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Efficient calibration methodology of the wastewater treatment plant model based on ASM3 and application to municipal wastewater

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ABSTRACT

Operation of wastewater treatment plants (WWTPs) can be comprehensively investigated and improved by mathematical modeling but the WWTP model needs to be calibrated. Usually, calibration has to be performed using a limited, scarce, and imperfectly obtained set of plant-measured data. The paper describes the calibration of a municipal WWTP dynamic model based on the activated sludge model No. 3 (ASM3) and Benchmark Simulation Model, thereby proposing a new calibration methodology. In order to achieve the calibration goal, a set of influent wastewater variables associated with a set of process and settler parameters were chosen and calibrated by optimization. Optimization based on a constrained sequential quadratic programming algorithm was used. As objective function, it considers the sum of the absolute differences between the effluent simulated and measured data for chemical oxygen demand, total nitrogen, and suspended solids. The WWTP model relies on the measured influent, plant configuration, and size data that originate from a Romanian municipal WWTP. The emerged municipal WWTP dynamic model using the ASM3 was calibrated, based on the new proposed calibration methodology. The calibrated model was tested both by steady state and dynamic simulations and the results show good agreement with the municipal WWTP behavior.

Keywords: Municipal wastewater treatment plant; Activated Sludge Model No. 3; Calibration

1. Introduction

1.1. Wastewater treatment and mathematical modeling

The aim of wastewater treatment is to substantially reduce pollutants in water that originates from human and industrial activities. This mission should be accomplished to such an extent that remaining pollutants have very low concentrations and they may be further degraded by the self-purifying potential of the receiving natural waters. Municipal wastewater treatment is a challenging task for every urban society from technical and economic points of view [1–5]. The most appreciated and widespread biological purifying process that is applied at municipal wastewater treatment plants (WWTPs) is the activated sludge technology [6]. According to its expected performance, the carbon, nitrogen, and phosphorous components are transformed and removed from the wastewater [7]. Supporting the wastewater treatment field, mathematical modeling contributes to the understanding, systematic investigation, and improvement of the processes that occur in the WWTPs [8–15]. International Water Association (IWA) proposed four complex mathematical models for the biological wastewater treatment: Activated sludge model No. 1, 2, 2 d, and 3 (ASM1, ASM2, ASM2d, and ASM3) [16–19]. Obviously, the models need to be calibrated for each particular application, because of WWTP size, configuration, and composition of

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the influent wastewater entering the plant change from one plant to another [20–22]. Different calibration approaches have been developed, as calibration of the models can be performed by different methodologies and optimization procedures [23,24].

Based on measured data from a Romanian plant, the paper presents a new calibration procedure applied to an anaerobic-anoxic-aerobic (A^2O) WWTP unit using ASM3 and the results of its modeling performance.

1.2. Activated sludge model no. 3

ASM3 was presented by Gujer et al. [25]. The model was designed to describe the removal of organic carbon and nitrogen and correct certain weaknesses that emerged from the application of the ASM1 model [26–30].

The growth of heterotrophic biomass in the ASM3 is achieved by considering the sequential two-step process [31,32]. The first step is the storage of the biodegradable substrate in the form of internal cellular storage products. During the second step, internal storage products are used for biomass growth. The storage process requires energy, which is obtained by aerobic or anoxic respiration [33]. In ASM1, the readily biodegradable substrate is also obtained by decomposing the nitrifying organisms, while this biodegradable substrate is used for the growth process of the heterotrophic biomass. Compared to ASM1, in ASM3, autotrophic and heterotrophic microorganisms are clearly separated. As a result, biodegradable carbon does not pass from one biomass type to the other [16].

2. Investigated Romanian municipal wastewater treatment plant

2.1. Configuration of the municipal wastewater treatment plant

The Romanian municipal WWTP under investigation has an A^2O configuration, whose layout is presented in Fig. 1. The wastewater entering the plant is firstly processed by mechanical filtration, followed by sand and fats separation, and the primary sedimentation. Water treatment is continued through the biological processes in the anaerobic, anoxic, and aerobic zones of the biodegradation basins. The secondary settlers represent the last purification step. Two recirculation streams operate in the WWTP. The first one is the nitrate recirculation (NR) stream (internal recirculation). It emerges from the end of the biodegradation basins and enters between the anaerobic and anoxic tanks. Its role is to return the nitrates that are formed in the aerobic basins in order to be processed by denitrification. The second one is the return activated sludge (RAS) stream (external recirculation), which is responsible for preserving the desired biomass in the biological tanks by returning the biomass from the secondary settlers to the anaerobic basin.

2.2. Measured influent, effluent, and plant sizes data

At the investigated municipal WWTP, the measurements of the flows and a part of the influent and effluent components concentration are carried out by special devoted instrumentation. Basically, they work with a sampling rate of 10 s (i.e., almost continuous measurements from the viewpoint of the overall WWTP rate-controlling time constants). Chemical oxygen demand (COD), nitrogen components (ammonium and ammonia, nitrates and nitrites, total nitrogen (N_{total})), phosphorus, and total suspended solids (SS) have dedicated instrumentation for their continuous measurements. The computer monitoring system is completed, or even doubled for part of the measurements, by specific daily or weekly laboratory measurements. For continuous measurements COD, nitrogen components (ammonium and ammonia, nitrates and nitrites, and N_{total}), phosphorus, and total SS the dedicated instrumentation is used. The influent and effluent flow rates, the flow rate of the air entering the aerated biodegradation basins, the flow rates of the NR and the RAS are also determined by the same fast sampling rate. The available measured data for the month of May 2016 was collected, analyzed, and reconciled. The average characteristic values of the main WWTP process variables for the first 22 d of this month are shown in Table 1.

In the period of May 2016, four primary clarifiers, four lines of the biological basins and four secondary settlers were in parallel operation. The main sizing characteristics of the

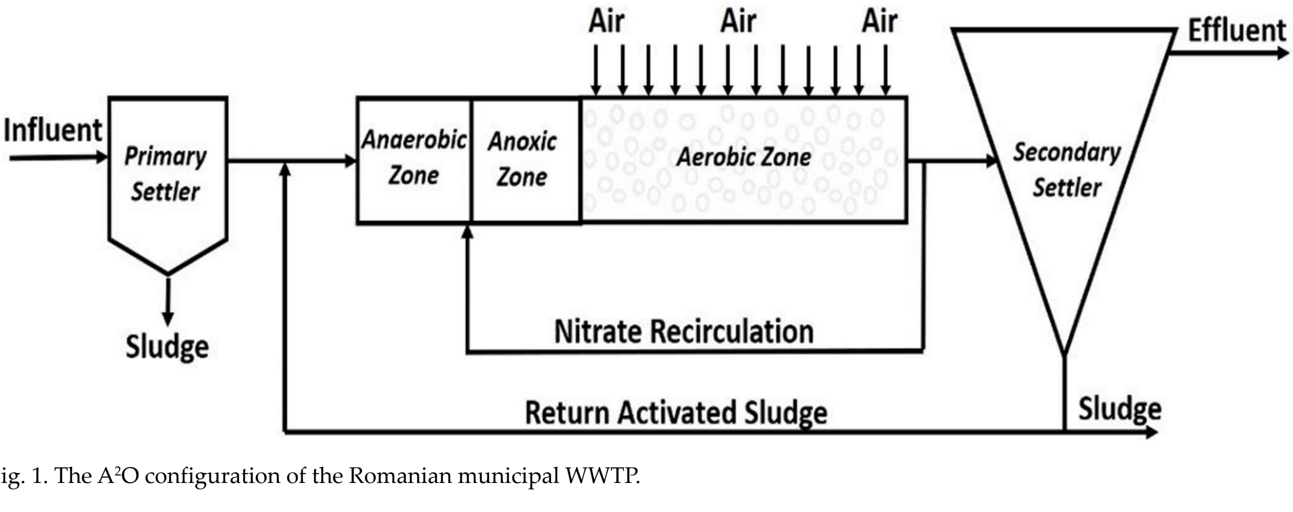

Fig. 1. The A^2O configuration of the Romanian municipal WWTP.

Table 1
Averaged measured data for the main influent, operating, and effluent variables

Variable	Average value
Influent	
COD, g COD/m^3	264.17
S_{NH_4}, g N/m^3	24.98
S_{NOX}, g N/m^3	2.34
N_{org}, g N/m^3	7.91
N_{total}, g N/m^3	35.23
X_{SS}, g SS/m^3	132
Q, m^3/d	119,221
Temperature, °C	15.83
pH	6.81
Air, recirculation, and waste flow rates	
Air entering into the aerobic tanks, m^3/d	383,325
NR, m^3/d	138,345
RAS, m^3/d	112,523
Waste, m^3/d	889
Effluent	
COD_S, g COD/m^3	4.84
S_{NH_4}, g N/m^3	0.17
S_{NOX}, g N/m^3	3.76
N_{org}, g N/m^3	1.77
N_{total}, g N/m^3	5.7
X_{SS}, g SS/m^3	12

Table 2
Sizing characteristics of the primary clarifiers, biodegradation basins, and secondary settlers

Parameter	Value
Primary clarifiers	
Area of one primary clarifier, m^2	531.2
Total area of the four primary clarifiers, m^2	2,125
Height of the primary clarifier, m	3.5
Biodegradation basins	
Volume of the operated anaerobic zone, m^3	9,015
Volume of the operated anoxic zone, m^3	12,678
Volume of the operated aerobic zone, m^3	33,066
Area of the operated aerobic zone, m^2	6,012
Secondary settlers	
Area of one secondary settler, m^2	16,956
Total area of the four secondary settlers, m^2	67,824
Height of the secondary settler, m	3

basins and settlers, which are considered in the developed WWTP model, are presented in Table 2.

3. Methods

3.1. Dynamic wastewater treatment plant model components

The developed model is composed of a primary clarifier [34] that relies on the Otterpohl and Freund model [35], five bioreactors connected in series and described by biological processes according to ASM3 [25] and a secondary settler based on the double-exponential settling velocity function approach [36].

The WWTP model was updated with the measured influent and operating data, considering the configuration, and sizing data collected from the Romanian municipal WWTP.

Matlab software and Simulink graphical programming software environment were used to develop the dynamic WWTP model based on the ASM3. The core of the WWTP model is the Benchmark Simulation Technique that was developed by the IWA Working Task Group on Benchmarking of Control Strategies [37]. The process equations were written in C programming language and implemented as compiled MEX MATLAB files. S-function blocks were used to incorporate the codes into Simulink. The algebraic and differential equations were solved using the ODE15s stiff problem solver from Matlab.

3.2. Proposed ASM3 model calibration methodology

Models and simulators in wastewater treatment have become very useful tools, but they require the calibration of each WWTP model in order to provide trusting information [38,39]. This implies finding the appropriate values for the parameters of the model, such as the simulated data fits to the process measured data [40,41]. Frequently, a set of the model parameters, which are considered as decision variables, is selected and their appropriate values are computed as a result of an optimization procedure, carried out to minimize a suitable objective function.

As revealed by the literature, different calibration procedures may be applied for building wastewater treatment models for different types of wastewater [42–49]. The common, usually recursive steps of each calibration protocol consist of goal definition of the calibration procedure, collection, analysis and reconciliation of the process measured data, selection of the model structure and the parameters to fit, the achievement of the steady and dynamic calibration, and finally, assessment of the calibrated model performance [43]. A significant particularity of the WWTPs calibration protocols is the consideration of calibrating both the influent wastewater characteristics and the process model parameters. For example, according to the Department of Applied Mathematics, Biometrics and Process Control, Ghent University, Belgium (BIOMATH) group, the characterization of the influent wastewater may be based on respirometry tests. Explicitly, the influent readily biodegradable organic substrate concentration (S_S) is determined directly by respirometry experiments and the influent content of inert particulate organic material (X_I) is calibrated by optimization. Optimization is also used to find other process parameters that are related to the heterotrophic organisms (X_{STO}) characteristics [50]. The Dutch Foundation of Applied Water Research, The Netherlands (STOWA) calibration protocol focuses on the biochemical oxygen demand measurements in order to determine the COD's biodegradable part [51].

According to this approach, X_I is calculated from the mass balance, without any need of additional lab-scale experiments. The Hochschulegruppe calibration procedure is a combination of the BIOMATH and STOWA calibration protocols [52]. The influent characterization is based on STOWA and the model parameter estimation relies on the BIOMATH approach. Water Environment Research Foundation, North America (WERF) protocol combines the influent wastewater characterization based on oxygen uptake rate (OUR) measurements and physical-chemical analyses. Estimation of the parameters influencing the nitrification process is achieved using optimization [53].

Considering the calibration procedures that are reported in the literature, available municipal WWTP measured data, previous simulation and modeling experience, a new calibration approach is proposed in this work and the performance of the calibrated WWTP model is assessed. The calibration methodology is presented in Fig. 2. Fig. 2 presents an insight into calibration methodology. It shows both the general calibration steps and the details specific to its application at the investigated municipal WWTP case study.

The novelty of the calibration approach lies in (i) the particular selection of the influent variables, bioreactors, and settler parameters to be calibrated using the available measured data, (ii) the specification of the optimization performance index form, and (iii) the formulation of the additional equations that are used for the computation of the rest of the variables that are to be calibrated. The proposed calibration methodology makes a well-balanced trade-off between the ASM features, available WWTP measurements, and optimization performance. In the present research, 11 variables and parameters (five influent variables characteristics, three biodegradation reactor process model parameters, and three settler model parameters) were chosen for performing the steady-state model calibration.

In the ASM3 model, 13 WWTP state variables are considered by the basic model, but only a part of these variables are output variables that can be directly measured at

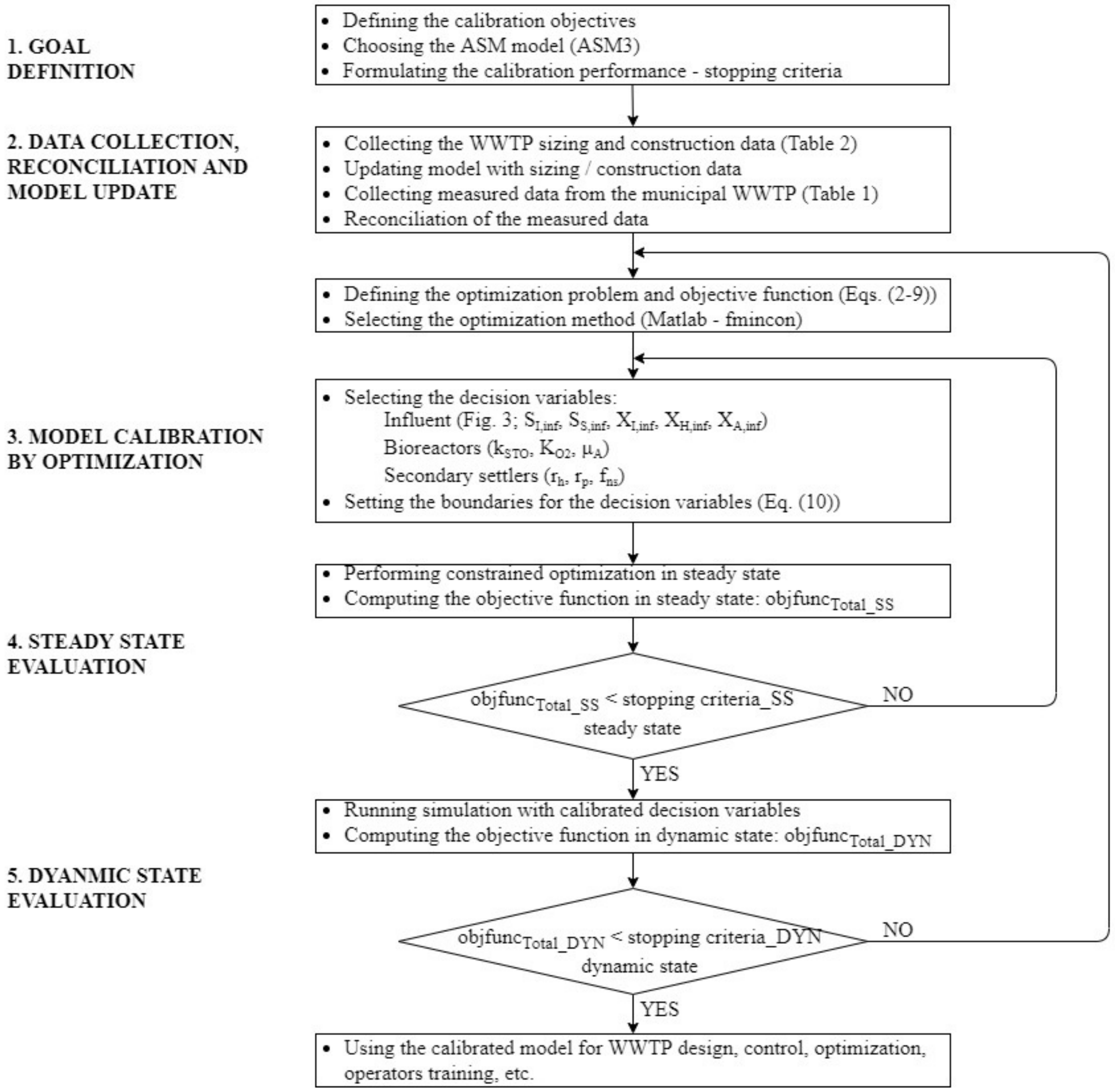

Fig. 2. The proposed calibration methodology.

the investigated municipal WWTP. The calibration approach proposed in this research for the influent organic compounds presents in Fig. 3 the influent components of ASM3 that are measured, calculated, and calibrated.

Considering the carbon-related variables and their importance, the main total chemical oxygen demand ($\mathrm{COD_{tot}}$) influent variable is determined by measurements. Based on the $\mathrm{COD_{tot}}$ measurement, the calibration of the soluble chemical oxygen demand (COD_S) and particle COD_X components becomes necessary. The components of both soluble and particulate COD are revealed in Fig. 3. Consequently, in this work, five influent COD variables (as components of the soluble and particulate COD) have been proposed for calibration by optimization. They are inert soluble organic material (S_I, noted with x_1), readily biodegradable organic substrates (S_S, noted with x_2), inert particulate organic material (X_I, noted with x_3), heterotrophic biomass (X_H, noted with x_4) and nitrifying biomass (X_A, noted with x_5). These five influent COD variables are calibrated as constant fractions of the measured influent $\mathrm{COD_{tot}}$ concentration. The cell's internal storage product of heterotrophic organisms (X_{STO}) is neglected in the influent wastewater [16] and the slowly biodegradable COD substrate (X_S) is calculated from the other variables according to Eq. (1).

$$X_s = \mathrm{COD_{tot}} - S_I - S_S - X_I - X_H - X_A \quad (1)$$

The nitrate plus nitrite nitrogen (S_{NOX}) and the ammonium plus ammonia nitrogen ($S_{\mathrm{NH_4}}$) components concentration in the influent wastewater were directly measured. The organic nitrogen fractions are neglected in the ASM3 [16].

Six process and settler parameters were selected to be calibrated. The three process parameters include storage rate constant (k_{STO}, noted with x_6), saturation constant for dissolved oxygen ($K_{\mathrm{O_2}}$, noted with x_7), and autotrophic maximum growth of the nitrifying organisms (μ_A, noted with x_8) and these are associated to three settler parameters, which are the hindered zone settling parameter (r_h, noted with x_9), flocculant zone settling parameter (r_p, noted with x_{10}), and the non-settleable fraction (f_{ns}, noted with x_{11}).

The dynamic WWTP model was calibrated using the influent and effluent data measurements for the COD, N fractions, and SS variables, collected from the municipal WWTP under study.

The eleven influent wastewater variables, process parameters, and settler parameters that are chosen to be calibrated are the decision variables of the overall objective function ($\mathrm{objfunc_{total}}$). The latter is consisted within the sum of three sub-objective functions. They are the effluent soluble COD, effluent nitrogen fractions, and effluent SS concentrations, as described by Eqs. (2)–(4). The task of the optimization problem was to find the values of the unknown decision variables that minimize the overall objective function, while a set of inequality constraints are also satisfied.

$$\min_X \left[\mathrm{objfunc_{total}} \left(x_1, x_2, x_3, x_4, x_5, x_6, x_7, x_8, x_9, x_{10}, x_{11} \right) \right] \quad (2)$$

$$X = \left[x_1\ x_2\ x_3\ x_4\ x_5\ x_6\ x_7\ x_8\ x_9\ x_{10}\ x_{11} \right] \quad (3)$$

$$\mathrm{objfunc_{total}} = \mathrm{objfunc_{COD\,s}} + \mathrm{objfunc}_N + \mathrm{objfunc_{SS}} \quad (4)$$

The sub-objective function of the soluble COD ($\mathrm{objfunc_{CODs}}$) is equal to the absolute difference between the measured effluent soluble COD ($\mathrm{COD_{s,eff,WWTP}}$) and the simulated value of soluble COD ($\mathrm{COD_{s,eff,model}}$), Eq. (5). The sub-objective function of nitrogen fractions ($\mathrm{objfunc_N}$) is computed as a weighted sum, considering the nitrates and nitrites objective function term ($\mathrm{objfunc_{NOX}}$) and the objective function term of the ammonia and ammonium nitrogen ($\mathrm{objfunc_{NH_4}}$). The sub-sub-objective function $\mathrm{objfunc_{NH_4}}$ is multiplied by the factor of 10 in order to bring $\mathrm{objfunc_{NH_4}}$ term to the same order of magnitude as $\mathrm{objfunc_{NOX}}$ term. The objective functions of the nitrogen fractions are also considered as absolute

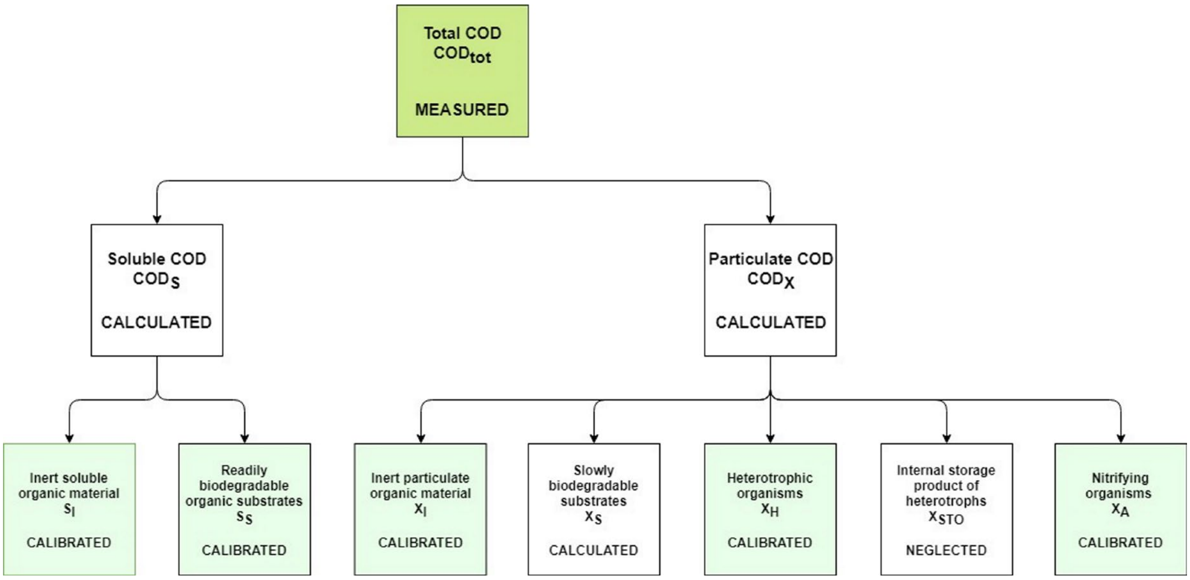

Fig. 3. Measured, calibrated, and calculated influent organic compounds in the proposed calibration methodology.

values of the differences between the WWTP measured data and the values that are obtained by simulation. The equations of the sub-objective functions for the nitrogen fractions are described by Eqs. (6)–(8). The sub-objective function of the SS ($\text{objfunc}_{\text{SS}}$) is shown in Eq. (9) and it is also consisted in the absolute difference between the measured municipal WWTP effluent SS and the simulated effluent SS data.

$$\text{objfunc}_{\text{COD}\,s} = \left|\text{COD}_{s,\text{eff,WWTP}} - \text{COD}_{s,\text{eff,model}}\right| \tag{5}$$

$$\text{objfunc}_{N} = \text{objfunc}_{\text{NOX}} + 10 \times \text{objfunc}_{\text{NH}_4} \tag{6}$$

$$\text{objfunc}_{\text{NOX}} = \left|\text{NOX}_{\text{eff,WWTP}} - \text{NOX}_{\text{eff,model}}\right| \tag{7}$$

$$\text{objfunc}_{\text{NH}_4} = \left|\text{NH}_{4,\text{eff,WWTP}} - \text{NH}_{4\text{eff,model}}\right| \tag{8}$$

$$\text{objfunc}_{\text{SS}} = \left|\text{SS}_{\text{eff,WWTP}} - \text{SS}_{\text{eff,model}}\right| \tag{9}$$

As presented in Eq. (10), in order to obtain feasible values for the calibrated parameters and influent variables, both lower bounds (LB) and upper bounds (UB) for the independent optimization variables have been taken into account and specified. The values for the LB and UB were chosen based on a literature survey [16,25,37,54].

$$\text{LB} \le X \le \text{UB} \tag{10}$$

Optimization was carried out taking into consideration both the steady-state values that were obtained by running the simulation for 150 d and the averaged measured data that were collected from the municipal WWTP under study.

The constrained optimization algorithm that was implemented in Matlab software was considered in this research. It uses the interior point algorithm which combines the direct Newton with the conjugate gradient optimum searching method.

Following the optimization step, the dynamic WWTP model was updated with the calibrated influent variables, process, and settler parameters that were obtained by optimization. Performance of the calibrated model was assessed equally in a steady and dynamic state. For the dynamic evaluation, the 10 min-averaged municipal WWTP measured values of the influent wastewater variables, flow rates of air entering the aerated biodegradation basins, flow rates of NR and RAS were used in the dynamic simulations. They created the time-varying validation scenario. The effluent data results obtained by running the dynamic simulations were compared with the 10 min-averaged measured effluent data that was collected from the Romanian municipal WWTP.

4. Results and discussion

4.1. Calibration and steady-state simulation results

Firstly, the five selected influent variables, three process parameters, and three settler parameters were calibrated by optimization, using the steady-state values computed for the effluent variables. The calibrated values obtained by optimization for the selected influent variables, process, and settler parameters are presented in Table 3.

The steady-state values that were obtained by simulation after 150 d of WWTP simulation time were collected and analyzed. The results are presented as follows.

For the influent, according to the calibrating results, the influent total COD was equal to 264.17 g COD/m^3, which is a value that corresponds to the averaged total COD that was measured at the WWTP. The inert soluble organic matter (S_I) fraction of` the total COD had a value of 0.0183, while for the fraction of the readily biodegradable organic substrates (S_S), a value of 0.19 was obtained. According to the calibration results, almost 21% of the total COD is represented by the soluble organic matter, which corresponds to the values reported in the literature (Pasztor et al. [54]). The influent concentration of the heterotrophic (X_H) and nitrifying (X_A) organisms are small and may be considered almost negligible. The inert particulate organic matter represented 6.5% of the total influent COD, while the concentration of the influent slowly biodegradable COD substrate (X_S) had the highest contribution. Its value was equal to 190.09 g COD/m^3 and it corresponds to 72% of the influent total COD.

The calibrated values of the process parameters show values that are similar to those found in the literature [16]. The autotrophic maximum growth rate of the nitrifying organisms is situated in the interval between 0.35 and 1 d^{-1}, as reported in the literature. The storage rate constant is slightly smaller than the value of 2.5 g COD_{XS}/(g COD_{XH} d), while the saturation constant for dissolved oxygen had a value of 0.666 g O_2/m^3. These values of the calibrated process parameters are considered to reveal both the typical and the specific characteristics of the investigated Romanian municipal WWTP.

Likewise, the settler calibrated parameters have values of the same order of magnitude as the values that are reported in the literature [37]. This conclusion is drawn by noting that they have close values to the literature data of 0.000576 m^3/g SS for the hindered zone settling parameter, of 0.00286 m^3/g SS for the flocculant zone settling parameter, and of 0.00228 for the non-settleable fraction.

Moreover, when the main effluent COD, NOX, NH_4, and SS variables are considered, the comparison between the measured data that are collected from the Romanian municipal WWTP (for a period of 22 d) and the simulated effluent data that are obtained with the calibrated model reveals a very good agreement. This is shown in Table 4.

The outputs of the Otterpohl primary settler and Takács secondary settler models were also verified in order to fit the available measured data. The components' concentrations in the stream leaving the calibrated primary clarifier model correspond to the measured data that were recorded at the municipal WWTP. The value for the TSS concentration in the underflow of the calibrated secondary settler has similar values to those that were measured at the investigated municipal WWTP.

Table 5 presents the values of the overall and the sub-objective optimization function values that are obtained with the optimally calibrated influent variables, process, and settler parameters. They show reduced values. It can be concluded that steady-state calibration based on the selected optimization algorithm was accurately accomplished and the

Table 3
Calibrated values obtained by optimization for the selected influent variables characteristics, process, and settler parameters

Calibrated variable/parameter	Notation	Symbol	Calibrated value
Influent variables			
Inert soluble organic material, g COD/m^3	$S_{I,\mathrm{inf}}$	x_1	4.84
Readily biodegradable organic substrates, g COD/m^3	$S_{S,\mathrm{inf}}$	x_2	50.31
Inert particulate organic material, g COD/m^3	$X_{\mathrm{I,inf}}$	x_3	17.28
Heterotrophic organisms, g COD/m^3	$X_{\mathrm{H,inf}}$	x_4	0.89
Nitrifying organisms, g COD/m^3	$X_{\mathrm{A,inf}}$	x_5	0.76
Process parameters			
Storage rate constant, g COD$_{\mathrm{XS}}$/(g COD$_{\mathrm{XH}}$ d)	k_{STO}	x_6	1.71
Saturation constant for dissolved oxygen, g O$_2$/m^3	$K_{\mathrm{O_2}}$	x_7	0.666
Autotrophic max growth of the nitrifying organisms, 1/d	μ_A	x_8	0.638
Settler parameters			
Hindered zone settling parameter, m^3/g SS	r_h	x_9	0.0008
Flocculant zone settling parameter, m^3/g SS	r_p	x_{10}	0.0023
Non-settleable fraction	f_{ns}	x_{11}	0.0016

Table 4
Comparison between the measured effluent data at the investigated Romanian WWTP and the effluent data obtained by simulation with the calibrated model

Effluent variables concentration	Notation	Averaged measured effluent data for 22 d collected from WWTP	Simulated effluent data obtained with the calibrated model
Soluble chemical oxygen demand, g COD/m^3	COD$_S$	4.84	4.84
Nitrate and nitrite nitrogen, g N/m^3	S_{NOX}	3.76	3.56
Ammonium and ammonia nitrogen, g N/m^3	$S_{\mathrm{NH_4}}$	0.17	0.17
Suspended solids, g SS/m^3	X_{SS}	12.00	12.00

Table 5
Values obtained for the optimized performance indices of the proposed calibration

Objective function	Value of the objective function
Objective function for COD$_S$	5.13×10^{-5}
Objective function for N fractions	2.01×10^{-1}
Objective function for SS	5.43×10^{-9}
Overall objective function	2.01×10^{-1}

proposed calibration procedure can be used for the calibration of WWTP ASM3-based models.

4.2. Dynamic state simulation results

Dynamic simulations were carried out in order to test the performance of the calibrated WWTP model in dynamic state conditions. For the dynamic simulations, the 10 min-averaged WWTP measured values were used for the influent, airflow, RAS flow, and NR flow rates. The simulation results for the validation period of 22 d were compared with the effluent measured data that were collected from the investigated municipal WWTP. For the set of main WWTP variables, the measured effluent data show a good similarity to the simulated effluent data. As representative results, the soluble COD$_S$ and the nitrate and nitrite nitrogen concentrations S_{NOX} of the effluent for the first 17 d period are presented in Figs. 4 and 5.

It may be observed that in the dynamic state as well, simulated effluent values for the COD$_S$ and S_{NOX} are comparable to the measured effluent data.

Furthermore, the mean absolute and relative errors were calculated for the same period, considering the values at multiples of 10 min sampling time. The absolute error is the absolute difference between measured effluent concentration ($c_{\mathrm{eff,measured}}$) and simulated effluent concentration ($c_{\mathrm{eff,simulated}}$), which is given by Eq. (11). The relative error is computed as the ratio of the absolute error to the measured effluent concentration, as given by Eq. (12).

$$\varepsilon_{\mathrm{ads}} = \left| C_{\mathrm{eff,measured}} - C_{\mathrm{eff,simulated}} \right| \tag{11}$$

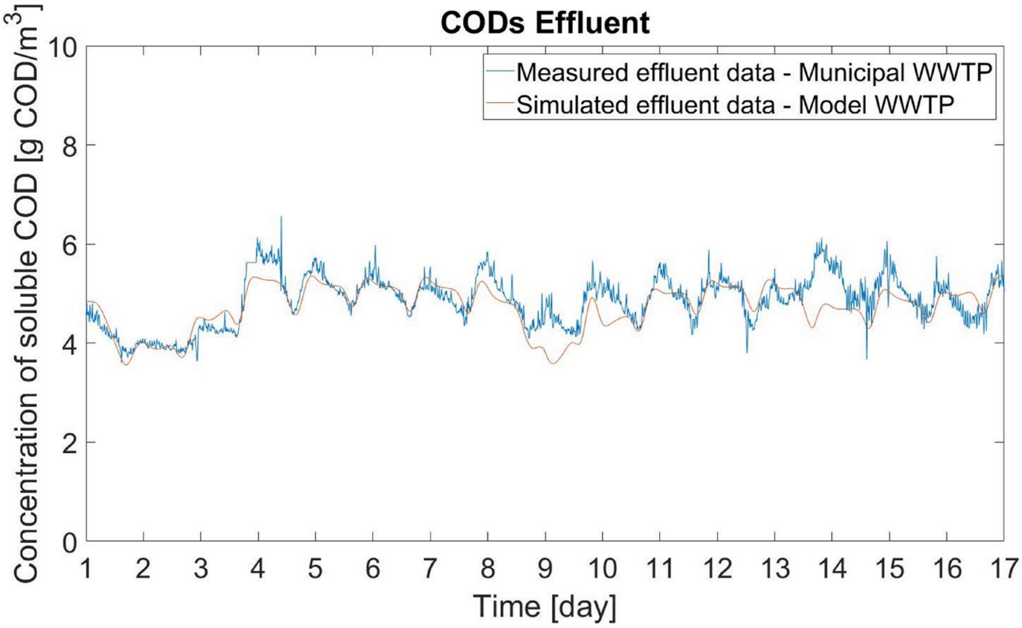

Fig. 4. Comparison between the measured effluent soluble COD_S at the Romanian municipal WWTP and the simulated effluent results obtained with the calibrated model.

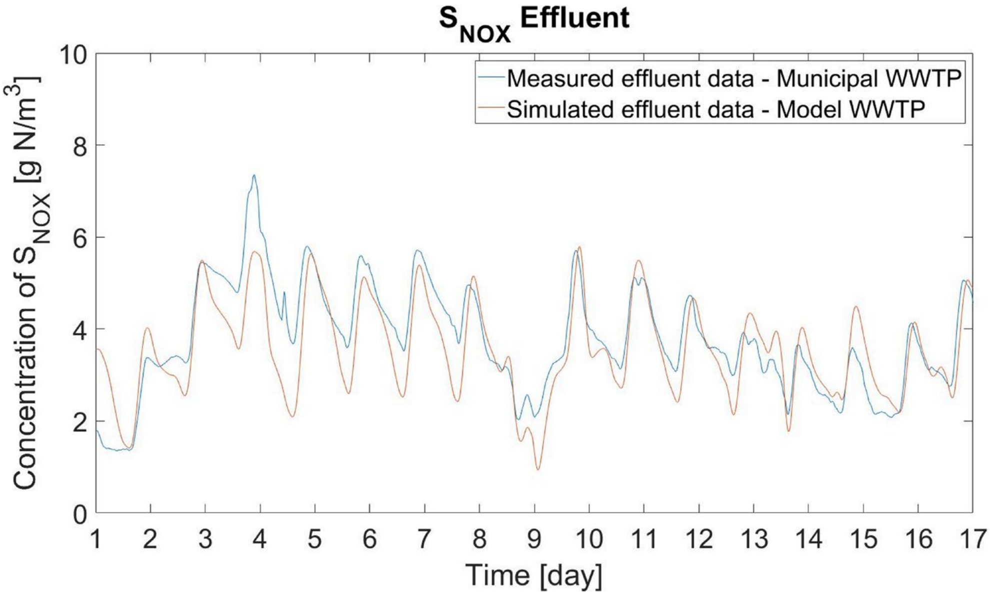

Fig. 5. Comparison between the measured effluent nitrate and nitrite nitrogen S_{NOX} concentration at the Romanian municipal WWTP and the simulated effluent results obtained with the calibrated model.

$$\varepsilon_{rel} = \frac{\left|C_{eff,measured} - C_{eff,simulated}\right|}{C_{eff,measured}} 100 \tag{12}$$

The mean absolute error for soluble COD_S is 0.3003, while the mean relative error for COD_S is equal to 6.36%. The calculated mean absolute error for nitrate and nitrite nitrogen (S_{NOX}) is equal to 0.5672, while the mean relative error for S_{NOX} is 16.52%.

Considering the complexity of the activated sludge process and its associated ASM3 model, it may be concluded that the developed WWTP model was successfully calibrated and both the steady state and dynamic simulation results are in good agreement with the municipal WWTP behavior.

5. Conclusions

Mathematical modeling of WWTP implies that there is a requirement for calibration in order to attain reliable WWTP models, which usually rests on field data that are affected by scarcity and measurement errors.

The objectives of this research were aimed to build a dynamic WWTP model based on the ASM3, in order to calibrate the model based on a new calibration approach using mathematical optimization and also to validate the calibrated simulation instrument with WWTP data, in both steady and dynamic state. Firstly, data describing the plant configuration, biodegradation reactors, settlers, and equipment size characteristics were collected. Secondly, measurements of influent and effluent variables were acquired from the investigated Romanian WWTP. They served as prerequisites for the calibration and validation procedure.

The new calibration approach was proposed to obtain the desired fit of the model results to the WWTP measured data. A set of unknown influent variables composition, together with a set of process and settler parameters, were appropriately selected for optimization. The optimization objective function and its components were properly defined for the WWTP most important COD and nitrogen effluent variables. The eleven designated variables and parameters to be calibrated were inert soluble organic material, readily biodegradable organic substrates, inert particulate organic material, heterotrophic organisms, nitrifying organisms' concentrations associated to the storage rate constant, saturation constant for dissolved oxygen, autotrophic maximum growth rate of nitrifying organisms, hindered zone settling parameter, flocculant zone settling parameter, and non-settleable fraction parameters. The calibrated values of these decision variables were computed by optimization. The steady state and dynamic simulation results that were obtained with the calibrated model revealed the significant similarity to the municipal WWTP main effluent measured values. The same conclusion is proved by dynamic simulations, as low values were obtained for the optimization sub-objective functions, the reduced mean absolute and relative errors that were demonstrated during the validation time period.

It may be concluded that the development and calibration of the dynamic WWTP model based on ASM3 were appropriately accomplished. The calibrated WWTP model may be used for design, optimization, and control of investigations. The proposed calibration methodology can be considered efficient and may be applied for the calibration of other WWTP ASM3-based models.

Notations

A^2O — Anaerobic-Anoxic-Oxic
ASM1 — Activated Sludge Model No. 1
ASM2 — Activated Sludge Model No. 2
ASM2d — Activated Sludge Model No. 2d
ASM3 — Activated Sludge Model No. 3
BIOMATH — Department of Applied Mathematics, Biometrics and Process Control, Ghent University, Belgium
BSM1 — Benchmark Simulation Model No. 1
COD — Chemical Oxygen Demand, g COD/m^3
$\mathrm{COD_S}$ — Soluble Chemical Oxygen Demand, g COD/m^3
eff — Effluent
f_{ns} — Non-settleable fraction
HSG — Hochschulegruppe—a group of researchers from German speaking countries
inf — Influent wastewater
IWA — International Water Association
k_{STO} — Storage rate constant, g $\mathrm{COD_{XS}}$/(g $\mathrm{COD_{XH}}$ d)
$k_{\mathrm{O_2}}$ — Saturation constant for nitrite nitrogen, g O_2/m^3
$\mathrm{NH_4}$ — Ammonium plus ammonia nitrogen, g N/m^3
$\mathrm{N_{org}}$ — Organic nitrogen, g N/m^3
NOX — Nitrate plus nitrite nitrogen, g N/m^3
NR — Nitrate Recirculation
$\mathrm{N_{total}}$ — Total nitrogen, g N/m^3
objfunc — Objective function
Q — Flow rate, m^3/d
RAS — Return Activated Sludge
r_h — Hindered zone settling parameter, m^3/g SS
r_p — Flocculant zone settling parameter, m^3/g SS
S_{COD} — Soluble Chemical Oxygen Demand, g COD/m^3
S_I — Inert soluble organic material, g COD/m^3
$S_{\mathrm{NH_4}}$ — Ammonium plus ammonia nitrogen, g N/m^3
S_{NOX} — Nitrate plus nitrite nitrogen, g N/m^3
S_S — Readily biodegradable organic substrates, g COD/m^3
SS — Suspended solids, g SS/m^3
STOWA — The Dutch Foundation of Applied Water Research, The Netherlands
WERF — Water Environment Research Foundation, North America
WWTP — Wastewater Treatment Plant
X_A — Nitrifying organisms, g COD/m^3
X_H — Heterotrophic organisms, g COD/m^3
X_I — Inert particulate organic material, g COD/m^3
X_S — Slowly biodegradable COD substrate, g COD/m^3
X_{SS} — Suspended solids, g SS/m^3
μ_A — Autotrophic maximum growth rate of the nitrifying organisms, 1/d

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