, input, output and energy consumption sub-models, and was calibrated by use of an extensive step-wise calibration process. Short-term predictability of the calibrated model was confirmed by comparing the dynamics of simulated and measured TSS, N-NH_4 and N-NO_3 effluent concentrations as well as their removal efficiencies. The uncertainty of the model was investigated by Monte Carlo Analysis (MCA). The results of the MCA emphasized the impact of data quality and quantity problem on uncertainty of developed model by showing high variances of effluent concentrations in MCA results. Considering the MCA results, additional tests, sampling and measurements were proposed to improve the modelling results.

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Appendix:

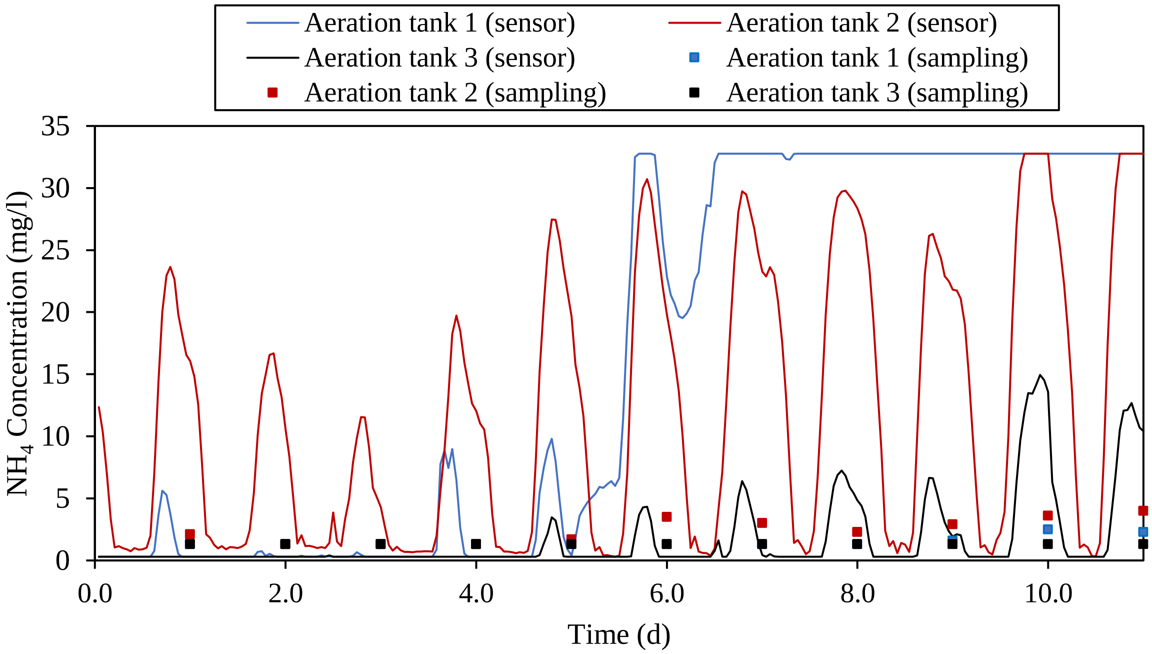

Fig. A.1. Comparison of sensor and sampling results for effluent NH_4 at 3 aeration tanks within the sampling campaign period (26.10-21.11.2016)