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WWTP MODEL CALIBRATION BASED ON DIFFERENT OPTIMIZATION APPROACHES

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Abstract

There is a significant interest in modelling the wastewater treatment plants (WWTP) because with a calibrated model a large variety of operational strategies can be evaluated, the control system design may be improved and enhanced constructive alternatives may be proposed. The Activated Sludge Model No. 1 (ASM1) has the potential of describing the biochemical processes taking place in WWTPs, in association with the Benchmark Simulation Model No. 1 (BSM1) which adds the description of the involved physical processes. An important challenge for reliable simulators development is the dynamically changing composition of the influent wastewater, also varying from one WWTP to another. Due to this reason, it is necessary to fit the model for each WWTP. This paper proposes a new methodology for the dynamic simulator calibration of a municipal WWTP. Different optimization methods are used for the simulator calibration and results of the different approaches are comparatively presented. Based on WWTP measurements a set of influent variables, bioreactor parameters and settler parameters are calibrated. Optimization was carried out based on classical, genetic, hybrid and Pareto multiobjective algorithms and their performance is discussed, revealing their strengths and limitations.

Key words: activated sludge model no. 1, model calibration, optimization methods, wastewater treatment

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1. Introduction

The increase of industrialization and urbanization associated to the rapid population growth results in the production of huge quantities of wastewaters which may consist in thousands tons of suspended matters (high value of Total Suspended Solids, TSS) and organic compounds (high values of Chemical Oxygen Demand, COD) (Chan et al., 2009; Zaharia and Jufa, 2017). Raw or treated wastewater is discharged into rivers, lakes and this produces changes in ecological equilibrium or biological diversity, often causing environmental hazards (Ani et al., 2010, Cristea et al., 2010; Zou et al., 2018). These facts make wastewater treatment a very challenging issue (Einschlag, 2011).

One of the most important parts of every urban infrastructure is the municipal Wastewater Treatment Plant (WWTP). Municipal wastewater is the mixture of different types of wastewaters such as domestic wastewater, small amounts of industrial and agro-zootechnical wastewater, storm water, drain water, surface infiltration and ground water (Wiesmann et al., 2007). The main compounds which must be removed from water during treatment are: organics, dissolved molecules, colloids and solid particles; inorganic, dissolved compounds containing nitrogen (NH_4^+, NO_2^-, NO_3^-) and phosphorus (PO_4^{3-}). All these

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compounds may be removed by the activated sludge process.

The Activated Sludge Model No. 1 (ASM1) developed by the IAWQ group was firstly presented in 1987 and describes the following set of dynamic processes: aerobic growth of heterotrophs, anoxic growth of heterotrophs, aerobic growth of autotrophs, decay of heterotrophs, decay of autotrophs, ammonification of soluble organic nitrogen, hydrolysis of entrapped organics and hydrolysis of entrapped organic nitrogen (Jeppsson, 1996). Modelling of activated sludge processes has become a common part of the design and operation of wastewater treatment plants. Featuring a continuously expanding trend, the models are being used in design, control, teaching and research (Gernaey et al., 2004; Henze et al., 2002; Ostace et al., 2012).

The general overview of the ASM1 is presented in Fig. 1. As shown, the ASM1 state variables consist of organic matter and nitrogen components, in either biodegradable and non-biodegradable or soluble and particulate forms, associated to active heterotrophic and autotrophic biomass (Alex et al., 2008). Calibration of WWTP models is needed, because not all variables, parameters and influent composition are directly measured and many of them are not thoroughly known at the most of the wastewater treatment plants (Grau et al., 2007; Martin and Vanrolleghem, 2014). The WWTP models can be fitted by different optimization methods. Fitting the model may imply several stages, such as: defining the objective functions, plant survey, data analysis, model structure selection, process characterization, model calibration and its evaluation (Corominas, 2006; Langergraber et al., 2004).

The aim of this paper is to propose a new calibration methodology for WWTP models and to comparatively investigate four optimization methods which have been tested for calibration of a municipal WWTP case study. The proposed and analysed optimization methods used for WWTP calibration were based on classical, genetic, hybrid and Pareto multiobjective algorithms. Their performance is shown in the present work. The results of the different calibration methodologies also reveal the limitations and potential benefits of the considered model-type to plant-configuration association, when the trade-off between simplicity and accuracy is needed.

2. Material and methods

2.1. Process Description of the Investigated Municipal WWTP

The flow diagram of the municipal WWTP, for which different calibration methods were investigated, is presented in Fig. 2. This wastewater treatment unit has an Anaerobic-Anoxic-Oxic (A2O) configuration of the bioreactors. They are associated to the primary and secondary settlers. The wastewater flow leaving the primary settler mixes with the return activated sludge flow originating from bottom of the secondary settler and enters the first reactor of the denitrification zone, i.e. the anaerobic bioreactor.

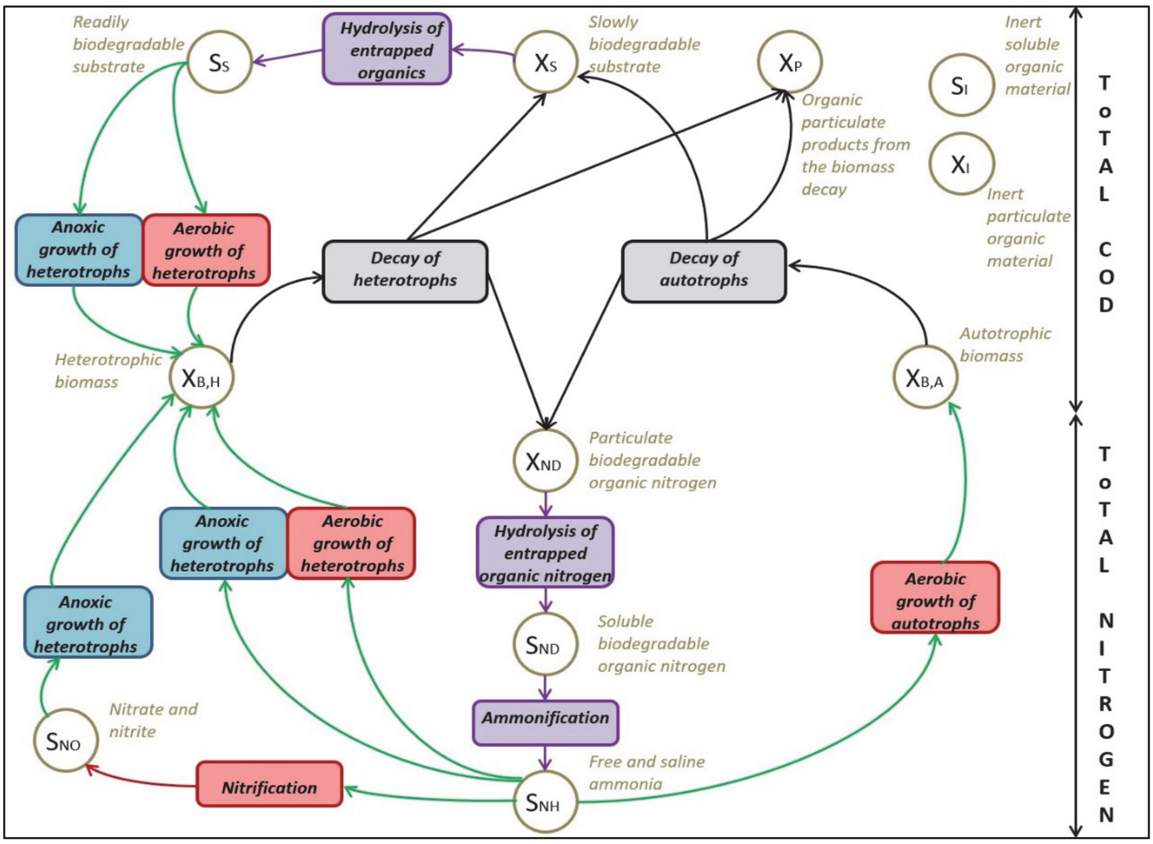


Fig. 1. General overview of ASM1

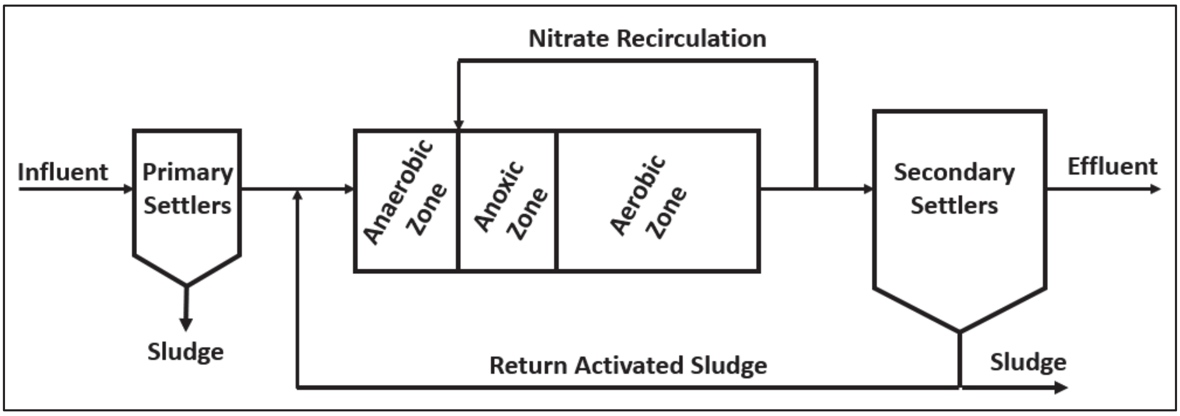


Fig. 2. Process flow diagram of the investigated municipal WWTP

The outlet flow of this bioreactor mixes with the nitrate recirculation flow emerged from aerobic reactor and enters the second reactor of the denitrification zone, i.e. the anoxic bioreactor. Subsequently, the wastewater enters the nitrification zone of the aerated bioreactor (Alasino et al., 2007; Ostace et al., 2011; WEF, 2007). Part of the water outlet flow of the nitrification bioreactor is recirculated in the denitrification zone and part is sent to the secondary settler for removing the solid particles. From the secondary settler the clear water is discharged into the emissary river and the sludge flow is split between the return activated sludge flow and the flow sent to the anaerobic digestion unit.

2.2. Simulator software implementation

The simulator was developed based on the Benchmark Simulation Technique provided by COST Action 682 and the IWA Working Task Group on Benchmarking of Control Strategies for WWTPs (Copp, 2002), with modifications implied by the A2O WWTP configuration under study and the supplement of the primary settler. The core of the model is ASM1. The MATLAB software and the graphical programming extension SIMULINK was used in the present research. The 8 process equations for the bioreactors and the equations for the primary and the secondary settlers were written in C programming language to reduce the simulation time and to spare computing resources. The codes were compiled and incorporated into the Simulink environment by S-function blocks. Simulink ODE15s and ODE23s solvers of MALAB were used for solving the differential and algebraic equations of the model.

2.3. Model calibration

2.3.1. Model and data used

Data were collected from the investigated municipal WWTP. The reactor-settler stream flow configuration of the process and data on the equipment characteristics were taken from the WWTP unit. Scarce influent wastewater and effluent water data measurements were considered. All available measured data were firstly analyzed.

The proposed and developed model is a combination of a primary clarifier and the modified BSM1 model, which includes 5-compartment activated sludge reactor composed of an anaerobic and an anoxic zone followed by 3 aerobic tanks, associated to the secondary settler (Alex et al., 2008). As a consequence, the original BSM1 WWTP recycle streams configuration was changed by relocating the nitrate recirculation fed-point between the anaerobic and anoxic tanks and by adding the primary settler.

The primary clarifier in the present model is a nonreactive settler, which is based on the Otterpohl's primary clarifier model. It describes the changes of sludge water concentrations, buffered by the clarifier and the partial removal of COD particulate fractions according to the influent flow (Otterpohl and Freund, 1992). The bioreactors are arranged in series and the aerated compartments consider fixed oxygen transfer coefficient (Henze et al., 1987). The secondary settler is represented by a configuration with 10-layers and the model is based on Takács's double-exponential settling velocity function (Takács et al., 1991). The main geometrical characteristics of the modelled WWTP are presented in Table 1.

As presented in literature, different procedures are used for the WWTP influent characterization and parameter estimation (Ekama et al., 1986; Henze, 1992; Henze et al., 1987; Hulsbeek et al., 2002; Melcer et al., 2003; Spanjers and Vanrolleghem, 1995; Vanrolleghem et al., 2003). By most of the influent wastewater calibration procedures, the X_{BH} and X_{BA} influent variables are considered to be negligible, whereas S_I is equal to the soluble COD from the effluent flow.

In the BIOMATH procedure a respirometry test is introduced for the determination of S_S fraction directly and X_I is calibrated, the other influent variables being calculated from mass balance. According to the protocol of Henze et al. (1987), mass balance is used to get the soluble and particulate COD fractions, and X_I is subject to calibration. In the STOWA protocol a long BOD test is used for the determination of X_S and no calibration was required for X_I. The mass balance was used for the calculation of X_I and S_S variables (Corominas, 2006).

Table 1. Reactors and settlers geometrical characteristics

Parameter	Value
Primary settler	
Area of the primary settler (A)	2125 m^2
Height of the primary settler (H)	3.5 m
Bioreactors	
Volume of the 1st reactor – anaerobic zone (V)	9015 m^3
Volume of the 2nd reactor – anoxic zone (V)	12678 m^3
Volume of the 3th reactor – aerobic tank (V)	11022 m^3
Volume of the 4th reactor – aerobic tank (V)	11022 m^3
Volume of the 5th reactor – aerobic tank (V)	11022 m^3
Area of 3th, 4th, 5th reactors – aerobic tanks (A)	2004 m^2
Secondary settler	
Area of the secondary settler (A)	11304 m^2
Height of the secondary settler (H)	3 m

For the WWTP under study, the Chemical Oxygen Demand (COD), ammonia (NH), nitrates and nitrites (NO), total nitrogen (N_{tot}) and total suspended solids (TSS) fractions of the influent and the effluent wastewater are measured. Data collected during the month of May 2016 were used for the calibration and simulations in this work.

The measured influent variables are shown in Table 2. They are average values computed for the considered 22 days' time period, based on available measured daily data or measured data based on 10 minutes averaged values. The flow rate of the air entering the aerated tanks, the flow rates of the nitrate recycle and the return activated sludge recycle (RAS), as well as the flow rate of the wasted sludge were also collected from measurements made at the WWTP under study. The average values of these variables are: Q_{air} = 127775 m^3/day, $Q_{nitrate\ recycle}$ = 138345 m^3/day, Q_{RAS} = 112523 m^3/day, Q_{waste} = 889 m^3/day.

The calibration was performed with the three control loops present in the municipal WWTP. The first one is the Proportional-Integral (PI) dissolved oxygen (DO) control in the aerated reactors, having the air flow rate as manipulated variable. The others two are ratio (feedforward) control loops, having the recycle flow rates, i.e. the nitrate recirculation and return activated sludge flow rates, as controlled variables and the wastewater inflow as the leading (disturbance) flow rate.

2.3.2.New calibration methodology for influent characterization

To obtain the required values of the influent state variables for ASM1, a new approach was proposed. This was created based on literature, experimental data and previously simulations experience. It also accounted for the limited amount and relatively poor quality of the available measured data from the WWTP under study.

It was considered that the quantity of the soluble non-biodegradable material (S_I) in the influent wastewater is equal to the soluble COD from the effluent water ($COD_{S,eff}$) (Eq. 1). The latter was calculated from the value of total COD and TSS of the effluent water (Eq. 2). $COD_{S,inf}$ and $X_{I,inf}$ were calibrated by optimization, S_S and X_S were calculated based on mass balance Eqs. (3-4). X_{BH} and X_{BA} fractions in the influent were neglected. Fig. 3 presents the proposed influent calibration procedure for the organic matter fractions.

As the S_{NO} and S_{NH} concentrations in the influent were directly measured, the organic fractions only needed to be calculated. The soluble organic fraction (S_{ND}) and particulate organic fraction (X_{ND}) were computed from the total Kjeldahl nitrogen (TKN) and COD fractions according to Eqs. (6-7). They are presented in Fig. 4 (Hellstedt, 2005; Petersen et al., 2002; Vanrolleghem et al., 2003).

Table 2. The average values of the measured influent variables

Variable	*Average Value*
Chemical Oxygen Demand (COD)	264.17 g COD/m^3
Free and saline ammonia (S_{NH})	24.98 g N/m^3
Nitrates and nitrites (S_{NO})	2.34 g N/m^3
Total nitrogen (N_{tot})	35.23 g N/m^3
pH	6.81
Total suspended solids (TSS)	132 g SS/m^3
Flow rate (Q)	119221 m^3/day
Temperature (T)	15.83°C
Organic nitrogen (N_{org})	7.91 g N/m^3

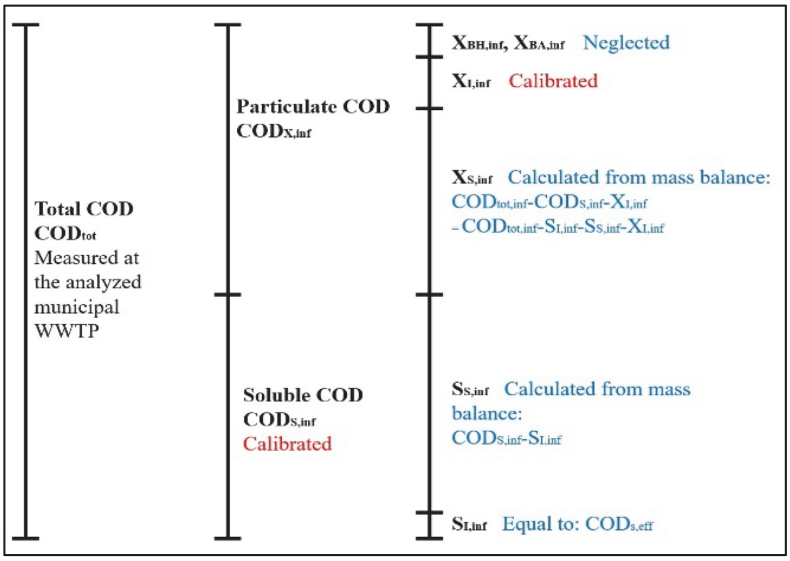


Fig. 3. Proposed calibration procedure for the influent organic matter fractions

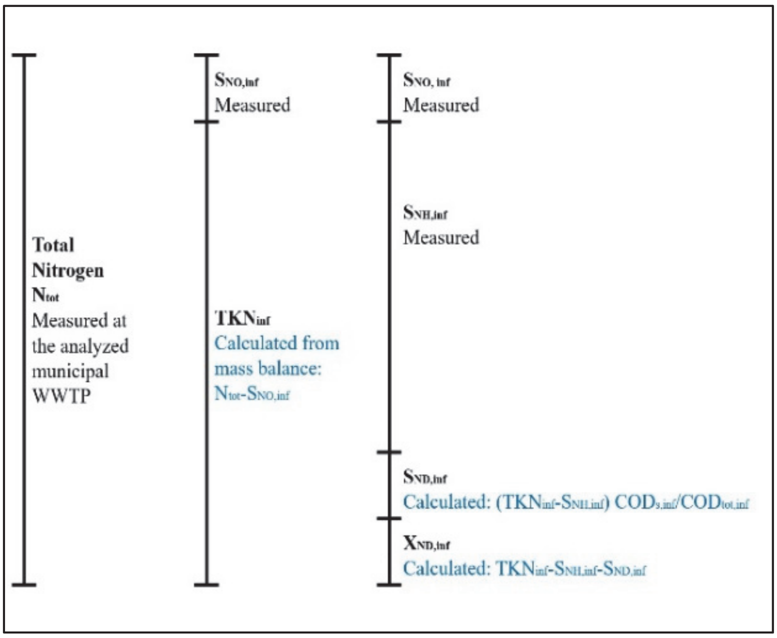


Fig. 4. Proposed calibration procedure for the influent nitrogen fractions

Summarizing, the proposed equations for model calibration are (Eqs. 1-7):

$$S_{I,\inf} = COD_{S,eff} \tag{1}$$

$$COD_{S,eff} = COD_{tot,eff} - COD_{X,eff} = COD_{tot,eff} - \frac{TSS_{eff}}{0.75} \tag{2}$$

$$S_{S,\inf} = COD_{S,\inf} - S_{I,\inf} \tag{3}$$

$$TKN_{\inf} = S_{NH,\inf} + S_{ND,\inf} + X_{ND,\inf} \tag{4}$$

$$X_{S,\inf} = COD_{tot,\inf} - S_{I,\inf} - S_{S,\inf} - X_{I,\inf} \tag{5}$$

$$S_{ND,\inf} = \frac{COD_{S,\inf}}{COD_{tot,\inf}} \cdot \left(TKN_{\inf} - S_{NH,\inf}\right) \tag{6}$$

$$X_{ND,\inf} = \left(TKN_{\inf} - S_{NH,\inf}\right) - S_{ND,\inf} \tag{7}$$

The novelty of the proposed and applied calibration procedure consists in the particular selection of the influent variables and process parameters to be calibrated with available measured data, the specification of the additional equations needed for the computation of the rest of the influent variables, the formulation of the optimization indices and the investigation of the Pareto multiobjective optimization approach for WWTP calibration.

2.3.3. Optimization methods used for model calibration

As it is not possible to determine all ASM1 influent variables and model parameters using the available WWTP measurements, some influent variables and model parameters have been considered decision variables and calibrated by optimization (Boyd and Vandenberghe, 2004; Funamizu et al., 1987; Zawilski and Brzezinska, 2009). The set of decision variables of the optimization problem has been chosen as a minimum set of influent variables and model parameters needed for calibration. They were decided as a result of (i) an analysis of the computation relationships required for calculating the influent variables, Eqs. (1-7), (ii) considering the main subunits of the plant and (iii) managing the available measurements collected from the municipal WWTP. In the present work 2 influent variables, 2 bioreactor process parameters and 3 settler model parameters were selected for fitting the plant model simulation results with the WWTP measurements. These variables and parameters are: COD soluble influent fraction ($COD_{sol,inf}$, denoted by x_1), particulate inert influent organic matter fraction ($X_{I,inf}$, denoted by x_2), heterotrophic decay rate (b_H, denoted by x_3), autotrophic decay rate (b_A, denoted by x_4), hindered zone settling parameter (r_h, denoted by x_5), flocculent zone settling parameter (r_p, denoted by x_6) and non-settleable parameter (f_{ns}, denoted by x_7). The model was calibrated on the basis of the COD, N and TSS influent and effluent measurements from the municipal WWTP.

The optimization problem is described by the following equations (Eqs. 8-17):

$$\min_{\mathbf{X}} objfunc_{total}(\mathbf{X}) \tag{8}$$

$$\mathbf{X} = [x_1\ x_2\ \ldots\ x_7]^T \tag{9}$$

$$objfunc_{total} = objfunc_{CODsol} + objfunc_N + objfunc_{TSS} \tag{10}$$

$$objfunc_{CODsol} = \left|COD_{sol,eff,\mathrm{WWTP}} - COD_{sol,eff,\mathrm{model}}\right| \tag{11}$$

$$objfunc_N = objfunc_{NO} + objfunc_{Norg} + 10 \cdot objfunc_{NH} \tag{12}$$

$$objfunc_{NO} = \left|NO_{eff,\mathrm{WWTP}} - NO_{eff,\mathrm{model}}\right| \tag{13}$$

$$objfunc_{Norg} = \left|Norg_{eff,\mathrm{WWTP}} - Norg_{eff,\mathrm{model}}\right| \tag{14}$$

$$objfunc_{NH} = \left|NH_{eff,\mathrm{WWTP}} - NH_{eff,\mathrm{model}}\right| \tag{15}$$

$$objfunc_{TSS} = \left|TSS_{eff,\mathrm{WWTP}} - TSS_{eff,\mathrm{model}}\right| \tag{16}$$

$$\mathbf{LB} \le \mathbf{X} \le \mathbf{UB} \tag{17}$$

The examined influent variables, process and settler parameters are associated to the overall objective function ($objfunc_{total}$), which is the sum of the sub-objective functions for COD, Nitrogen and TSS variables. The objective function for Nitrogen is composed of three sub-subobjective functions for: nitrates and nitrites (NO), organic nitrogen (N_{org}) and free and saline ammonia (NH). In order to make an approximately equal weighting between the three sub-subobjective terms of the total nitrogen subobjective function ($objfunc_N$), where the ammonia sub-subobjective term ($objfunc_{NH}$) is about 10 times lower compared to the two other sub-subobjective terms and due to the required accuracy for the ammonia concentration calibration, the weighting factor of 10 was introduced for $objfunc_{NH}$. These objective functions are represented by the absolute differences between the industrial effluent measured data and the corresponding value obtained by model simulation. The objective functions are presented in Eqs. (10-16). The lower and upper bound of the constrained optimization problem are specified in (Eq. 17).

Four optimization methods were used in this research. First, an optimization method based on the classical interior point algorithm which combines a direct Newton step with a conjugate gradient step was used. At each iteration a single point is generated and an optimal solution is approached by the sequence of points. The next point in the sequence is selected by a deterministic computation approach. The Matlab *fmincon* function was used for implementing this optimization algorithm.

The second optimization method was based on the genetic algorithm, in which a population of points is generated at each iteration. An optimal solution is approached by the best point (individual) in the population. In this optimization approach, the next population is generated using mutation and crossover of the current generation elite individuals. The algorithm stops when best individual of the new generation accomplishes a desired fitness value. The Matlab *ga* function was used for implementing this optimization algorithm.

The third investigated optimization method was the hybrid method which combines the genetic algorithm method with the classical algorithm method. This optimization has two parts: the genetic algorithm finds a point close to the optimal solution and then the classical algorithm uses it as its initial search point to improve the value of the objective function. The Matlab *hybrid* function was used for implementing this optimization algorithm.

A fourth optimization method was also investigated. For this multiobjective optimization approach were used the same and all three subobjective terms shown in (Eq. 10), also considered in the previously presented optimization methods. This optimization method finds the local Pareto minima of the multiple objective functions using genetic algorithms. The Matlab *gamultiobj* function was used for implementing this optimization algorithm.

In all cases the lower and upper bounds (**LB** and **UB**) were defined for the optimization variables and parameters. They were chosen based on literature survey (Pasztor et al., 2009). It is worthy to note that for the classical algorithm it was needed to provide a starting initial point for all optimization variables and parameters, whereas in the case of the genetic algorithm only the population size and the number of generations were initially defined. The initial point values for the classical algorithm have been set within the range of values of the corresponding decision variables reported in literature (Copp, 2002; Henze et al., 2002; Pasztor et al., 2009).

2.3.4. Calibration procedure

The calibration procedure started with choosing the variables and parameters which needed to be optimized. Afterwards, the influent measured data were converted to ASM units and the model was updated with the collected data, associated to the geometrical characteristics of the equipment from the municipal WWTP. Steady state optimization was carried out with the mentioned optimization methods, comparing the effluent data from the model simulation (obtained after 150 days) with the averaged effluent measured data from the municipal WWTP. Subsequent to the optimization step and based on the obtained results, the simulator was updated with the calibrated process parameters. Matlab and Simulink software were used for performing both dynamic simulations and optimization.

2.3.5. Evaluation of the calibrated model

The IWA Task Group created dry, rain and storm weather influent flow and composition timely changing profiles, saved in special influent files to be used in dynamic simulations. Analyzing both these dynamic influent profiles and the data from the municipal WWTP, it can be observed the daily pattern, the weekend effect, the seasonal specific periodic profiles and the particular behaviour during holiday periods (Gernaey et al., 2005; Wang et al., 2017).

For the evaluation of the steady state calibrated model, dynamic simulations were performed with constant inputs, until steady state was reached. Subsequently, the calibrated model was tested for assessing its dynamic behaviour performance. From the municipal WWTP the dynamic influent data measurements were available with averaged values over 10 minutes. The influent COD, total nitrogen, nitrate and nitrite and ammonia measurements were considered. Selectively, the influent COD and NH data are presented in Fig. 5.

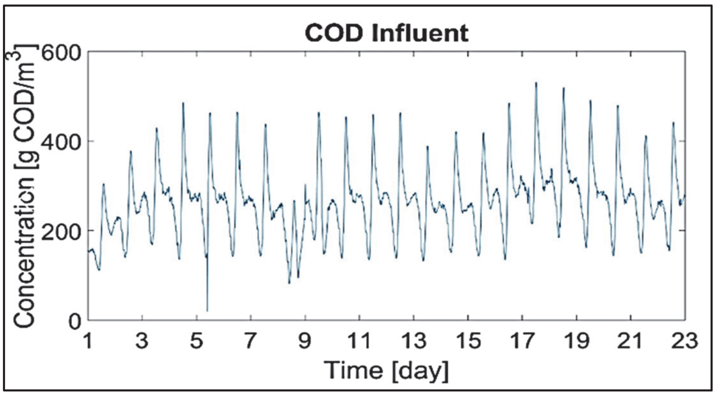
The measured data for the flow rates of the air entering the aerobic tanks, the nitrate recycle, the returned activated sludge recycle and the waste flow rate were also considered. The influent flow rate and the flow rates of recycle streams (nitrogen recycle and activated sludge return flow rate) are shown in Fig. 6. Based on 10 minutes averaged values, effluent data of soluble COD, total nitrogen, nitrate and nitrite, ammonia and flow rates were also collected and used for optimization. On the basis of these data, the time-changing influent files were created for the municipal WWTP and used for the dynamic performance evaluation of the calibrated model. Afterwards, dynamic simulations were made for a period of 22 days with time varying influent data.

The dynamic state simulations were performed using influent measured data with a sampling time of 10 minutes (averaged measured data over the 10 minutes time interval) assuming the same ratio of COD_S and X_I to COD_{tot} emerged from calibration. All influent concentrations used for the dynamic state results were changing at time moments represented by multiples of 10 minutes. Consequently, the WWTP effluent variables obtained by simulating the calibrated model were computed with the same 10 minutes averaged values. The effluent data from the calibrated model and the measured effluent data from the analysed WWTP were compared and the comparison is presented in the Results and Discussion section.

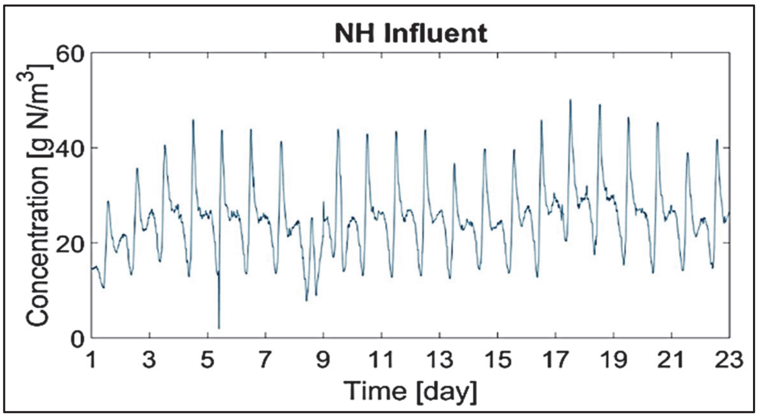
3. Results and discussion

3.1. Steady state results

Before the assessment of the calibrated model performance, values from the literature survey for the analyzed variables and parameters were summarized and presented in Table 3 (Bagheri et al., 2015; Pasztor et al., 2009). They represent the first indicator for the fitness of the calibrated model simulation results to the WWTP behaviour, as reflected by literature reported data.

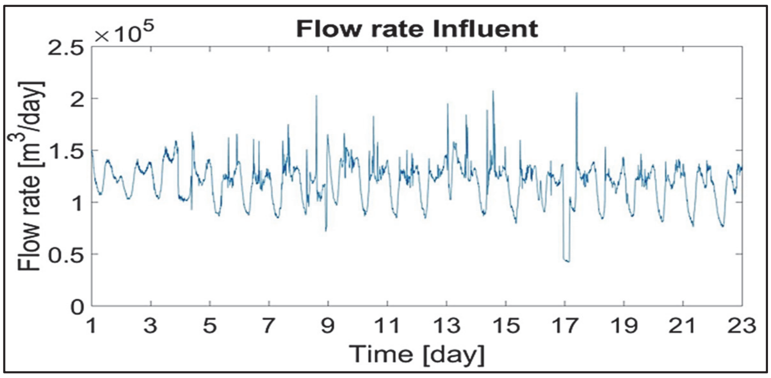


(a)

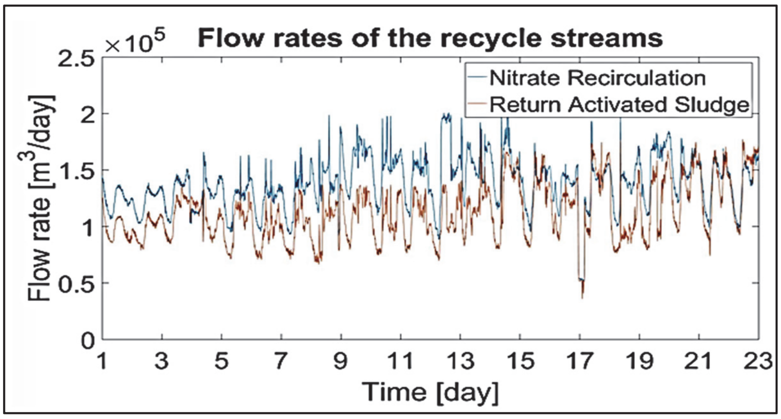


(b)

Fig. 5. (a) COD Influent Data; (b) NH Influent Data



(a)



(b)

Fig. 6. (a) Influent flow rate data; (b) Flow rates of the recycle streams

The results of the different optimization methods investigated in the present research work, showing comparatively the values of the fitted variables and parameters are also presented in Table 3. The influent COD_{sol} and X_I obtained by optimization are expressed as fractions of the influent COD_{tot}. Examining Table 3, it can be observed that the soluble COD is around 50% of total COD in the influent wastewater for the cases of optimization by classical algorithm, genetic algorithm and hybrid method.

The calibrated $X_{I,inf}$ influent variable, b_H and b_A model parameters are in the range of values reported in the literature, for all three calibration methods. The settler model parameters r_h, r_p and f_{ns} are also comparable with the values reported in literature. Comparison between the effluent soluble COD, TKN, NO, organic nitrogen (N_{org}), NH and TSS values obtained from the calibrated model and the measured values from the municipal WWTP is shown in Table 4.

Table 3. Summarized literature values for the calibrated variables and parameters, respectively comparative model calibration results using different algorithms

Influent Variable / Process Parameter / Settler Parameter	***Notation***	***Value from literature***	***Value obtained by calibration with classical algorithms***	***Value obtained by calibration by genetic algorithms***	***Value obtained by calibration with hybrid method***	***Unit***
Soluble influent COD	$COD_{sol,inf}$	0.08 – 0.49	0.449	0.486	0.519	fraction
Particulate inert organic matter	$X_{I,inf}$	0.1 – 0.2	0.164	0.159	0.139	fraction
Heterotrophic decay rate	b_H	0.05 – 1.6	0.253	0.317	0.303	1/day
Autotrophic decay rate	b_A	0.05 – 0.2	0.0746	0.0694	0.0759	1/day
Hindered zone settling parameter	r_h	0.00048	0.000613	0.000715	0.000673	$m^3/(g\ SS)$
Flocculent zone settling parameter	r_p	0.00286	0.00615	0.00705	0.00777	$m^3/(g\ SS)$
Non-settleable parameter	f_{ns}	0.00228	0.00204	0.00210	0.00221	dimensionless

Table 4. Comparison between the effluent data obtained with the calibrated model and the effluent data from the municipal WWTP measurements

Effluent variable	***Average measured value at the analysed WWTP***	***Value obtained by calibration with classical algorithms***	***Value obtained by calibration by genetic algorithms***	***Value obtained by calibration with hybrid method***	***Unit***
COD_{sol}	4.84	4.65	4.89	4.84	$g\ COD/m^3$
TKN	1.94	1.89	2.03	2.01	$g\ N/m^3$
NO	3.76	3.70	3.30	3.14	$g\ N/m^3$
N_{org}	1.77	1.74	1.89	1.84	$g\ N/m^3$
NH	0.17	0.15	0.15	0.17	$g\ N/m^3$
TSS	12.00	12.31	12.23	12.00	$g\ SS/m^3$

Table 4 reveals that effluent values obtained with the calibrated model, using all three optimization methods, and the average values of the measured effluent from the municipal WWTP are in good agreement. The results obtained by the Pareto multiobjective optimization, considering the same three sub-objective functions, were also examined. From the Pareto fronts the one considered most representative and important for the selection of the best optimization point was presented. This obtained Pareto front is shown in Fig. 7 for two objective functions of the multiobjective one. The first objective function (shown on the abscissa) is representing the soluble COD ($objfunc_{CODsol}$), while the second objective (shown on the ordinate) is corresponding to the N fractions ($objfunc_N$). They were described in Eqs. (10-16).

Following the analysis of all three Pareto fronts, the front presenting the first two subobjective terms of (Eq. 10), i.e. objective functions for the soluble COD and N fractions, was considered most important and it was presented in Fig. 7. This figure also reveals two of the Pareto optimal solutions (points) that were selected from the Pareto front. These two points belonging to the presented Pareto front were chosen to have associated the most reduced values of the sum of all the three subobjective functions. The trade-off for this selection of the Pareto front points considered the most important calibration targets the soluble COD and N fractions, as they correspond to the main WWTP effluent variables.

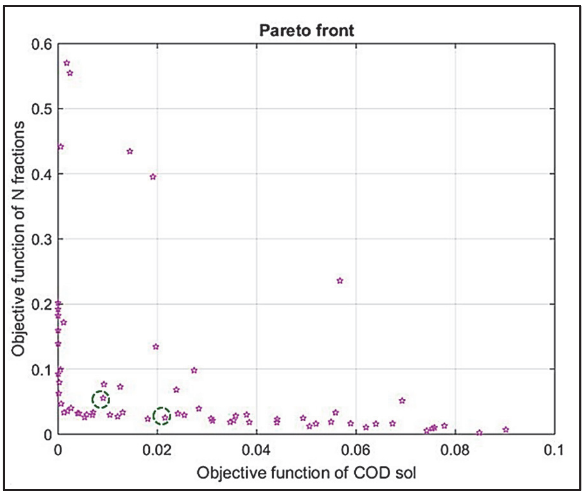


Fig. 7. The Pareto front obtained by the multiobjective optimization for the soluble COD and N sub-objective functions

They were considered to make the best trade-off between the three implied sub-objective functions.

The values of their corresponding influent variables and parameters (i.e. the model calibration results) were further used for simulations. The selected points are characterized by the most reduced values for the multiobjective function presented in (Eq. 10). Table 5 shows the values obtained by Pareto optimization for the fitted influent variables/parameters.

The effluent data obtained by simulating the calibrated model for the selected Pareto optimal points are presented in Table 6. They are comparatively shown to the WWTP effluent measured data. It can be observed that the effluent values obtained with the calibrated model by Pareto optimization very well approximate the measured effluent values at the municipal WWTP. Accordingly, the multiobjective Pareto optimization method can be considered a very effective optimization approach.

Table 3 and Table 5 reveal that the best fit was obtained with the Pareto multiobjective method while the genetic algorithm provided the worst results. The values of the influent soluble COD and particulate inert organic matter fractions obtained by optimization are corresponding to the data found in literature (Derco et al., 2011; Pasztor et al., 2009). The value of the heterotrophic decay rate and the autotrophic decay rate process parameters are also situated in the range reported in literature (Copp, 2002; Henze et al., 1987; Vivekanandan and Seshagiri Rao, 2017). The optimization performance indices for all presented optimization methods are shown in Table 7.

Analyzing the calibration results, it may be stated that the best overall results were obtained by the Pareto multiobjective optimization. Examining individually the obtained values for the objective functions, the calibration using the Pareto multiobjective optimization method showed the best performance index values for all of the N fractions, while the best performance indices for soluble COD and TSS were obtained with the calibration using the hybrid optimization method. Nevertheless, the model was calibrated with the parameters emerged from the Pareto multiobjective optimization approach as it revealed the most reduced value for the overall objective function.

3.2. Dynamic state results

The previously steady state best calibrated model was also tested for investigating its dynamic behaviour by dynamic simulations. The influent data used for the dynamic simulations were obtained by online and laboratory measurements.

Influent NH and NO were measured with online sensors, while the influent COD and TSS dynamic profiles were built based on laboratory determinations. A constant ratio was assumed for the soluble COD to the total COD concentrations, both for the calibration step and for the dynamic simulations. Simulation results are presented in Fig. 8 for a period time of one week starting from day 5 to 12.

As it may be observed from Fig. 8, the output values of the calibrated model show a fairly good similarity with the data measured at the real plant for the dynamic case, too. Comparable results were obtained in the case of soluble COD concentration, total nitrogen concentration, the nitrate and nitrite concentration and in the case of effluent flow rate.

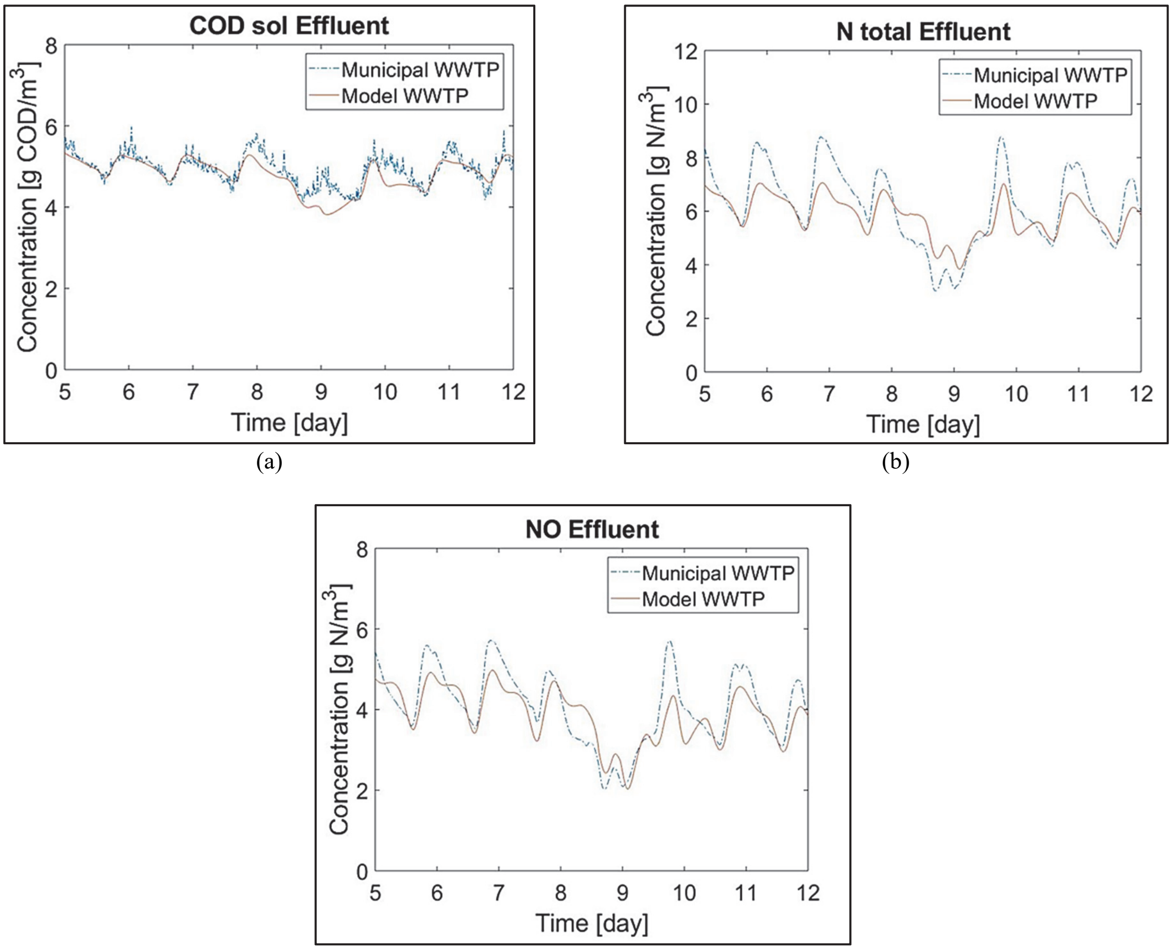
4. Conclusions

The goal of this research was to calibrate the selected WWTP model based on a new model calibration approach and then to make a comparison between the investigated optimization methods. The originality of the presented WWTP calibration approach consists in the (i) influent variables and model parameters selection, (ii) equations used for the computation of part the influent variables, (iii) performance indices structure and (iv) comparison between different optimization methods.

Models of the wastewater treatment plant based on the activated sludge technology are very useful tools for analyzing, revealing and understanding the complex mechanisms of the processes involved, and have become very efficient means for designing, upgrading and controlling WWTPs. It is quite frequently that only a part of the state variables required by ASM model are directly measured at the WWTP. By optimization procedures, the implied state variables may be calibrated in order to obtain a robust WWTP model. In this work, the unknown influent COD and N fractions associated to a set of process and settler parameters were considered and computed by optimization in order to achieve a good fit between the ASM1 model and the measured data from the municipal WWTP under study. Due to the fact that obtained effluent data from simulations show a reasonable fit with the measured effluent data, it may be concluded that the model calibration of the analyzed WWTP was successfully accomplished.

Table 5. Model calibration results obtained by the Pareto multiobjective optimization

Influent Variable /Parameter	*Value for the 1st Pareto optimum point*	*Value for the 2nd Pareto optimum point*	*Unit*
$COD_{sol,inf}$	0.427	0.425	fraction
$X_{I,inf}$	0.176	0.175	fraction
b_H	0.301	0.298	1/day
b_A	0.08	0.08	1/day
r_h	0.000612	0.000614	m^3 /(g SS)
r_p	0.00634	0.00631	m^3 /(g SS)
f_{ns}	0.00202	0.00202	dimensionless



(a) (b)

(c)

Fig. 8. Comparison between the effluent measured data at the municipal WWTP and the results obtained from the best calibrated model: (a) soluble COD; (b) total nitrogen; (c) nitrate and nitrite concentrations

Table 6. Comparison between the effluent data obtained with the calibrated model by the Pareto multiobjective optimization and the effluent data from the municipal WWTP measurements

Effluent variable	*Measured value at the analysed WWTP*	*Value obtained with the 1st Pareto optimum*	*Value obtained with the 2nd Pareto optimum*	*Unit*
COD_{sol}	4.84	4.83	4.82	g COD/m^3
TKN	1.94	1.99	1.98	g N/m^3
NO	3.76	3.76	3.76	g N/m^3
N_{org}	1.77	1.82	1.81	g N/m^3
NH	0.17	0.17	0.17	g N/m^3
TSS	12.00	12.00	12.00	g SS $/m^3$

Table 7. Optimization performance indices for all optimization approaches analyzed in this work

Optimization method	*Objective function of COD_{sol}*	*Objective function of N fractions*	*Objective function of TSS*	*Total objective function*
Calibration by classical algorithm	0.1928	0.2681	0.3056	0.7665
Calibration by genetic algorithm	0.0504	0.7997	0.2299	1.0800
Calibration by hybrid method	0.0047	0.6963	0.0002	0.7012
Multiobjective calibration (1st point)	0.0104	0.0534	0.0018	0.0656
Multiobjective calibration (2nd point)	0.0201	0.0431	0.0025	0.0657

Considering the measured data available, the proposed model calibration strategy proved to be efficient for the case study of the analyzed municipal WWTP, but it may also serve as a good methodology for model calibration of other WWTPs.

The present study also investigated different optimization methods used for model calibration and comparison was made to assess their efficiency. Four optimization methods were analysed considering an overall objective function consisting in three sub-objective functions. These sub-objective functions addressed the minimization of the model simulated effluent soluble COD, nitrogen fractions and TSS fraction deviations from their WWTP measured values. These optimization approaches for model calibration were conducted by the classical, genetic, hybrid and Pareto multiobjective algorithms. Optimization performed by the Pareto multiobjective algorithm proved to be the most efficient method for the presented case study.

An advantage demonstrated by this method was the possibility to be extracted from the Pareto front the optimum point that best meets desired trade-off criteria. Every tested optimization method provided good calibration results. The best results for soluble COD objective function were obtained by calibration with the hybrid optimization method but for nitrogen fractions and for the overall optimization function the best model fit was obtained by calibration with the Pareto multiobjective optimization method.

The WWTP data on compositions measured and averaged at every 10 minutes were compared with the values predicted by the dynamic simulation. Despite the process complexity, simulation results also reveal a fairly good dynamic behaviour and performance of the calibrated model, demonstrating the efficiency of the proposed calibration method and the optimization algorithms tested.

Nomenclature

A2O-Anaerobic-Anoxic-Oxic
ASM1-Activated Sludge Model No. 1
b_A-Autotrophic decay rate 1/day
b_H-Heterotrophic decay rate 1/day
BSM1-Benchmark Simulation Model No. 1
COD-Chemical Oxygen Demand g COD/m^3
COD_S-Soluble Chemical Oxygen Demand g COD/m^3
COD_{sol}-Soluble Chemical Oxygen Demand g COD/m^3
COD_{tot}-Total Chemical Oxygen Demand g COD/m^3
COD_X-Particulate Chemical Oxygen Demand g COD/m^3
DO-Dissolved Oxygen g O_2/m^3
f_{ns}-Non-settleable parameter
IAWQ-International Association on Water Quality
LB-Lower bound of the constrained optimization problem
NH-Free and saline ammonia g N/m^3
NO-Nitrate and nitrite nitrogen g N/m^3
N_{org}-Organic nitrogen g N/m^3
N_{tot}-Total nitrogen g N/m^3
$objfunc_{total}$-Total objective function
$objfunc_{CODsol}$-Objective function of soluble COD
$objfunc_N$ -Objective function of nitrogen fractions
$objfunc_{NH}$-Objective function of free and saline ammonia
$objfunc_{NO}$-Objective function of nitrates and nitrites
$objfunc_{Norg}$-Objective function of organic nitrogen
$objfunc_{TSS}$-Objective function of total suspended solids
PI-Proportional-Integral
Q-Flow rate m^3/day
Q_{air}-Flow rate of the air entering the aerated tanks m^3/day
$Q_{nitrate\ recycle}$-Flow rate of the nitrate recycle m^3/day
Q_{RAS}-Flow rate of the return activated sludge m^3/day
Q_{waste}-Flow rate of the wasted sludge m^3/day
RAS-Return activated sludge
r_h-Hindered zone settling parameter m^3/(g SS)
r_p-Flocculent zone settling parameter m^3/(g SS)
S_I-Soluble non-biodegradable material g COD/m^3
S_{ND}-Soluble organic nitrogen g N/m^3
S_{NH}-Free and saline ammonia g N/m^3
S_{NO}-Nitrate and nitrite nitrogen g N/m^3
S_S-Readily biodegradable substrate g COD/m^3
T-Temperature ^oC
TKN-Total Kjeldahl Nitrogen g N/m^3
TSS-Total Suspended Solids g SS/m^3
UB-Upper bound of the constrained optimization problem
WWTP-Wastewater Treatment Plant
x_1-COD soluble influent fraction g COD/m^3
x_2-Particulate inert influent organic matter g COD/m^3
x_3-Heterotrophic decay rate 1/day
x_4-Autotrophic decay rate 1/day
x_5-Hindered zone settling parameter m^3/(g SS)
x_6-Flocculent zone settling parameter m^3/(g SS)
x_7-Non-settleable parameter –
X_{BH}-Heterotrophic biomass g COD/m^3
X_{BA}-Autotrophic biomass g COD/m^3
X_I-Particulate non-biodegradable material g COD/m^3
X_{ND}-Particulate organic nitrogen g N/m^3
X_P-Organic particulate products from the biomass decay g COD/m^3
X_S-Slowly biodegradable substrate g COD/m^3

Subscripts

Inf-Influent
Eff-Effluent
WWTP-Measured data at the investigated wastewater treatment plant
Model-Simulated data with the developed model

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