Modeling and calibration of a full-scale wastewater treatment plant using GPS-X model (A case study of Tehran)

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Abstract:

Wastewater treatment plants (WWTPs) play a significant role in sustainability due to integration of resource recovery and health management during clean water production. Mathematical modeling has become a vital tool for sustainable wastewater management, especially for simulating complex procedures involved in activated sludge processes. Wastewater process modeling provides more options for upgrades and improvements of operational controls. In this paper, a systematic approach was undertaken to create a plant-wide model for a full-scale plant located in Tehran, Iran, namely the Southern Tehran WWTP, using GPS-X software. The characterization of the influent composition to satisfy the mass balance is the most critical step of modeling, which can have significant influence on simulation accuracy. Therefore, the influent wastewater was initially characterized and carefully analyzed carefully. Then, the model has been calibrated followed by model validation using the collected data. For calibration of the model, the sensitivity of various stoichiometric and kinetic parameters in the GPS-X was analyzed and screened. In this regard, the average absolute relative error was employed to show the agreement between the simulated and measured values. Finally, the calibrated model was validated using the actual input and output data. The results indicate that the model's accuracy was acceptable, and therefore the developed model can be applied for future studies.

1. Introduction

Due to urbanization and industrial development, the amount of wastewater entering treatment facilities has increased. Wastewater contains elements toxic to human beings and the ecosystem. Therefore, discharging untreated wastewater into natural water bodies leads to severe sustainability problems such as threatening life on land or in water and increasing treatment cost of the polluted water [1-3]. On the other hand, water scarcity, defined as a structural, persistent reduction in water availability, is one of the main problems societies face in the 21st century.

Water scarcity problems have increased in many regions since the 70s, and they likely continue over this century

due to the increasing human population, accelerated economic activity, and land-use changes [4].

Thus, water scarcity, along with water quality deterioration problems, have become two of the most critical threats for the sustainability of aquatic ecosystems in (semi-) arid areas and in other regions with excessive water abstraction [5-7].

In this regard, recycling and reuse of treated wastewater offers a strategy to prevent the entry of pollutants into the environment and decrease the water crisis from a circular economy perspective. Wastewater treatment plants (WWTPs) can be an important part of sustainability due to the integration of water resource recovery and ecosystem and human health issues.

Various treatment processes are used to treat wastewater in WWTPs. Conventional wastewater treatment consists of

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physical and biological processes to remove solids, organic matter, and nutrients from wastewater.

Biological processes are critical treatment methods for treating wastewater due to their eco-friendly and cost-effective properties. Among the different types of biological wastewater treatment technologies, the activated sludge process is the most widely used method as it removes organic matter and nutrients from the wastewater [2, 8]. However, biological processes are highly complex due to their nonlinear dynamics and uncertainty. The treatment efficiency is notably sensitive to many factors such as temperature, wastewater characteristics, and operating conditions [9]. Mathematical modeling of a wastewater treatment plant is an excellent tool for the simulation ofsimulating biological treatment processes in full-scale WWTPs [10].

Presently, there has been a strong demand for the application of mathematical models for the simulation of wastewater treatment processes in full-scale WWTPs [10]. By using computer simulation and advanced programs, it is possible to create a mathematical model of a real WWTP, run a simulation and subsequently interpret results under various conditions without interfering in the actual process performance [11]. Regardless of the process complexity, plant-wide modeling of WWTPs can be used as a base for future applications, optimization studies, or for developing a process for achieving the highest effluent quality levels and energy savings [12]. Furthermore, through careful calibration, modeling can optimize treatment processes and reduce the operating costs of wastewater treatment plants [13-14].

Many specialized simulator software solutions such as BioWin (EnviroSim Associates Ltd., Canada), STOAT® (WRc, Wiltshire, England), GPS-X® (Hydromantis Inc., Hamilton, ON), and WEST® (Mostforwater, Belgium) were developed for activated sludge modeling [15]. Among them, GPS-X is a robust tool for plant-wide modeling. The GPS-X model has recently been received significant attention due to its wide variety of pre-compiled treatment technologies, ease of use, and easily accessible training materials [16–17].

Simulation of wastewater treatment process comprises two steps of calibration and validation. Model calibration is necessary to adjust the value of various parameters to fit the targets and enhance simulation accuracy [18-19]. The widely used method for model calibration is carried out using practical operation data, fine-tuning the values of sensitive parameters until the simulation values are in agreement with the measured values [20].

In this study, the GPS-X software was applied to simulate a full-scale WWTP located in the south of Tehran, Iran, which is one of the largest plants in the Middle East. The main objective is to demonstrate a systematic approach to simulate and calibrate an actual biological wastewater treatment system. To the best of our knowledge, modeling an actual integrated activated sludge and nitrifying trickling filter process with an approximately long wastewater transfer line, resulting in changes in influent raw wastewater, is rare. In this regard, the characterization of the influent wastewater was carefully analyzed. In addition, the sensitivity of the stoichiometric and kinetic parameters in the GPS-X simulation was analyzed, screened, and validated based on the actual input and output data.

2. Materials and Methods

2.1 Description of the full-scale wastewater treatment plant

In this study, a full-scale WWTP located in Tehran Province, Iran, was simulated. The city of Tehran is one of the most populous cities in the world. According to Tehran's demand for water for various uses, refined wastewater has been used in the irrigation of green spaces and to fill the groundwater, especially in areas where the level has decreased [21].

The Southern Tehran Wastewater Treatment Plant (STWWTP), located south of Shahr-e-Rey, is planned to treat part of Tehran's municipal wastewater in 8 modules with a total capacity of 4,200,000,000 people. The first phase of this plant (modules 1-4) employs the completely mixed activated sludge process (CMAS) with an average design capacity of 450,000 cubic meters per day [22].

After passing the screening and grit chamber units, the input wastewater is divided into the four primary sedimentation tanks. These tanks have been designed as rectangular tanks with a sludge funnel at the feeding side of the tanks. Then, the wastewater enters into four biological tanks, including selector and aeration tanks. The total net volume of each biological tank is about 21920 cubic meters. The activated sludge reactors are followed by eight rectangular secondary sedimentation tanks. These tanks have been designed as cross-flow tanks with bottom feed and sludge draw-off by suction scrapers. Trickling filters are also employed for nitrification of ammonia contained in the recirculated part of the activated sludge stage effluent. Finally, after passing the disinfection units (chlorination), the effluent treated wastewater will be transferred to the Varamin channels to irrigate the Varamin plain. The general layout and process flow diagram of the plant, which was created in the GPS-X software, are shown in Fig. 1.
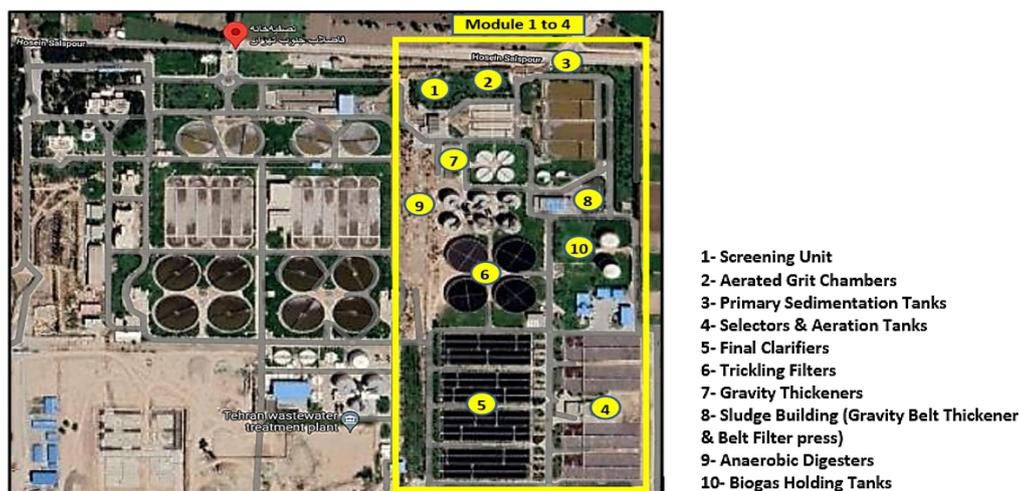
(a)
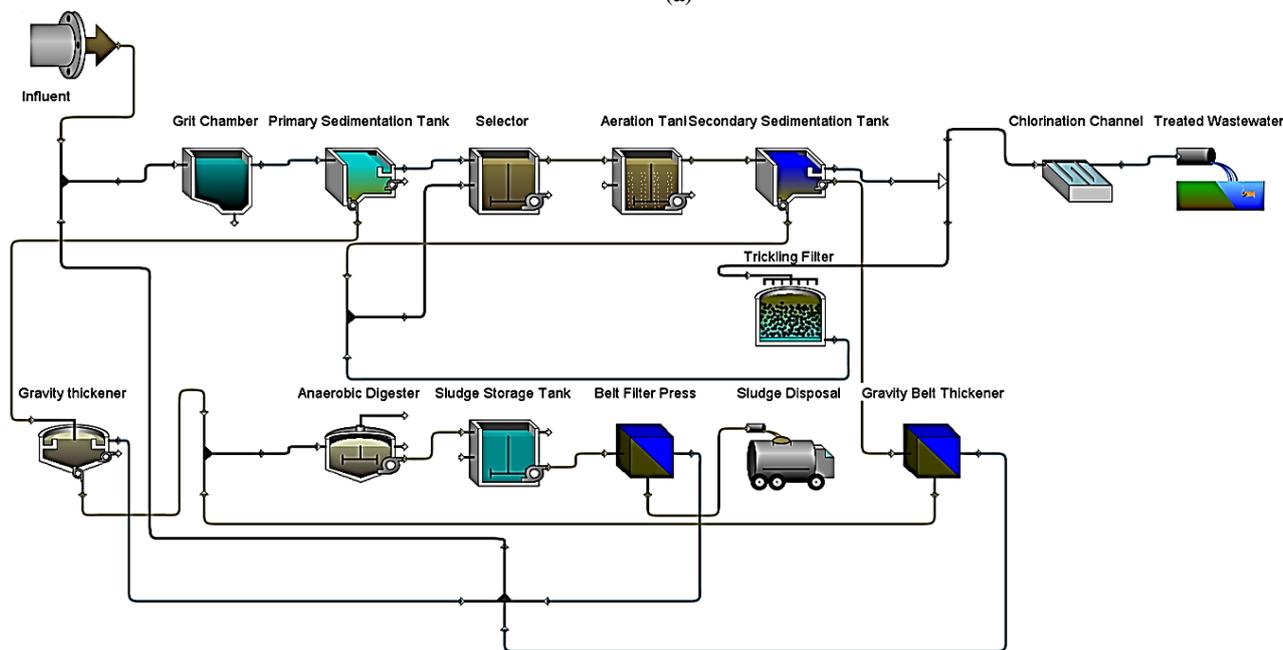
(b)

Fig. 1: (a) Geographic location, general layout, and (b) process flow diagram of the main processing units in STWWTP

2.2 Process Data

The input data for the simulation came from the STWWTP and comprised the period of three months from May to July. The data from 1st May to 30th June was used for the model calibration, and data of July from the following year was implemented for the validation step. The values of wastewater characteristics and operating parameters used for model calibration and validation are presented in Tables 1 and 2, respectively. Generally, the removal rates of the Biochemical Oxygen Demand (BOD), Chemical Oxygen Demand (COD), Total Suspended Solids (TSS), and Total Nitrogen (TN) during the calibration step were 97.8 ± 0.8%, 95.1 ± 1.2%, 93.2 ± 0.3% and 62.6 ± 2.2%, respectively.

2.3 GPS-X Model

The GPS-X software version 8.0.1 (education license) developed by the modeling software company Hydromantis was used in the present work. It is a widely used comprehensive standalone model built with integrated biological wastewater treatment processes and many others involving physical and chemical reactions. In this study, the model was designed in a carbon, nitrogen, and custom components library (cniplib) in the GPS-X software under the MANTIS and simple1d clarifier model.

With model constraints as per activated sludge model ASM1 [23], the assumptions adopted for developing the model in this research were as follows:

- The biological process operates at a content temperature.
- pH is steady and near-neutral value.

Table. 1: Characteristics of influent & effluent wastewater

Parameter	Unit	Values			
		During the period of the calibration step: from May to June		During the period of the validation step: July	
		Raw wastewater	Treated Effluent	Raw wastewater	Treated Effluent
Wastewater Flow rate	m3/d	429980 ± 18975	418090 ± 7623	434659 ± 34475	400516 ± 25272
Temperature	ºC	25.3 ± 2.6	26.4 ± 1.9	28.0 ± 0.3	29.0 ± 0.5
BOD5	mg/L	256.5 ± 26.9	5.7 ± 1.4	246.8 ± 27.3	5.4 ± 1.0
COD	mg/L	453.5 ± 39.1	22.3 ± 5.7	427.7 ± 56.3	23.6 ± 5.3
TSS	mg/L	168.2 ± 32.6	11.1 ± 3.6	139.9 ± 28.2	9.5 ± 2.2
VSS to TSS ratio	-	0.33 ± 0.05	N.A.	0.30 ± 0.07	N.A.
TN	mg/L	45.5 ± 4.4	16.8 ± 1.9	44.1 ± 5.5	15.1 ± 1.6
NH4-N	mg/L	37.1 ± 3.9	6.9 ± 2.7	36.4 ± 3.2	5.1 ± 2.3
TP	mg/L	6.3 ± 0.5	N.A.	6.3 ± 0.4	N.A.

N.A. = Not Available

Table. 2: Main Operational Data

| Parameter	Unit	Values	
		During the period of the calibration step: from May to June	During the period of the validation step: July
Return Sludge	m3/d	545043 ± 46145	515036 ± 52534
Excess Sludge	m3/d	10220 ± 1124	11425 ± 385
SVI of sludge in Aeration Tanks	g/L	102.5 ± 10.9	99.4 ± 6.6
DO in Aeration Tanks	mg/L	0.85 ± 0.32	0.76 ± 0.38

- There is sufficient mixing within the biological reactors.
- The model's coefficients are assumed to be constants for any influent characteristics.
- There are enough inorganic nutrients to ensure the sufficient growth of microorganisms.
- There is simultaneous hydrolysis of organic and nitrogenous compounds.

2.4 GPS-X Modeling Approach

Plant-wide modeling was undertaken via simulation in the GPS-X software using the following steps as shown in Fig. 2.

- Step 1: Collection of daily data required for the GPS-X modeling.
- Step 2: Portraying the existing plant in terms of physical and operational data of the process units.
- Step 3: Characterization of the influent wastewater quality parameters (inserting the values of available data, i.e., COD, NO2− & NO3−, free and ionized ammonia, TKN, and VSS/TSS ratio) and adjusting the influent fractionations using the GPS-X influent advisor to an acceptable state and composite variables mass balance.
- Step 4: Running the Model
- Step 5: a preliminary sensitivity analysis was carried out, selecting the different subsets of parameters in order to reduce the number of model parameters to be calibrated.
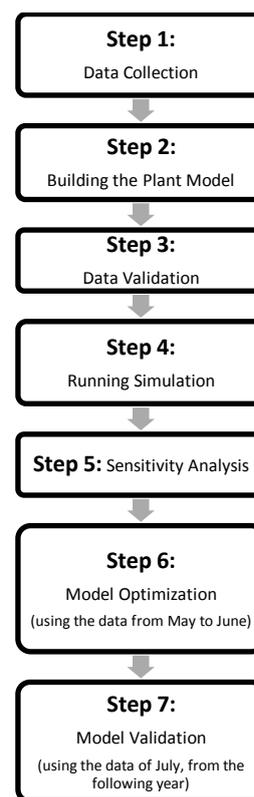
Fig. 2: GPS-X Modeling Approach

- Step 6: Time series-type optimization of the model via adjusting kinetic, stoichiometric, and other relevant parameters to fit the model to obtain the best matching between the predicted and measured values of target provided in the data file (effluent quality data including COD, BOD, TSS, and TN).

The model was fitted to the measured data using the "Maximum Likelihood" objective function.

- Step 7: The fits of measured and simulated data were evaluated quantitatively via plotting a graph of simulated versus measured data points and the absolute relative error (ARE).

2.5 Sensitivity Analysis

In this work, a preliminary sensitivity analysis was carried out to measure how the parameters used in the model calibration (kinetic or stoichiometric parameters) could influence the output variables (BOD, COD, TSS, and TN of effluent). This analysis is helpful because it mainly improves the model's prediction and reduces the number of model parameters to be calibrated. According to EPA guidelines [24], the normalized sensitivity coefficient ($S_{i,j}$) is defined as a ratio of the percentage change in the output variable (y_i) to a 10% change in the input variable (x_i):

$$S_{i,j} = \left| \frac{\Delta y_i / y_i}{\Delta x_i / x_i} \right| \qquad (1)$$

The influence of a parameter on the model output can be interpreted as follows: (1) $S_{i,j} < 0.25$ indicates that a parameter has no significant influence on the model output; (2) $0.25 < S_{i,j} < 1$ means that a parameter is influential; (3) $1 < S_{i,j} < 2$ means that a parameter is very influential; (4) $S_{i,j} > 2$ means that a parameter is extremely influential [25]. The mean square sensitivity measure (δ_j^{msqr}) is also used for sensitivity analysis measure, introduced by Brun et al. [26]. This sensitivity measure is designed to assess the individual parameter importance in a least-squares parameter estimation context and is defined as:

$$\delta_j^{msqr} = \sqrt{\frac{1}{n} \sum_{i=1}^{n} S_{i,j}^2} \qquad (2)$$

A high value of δ_j^{msqr} indicates that a parameter has an important influence on the simulation results. In contrast, the value of zero means that the simulation results do not depend on a parameter.

2.6 Model Calibration and Validation

The stoichiometric and kinetic parameters were revised for calibration of the model. The model was calibrated and then validated using the data acquired for a whole year, from May to June (60 days) and the first 25 days of July from the following year, respectively. The average absolute relative error (ARE) was also employed to show the agreement between the simulated and measured values. The following equation was employed to estimate the ARE [27].

$$ARE = \frac{1}{N} \sum_{i=1}^{N} \frac{|m_i - p_i|}{m_i} \times 100\% \qquad (3)$$

where, m_i denotes the measured values of the output variable, p_i denotes the simulated values of the output variable, and N is the number of samples.

3. Results and Discussion

3.1 Wastewater Characterization

The characterization of the influent wastewater is considered the most critical step of the modeling and needed careful analysis. Since the data available from the laboratory mainly concerned the total COD, total TKN, and total phosphorus, the model chosen for influent characterization was the "codstates." Using the "codstates" model, most state variables were calculated as fractions of the total COD. In this regard, the GPS-X already has default values for the COD fractions; but these default values were revised to achieve better calibration of the model. The main fractions of influent raw wastewater are listed in Table 3.

Table. 3: Main fractions of the influent wastewater

Parameter	Symbol	Unit	Default value	Calibrated value
Influent Fractions				
XCOD/VSS ratio	icv	gCOD/ gVSS	1.8 (raw) 1.8 (primary)	4.5
BOD5/BODultimate ratio	fbod	-	0.66 (raw) 0.75 (primary)	0.75
Organic Fractions				
Soluble inert fraction of the total COD	frsi	-	0.05 (raw) 0.08 (primary)	0.025
Readily biodegradable fraction of the total COD	frss	-	0.2 (raw) 0.32 (primary)	0.4
Particulate inert fraction of total the COD	frxi	-	0.13 (raw) 0.12 (primary)	0.10

Because of the long wastewater transfer line to STWWTP, there is enough time to convert the particulate material of

raw wastewater to soluble compounds through hydrolysis by various facultative and obligate anaerobes to provide a

source of the readily biodegradable soluble COD. Therefore, the default value of the readily biodegradable fraction of the total COD (frss) was increased to 0.4, as shown in Table 3. Consequently, the soluble COD (sCOD), which is a sum of the soluble inert fraction of the total COD (frsi) and the readily biodegradable fraction of the total COD (frss), was increased. The COD fractions of the influent wastewater that vary between different samples could cause significant influence on the simulation accuracy [28].

The influent TSS is a composite variable that mainly depends on the XCOD/VSS ratio (icv). This ratio was iteratively manipulated to obtain the actual TSS values, while the average value of the VSS/TSS ratio from the laboratory analyses was 0.33 during the studied period. As a result, the XCOD/VSS ratio was set as 4.5. In addition, the ratio of $BOD5/BOD_{ultimate}$ was also iteratively changed and finally was set as 0.75 for obtaining the actual influent BOD values.

3.2 Sensitivity Analysis

Sensitivity analysis enables the evaluation of the extent to which the parameters used in the model calibration can influence the model outputs. A parameter with high sensitivity is the one for which a slight variation in its value causes a considerable variation in the response predicted by the model. Analogously, a parameter with low sensitivity is the one that may be varied over a relatively wide range inducing only a relatively small variation in the predicted response [29].

In this study, the more sensitive kinetic and stoichiometric parameters in activated sludge models' calibration, as reported by several authors, were subjected to sensitivity analysis, including the heterotrophic yield coefficient (Y_H), the autotrophic yield coefficient (Y_A), the heterotrophic maximum specific growth rate ($\mu_{max,H}$), the heterotrophic decay rate (b_H), the autotrophic decay rate (b_A), the autotrophic maximum specific growth rate ($\mu_{max,A}$), the readily biodegradable substrate half-saturation coefficient ($K_{S,rbCOD}$), the ammonia half-saturation coefficient ($K_{HS,NH4}$), and the oxygen half-saturation coefficient ($K_{S,O}$) [29-31]. The values of the normalized sensitivity coefficient ($S_{i,j}$) with regard to the four mentioned output variables, if $S_{i,j}$ is higher than 0.1, are presented in Table 4. Results indicate that the values of $S_{i,j}$ were always below 0.25 (even lower than 0.1) for the kinetic and stoichiometric parameters of the active autotrophic biomass. Therefore, they were excluded from the optimization step. Among the studied parameters for the heterotrophic biomass, three of them (Y_H, b_H and $\mu_{max,H}$) can be classified as influential according to the classification proposed by Petersen et al. [25].

As similarly reported by several other researchers [29, 31-32], Y_H was the most influential parameter on the simulation results of TN. The higher heterotrophic yield would result in more nitrogen consumption for biomass synthesis and thus result in high removal efficiency of TN in wastewater [32]. Liwarska-Bizukojc & Biernacki [29] also emphasized the influential role of Y_H on the effluent BOD.

Table. 4: Sensitivity coefficients of model targets for the kinetic and stoichiometric parameters

Parameters	Unit	$S_{i,j}$			
		COD	BOD	TSS	TN
Active Heterotrophic Biomass					
Kinetic parameters					
$\mu_{max,H}$	1/d	-	0.25	-	-
$K_{S,rbCOD}$	mg COD/L	-	0.17	-	-
$K_{S.NH4}$	mg N/L	-	-	-	-
b_H	1/d	-	0.15	0.13	0.40
Stoichiometric parameters					
Y_H	g COD/g COD	0.41	0.69	0.32	1.95
Active Autotrophic Biomass					
Kinetic parameters					
μ_{maxA}	1/d	-	-	-	-
$K_{S,O}$	mg O2/L	-	-	-	-
b_A	1/d	-	-	-	-
Stoichiometric parameters					
Y_A	g COD/g N	-	-	-	-

In addition, results indicated that only Y_H with $\delta_j^{msqr} = 1.02$ had an important influence on the simulation results. The values of δ_j^{msqr} for other parameters were extremely low (0.22 for b_H and 0.13 for $\mu_{max,H}$) or near zero, which indicates that the simulation results did not depend on them.

3.3 Calibration and Validation of the Model

Simulation of the wastewater treatment process was done in two steps: model calibration followed by model validation. Based on the sensitivity analysis and also the revised components' fractions in influent wastewater (i.e., frss, frsi, frxi, icv, and fbod), the subsequent model simulation and calibration was performed for the first 60 days of time-series-data (from 1st May to 30th June). The default values for stoichiometric and kinetic parameters in GPS-X were firstly used to simulate the operation of STWWTP. However, the simulated data was relatively different from the measured data in the full-scale WWTP. Due to the discrepancies between the measured and simulated values, when the default parameters were used, calibration of the model parameters occurred to be necessary [29]. Therefore, the parameter optimization of the model was considered to estimate the kinetic and stoichiometric parameters to fit a specific set of treated wastewater quality data obtained from the experiment.

The model calibration and validation results are depicted in Fig. 3, which shows the measured and simulated values of BOD, COD, TSS, and TN in the effluent after model calibration with the selected parameters in the sensitivity analysis and also during the validation step.

ARE was employed to show the agreement between the simulated and measured values. Due to the high complexity of the process, ARE for the simulated and measured values of 7-15% is sufficient for indication of correct dynamic calibration [27].

As shown in Fig. 3, the base case scenario with the default values for kinetic and stoichiometric parameters indicated that the model results fit relatively well with the measured values, with ARE of 17.11%, 19%, 17.53%, 12.67% for BOD, COD, TSS, and TN, respectively. Indeed, there are some discrepancies between the model results and the measured values. In this regard, model calibration was conducted by automatic calibration using the optimizer in GPS-X to find the best set of parameter values to fit the prediction to the measured data.

As mentioned above, among the kinetic and stoichiometric parameters studied, three of them, namely the heterotrophic maximum specific growth rate ($\mu_{max,H}$), heterotrophic decay rate (b_H), and heterotrophic yield (Y_H) were considered to be more sensitive and selected for the process optimization.

By adjusting the critical kinetic and stoichiometric parameters ($\mu_{max,H}$, b_H, and Y_H) as presented in Table 5, the simulated values of COD, BOD, TSS, and TN in the treated effluents were calibrated.

After the calibration process, ARE for BOD, COD, TSS and TN were slightly decreased to 14.19%, 15.03%, 12.53%, and 12.53%. These results indicated the appropriateness and effectiveness of the parameter adjustment done to make the simulated values in line with the measured ones.
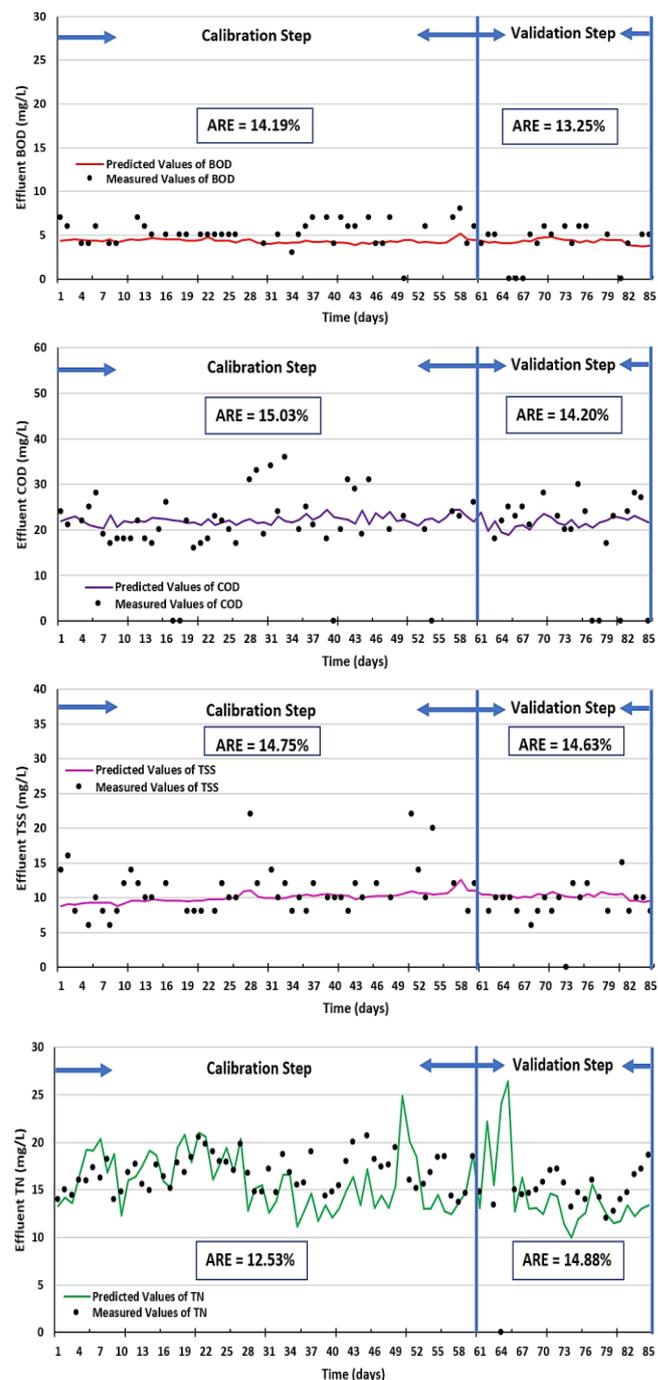

Fig. 3: Measured vs. simulated values of BOD, COD, TSS, and TN in the effluent after model calibration and also during the validation step

Table. 5: List of the kinetic/stoichiometric parameters in Mantis2 adjusted during model calibration in the GPS-x simulator

Parameter	Symbol	Unit	Default value	Calibrated value	Range in literature	
					value	reference
Kinetic Parameters						
Heterotrophic maximum specific growth rate	$\mu_{max,H}$	1/d	3.2	3.85	1-8	[33]
Heterotrophic decay rate	b_H	1/d	0.62	0.57	0.05-1.6	[34]
Stochiometric Parameters						
heterotrophic yield	Y_H	g COD/g COD	0.666	0.635	0.4–0.8	[35]

As a result (shown in Table 5), the heterotrophic maximum specific growth rate was elevated to 3.85 1/d, higher than the default value of 3.2 1/d.

One of the main reasons is that the actual operating temperature of the experiment (25.3 ± 2.6 ℃) was higher than the default value of the model (20℃), which was closer to the optimum temperature for microorganisms.

The heterotrophic yield (Y_H), which expressed the affinity of the heterotrophic biomass to the carbonaceous substrate, was set to 0.635 g COD/g COD which is slightly lower than the default value of 0.666 g COD/g COD. This finding shows that the affinity of biomass to the carbonaceous substrate was slightly lower than the same affinity for the typical municipal wastewater, as similarly observed in three of WWTPs located in the FVG region of Italy [19]. As shown, the majority of the kinetic and stoichiometric parameters of the model were employed without any changes.

Model validation was the next step. The model is considered to be validated when model predictions agree with measured values from an independent dataset within the acceptable tolerances [36]. The GPS-X software with the calibrated parameters was applied to calculate the effluent concentrations according to the quality data collected during July.

The model validation results, depicted in Fig. 3, indicate that the calibration was performed correctly, and the calibrated model can be regarded as valid. For validation data, ARE for BOD, COD, TSS, and TN were obtained 13.25%, 14.20%, 14.63%, and 14.88%, respectively.

4. Conclusion

In this study, the GPS-X software was satisfactorily applied for plant-wide modeling of the largest WWTP in Iran, namely the Southern Tehran WWTP. Some modifications were introduced to the default values of model parameters, including the influent wastewater characterization and kinetic and stoichiometric parameters.

It was found that the COD fractions of the influent wastewater, including the readily biodegradable fraction of the total COD (frss) and the soluble COD (sCOD), could have significant influence on the simulation accuracy. Because of the long wastewater transfer line to STWWTP, there is enough time to convert the particulate material of raw wastewater to soluble compounds through hydrolysis, which increases the frss and sCOD of the raw wastewater entering the WWTP.

With the help of sensitivity analysis approach, it was found that the heterotrophic maximum specific growth rate ($\mu_{max,H}$), heterotrophic decay rate (b_H), and heterotrophic yield (Y_H) were the most influential kinetic and stoichiometric parameters. The heterotrophic yield was the most influential parameter on the simulation results of TN since the higher heterotrophic yield would result in more nitrogen consumption for biomass synthesis. The heterotrophic maximum specific growth rate was increased to 3.85 1/d, which was due to the higher operating temperature of the wastewater (25.3 ± 2.6 ℃) compared to the default value of the model. The kinetic and stoichiometric parameters of the active autotrophic biomass had no significant influence on the model output, and subsequently, they were excluded from the optimization step.

ARE was used to measure the agreement between the measured and predicted data. This index indicated that the GPS-X results fit reasonably well with the measured values with an overall ARE of less than 15%. Furthermore, the results showed that the developed model could accurately predict changes in BOD, COD, TSS, and TN with ARE values in the range of 12-15% during both calibration and validation steps. Therefore, this case study can be used as a guide for future applications and optimization studies.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships influence that could have appeared in the work reported in this paper.

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