DEVELOPMENT AND CALIBRATION OF A CONCEPTUAL ACTIVATED SLUDGE BASED MBR MODEL FOR WASTEWATER TREATMENT

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ABSTRACT

The paper presents a conceptual activated sludge based MBR model for wastewater treatment. The model uses influent COD and operating conditions of MBR as input, and the model simulates the concentration of mixed liquor suspended solids and the effluent COD. Calibration of model parameters is performed by a global optimization method using the experimental data obtained from running a lab-scale MBR system treating primary effluent of a local wastewater treatment plant for 220 days. Results show that the simulation by the conceptual model has good agreement with the observed data using the optimized parameters, and analysis of residuals demonstrates patterns of normal distribution. The model assisted analysis of operating conditions helps to facilitate the optimization of MBR performance in wastewater treatment.

1. INTRODUCTION

Membrane bioreactor (MBR) process is gaining more and more attention in wastewater treatment because of its benefits such as supreme effluent quality and small footprint. Currently, mathematical models based on activated sludge model no. 1 (ASM1) are typically used as tools to simulate the response of MBR system. These models, describe every aspect of activated sludge and membrane process characteristics, however, are composed of numerous stoichiometric and kinetic parameters that need to be adjusted for different system environment, which make the calibration process computationally complicated and intractable unless those parameters are pre-defined in the models to reduce the complexity of variety. This generates new problems, however, when the pre-defined parameter values, which are usually obtained from published literatures, are used in the modeling process. Typical problems associated with parameter pre-assignment are the following: (1) the model does not fit the observed results well, and (2) the deterministic choices of parameters make the model calibration impossible. Reasons that may lead to the problems are the following: (1) the parameter values of MBR vary from one system to another due to differences of experimental conditions in published literatures and (2) cross influences of parameters in the system. The uncertainty of parameter values makes the pre-defined parameter values difficult to represent the real conditions of the to-be-modeled MBR. Therefore, a different approach for parameter adjustment is needed to enhance the frontier of MBR modeling study.

The objective of this study is to develop a conceptual MBR model by simplifying the theory of ASM1 and focusing on the COD removal. The model is developed by including eleven stoichiometric and kinetic parameters, which are biomass yield (Y), maximum substrate utilization rate ($\hat{q}$), half-saturation substrate concentration (K_S), biomass decay coefficient (b), inert fraction of biomass leading to soluble microbial products (f_d), maximum UAP utilization rate ($\hat{q}_{UAP}$), half-saturation UAP concentration (K_{UAP}), UAP formation coefficient (k_1), maximum BAP utilization rate ($\hat{q}_{BAP}$), half-saturation BAP concentration (K_{BAP}) and BAP formation coefficient (k_2). Two operating parameters hydraulic retention time (HRT) and solids retention time (SRT) together with influent COD are the model input. The model output is the effluent COD and the concentration of mixed liquor suspended solids (MLSS) in MBR. The stoichiometric and kinetic parameters used in the conceptual model are calibrated values based on the observed performance of a to-be-modeled lab-scale MBR system. Optimization of parameters is performed by Shuffled Complex Evolution (SCE-UA), a global optimization method. The conceptual model using optimized parameters is used to analyze the influences of operating conditions on the model output.

2. MODEL DEVELOPMENT

2.1. The To-be-modeled MBR System

A hollow fiber membrane bioreactor system is used in the modeling process. Schematic diagram of the MBR is shown in Fig. 1. The MBR has one membrane module, which theoretically retains all of the biomass in the reactor. The influent and effluent flow rates are the same to maintain a constant working volume. Biomass in the MBR is activated sludge from an aeration tank of a local wastewater treatment plant. Withdrawn of solids is regularly performed when measuring the MLSS concentration in the MBR.

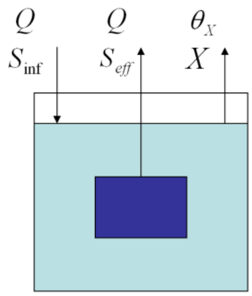

Fig.1: Schematic diagram of a conceptual MBR model

2.2. Data Acquisition

A lab-scale MBR was operated for 220 days in the Kappe Environmental Engineering Laboratory at University Park Wastewater Treatment Plant, State College, Pennsylvania, USA. The MBR had a working volume of 1.8 L and was fully aerated during the experiment. The membrane module had a pore size of 0.4 µm and a surface area of 0.03 m^2. Primary effluent from the treatment plant was used to feed the MBR, and a peristaltic pump was operated in an 8 minutes on and 2 minutes off manner to withdraw effluent from the system. The operation data of sampling time (t), flow rate (Q), influent COD (S_{inf}), MLSS (X) in the MBR, solids withdrawn frequency (Δt) and effluent COD (S_{eff}) was routinely monitored.

2.3. Modeling Approach

Numerous modeling approaches have been presented in literatures. A framework for modeling this MBR consists of the following steps as shown in Fig. 2.

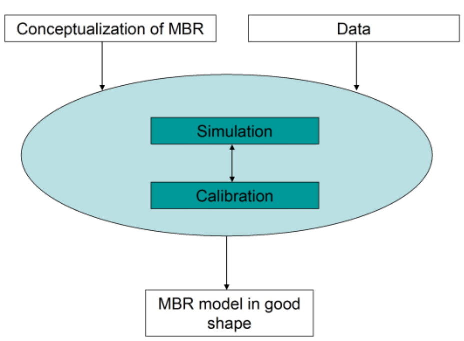

Fig. 2: Framework for the development of the MBR model

The conceptualization of the MBR system is performed by focusing on COD removal based on ASM1. Each variable parameter is pre-assigned a value from literatures to start the simulation. Then the simulated data are compared with the observed data. If the simulation performance does not meet certain criteria, values of variable parameters are adjusted. After each calibration of variable parameters, the model is evaluated again to examine whether the simulation performance is improved. Simulation and calibration are repeatedly performed until the simulation performance is the best. Then the model is considered to be in good shape to get the closest response of MBR. Table 1 gives a list of description for input, output, state and variable parameters for the model. The observation data of Q and S_{inf} is given as the input for the model while X and S_{eff} is the model output. HRT (θ) and SRT (θ_X) are operating parameters. $X_{act,0}$, $X_{int,0}$, S_0, UAP_0, BAP_0 are initial states, and Y, $\hat{q}$, K_S, b, f_d, $\hat{q}_{UAP}$, K_{UAP}, k_1, $\hat{q}_{BAP}$, K_{BAP} and k_2, are variable parameters.

Table 1: Description of parameters for the conceptual MBR model

Parameter	Symbol	Description	Unit	Range
Input	S_{inf}	Influent substrate concentration	mgCOD/L	Observation
	Q	Flow rate	L/day	Observation
	t	Days of operation	day	Observation
Output	S_{eff}	Effluent substrate concentration	mgCOD/L	Simulation
	X	Mixed liquor suspended solids concentration	mgSS/L	Simulation
Operational	θ	Hydraulic retention time	day	Observation
	θ_X	Solids retention time	day	Observation
	Δt	Solids withdrawn frequency	day	Observation
InState	$X_{act,0}$	Initial concentration of active biomass	mgSS/L	Observation
	$X_{int,0}$	Initial concentration of inert biomass	mgSS/L	0
	S_0	Initial concentration of effluent substrate	mgCOD/L	0
	UAP_0	Initial concentration of effluent UAP	mgCOD/L	0
	BAP_0	Initial concentration of effluent BAP	mgCOD/L	0
Variable	Y	Yield	mgSS/mgCOD	0 - 1
	$\hat{q}$	Maximum specific rate of substrate utilization	mgCOD/mgSS.d	1 - 10
	K_S	Half-saturation substrate concentration	mgCOD/L	10 - 100
	b	Biomass decay rate	day-1	0 - 1
	f_d	Inert fraction of biomass leading to SMP	Unitless	0 - 1
	$\hat{q}_{UAP}$	Maximum specific rate of UAP utilization	mgCOD/mgSS.d	0 -10
	K_{UAP}	Half-saturation UAP concentration	mgCOD/L	10 - 200
	k_1	UAP formation coefficient	Unitless	0 - 1
	$\hat{q}_{BAP}$	Maximum specific rate of BAP utilization	mgCOD/mgSS.d	0 -10
	BAP_0	Half-saturation BAP concentration	mgCOD/L	10 - 200
	k_2	BAP formation coefficient	Unitless	0 - 1

2.4. Computational Algorithm

The algorithm used in the model development is shown from Eq. 1 - 10. Different from an activated sludge based chemostat with no solid recycle that does not separate HRT and SRT, the MBR system obviously has different values for the two parameters because the membrane module achieves fully retention of biomass. HRT (θ) is an operating parameter that depends on the flow rate (Eq. 1). SRT (θ_X) is also an operating parameter, and its value is determined by how frequently a fixed volume (20 ml in this experiment) of solids is withdrawn from the MBR system (Eq. 2). COD of MBR effluent (S_{eff}) and concentration of MLSS (X) are calculated based on the theory of ASM1 using the input of flow rate (Q) and substrate concentration in the MBR influent (S_{inf}) and the eleven variable parameters, which values are pre-assigned based on available literature and are adjusted according to the simulation performance. Because of the long SRT, the influence of soluble microbial products (SMP) must be considered. SMP is composed of utilization associated products (UAP) and bacteria associated products (BAP). The concentration of MLSS is also composed of two parts: active biomass (X_{act}) and inert biomass (X_{int}). The model needs several initial states to start, and the value of $X_{act,0}$ was measured to be 1040 mg/L in this experiment. It is assumed that all biomass initially transferred from activated sludge were active biomass, and the influent wastewater does not have inert biomass, $X_{int,0}$=0. Other assumptions related with the initial states are: S_0 =0, UAP_0 =0, and BAP_0 =0. Eq. 3 shows the mass balance equations for the soluble substrate concentration. Eq. 4 gives the mass balance equation for the active biomass. The inert biomass (Eq. 5) is linearly related with the active biomass concentration, biomass decay rate and SRT. Eq. 6 and 7 show the mass balance equations for BAP and UAP. MATLAB (The Mathworks, Inc.) is the script language to code the MBR system. The code could be obtained from the authors. Graphical User Interface (GUI) will be developed if another funding source is available.

Eq. 1:

$$\theta = \frac{V}{Q}$$

Eq. 2:

$$\theta_X = \frac{V \times \Delta t}{20}$$

Eq. 3:

$$V\frac{dS}{dt} = QS^0 - QS + \frac{\hat{q}SX_{act}}{K+S}V$$

Eq. 4:

$$V\frac{dX_{act}}{dt} = QX_{inf} - QX_{eff} + Q(S_{inf} - S_{eff)}Y - bX_{act}V$$

Eq. 5:

$$X_{int} = X_{int}^0 + X_{act}(1 - f_d)b\theta_X$$

Eq. 6:

$$X = X_{act} + X_{int}$$

Eq. 7:

$$V\frac{dBAP}{dt} = -k_1X_{act}V - \frac{\hat{q}_{BAP}}{K_{BAP} + BAP}X_{act}V - Q \times BAP$$

Eq. 8:

$$V\frac{dUAP}{dt} = -k_2\frac{S_{inf} - S}{\theta}V - \frac{\hat{q}_{UAP}UAP}{K_{UAP} + UAP}X_{act}V - Q \times BAP$$

Eq. 9:

$$SMP = BAP + UAP$$

Eq. 10:

$$S_{eff} = S + SMP$$

2.5. Model Evaluation

Root Mean Squared Error (RMSE), which is defined in Eq. 11, is used to evaluate the simulation performance of the MBR model. In this study, RMSEs of both effluent COD and concentration of MLSS in MBR are calculated and their values are multiplied by a weight factor to reflect the difference of magnitude and are added together to indicate the direction of simulation effort (Eq. 12).

Eq. 11:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(O_{sim} - O_{obs})^2}{n}}$$

Where
O_{sim} is the simulated system output
O_{sim} is the observed system output
n is the number of data points

Eq. 12:

$$RMSE = 0.01 \times \sqrt{\frac{\sum_{i=1}^{n}(X_{sim} - X_{obs})^2}{n}} + 0.99 \times \sqrt{\frac{\sum_{i=1}^{n}(S_{eff,sim} - S_{eff,obs})^2}{n}}$$

Where
X_{sim} is the simulated MLSS concentration
X_{obs} is the observed MLSS concentration
$S_{eff,sim}$ is the simulated effluent COD
$S_{eff,sim}$ is the observed effluent COD
n is the number of data points

2.6. Parameter Optimization

The Shuffled Complex Evolution (SCE-UA), a global optimization method, is an efficient approach for parameter optimization. The method requires the initial selection of a population of parameter sets in the feasible parameter spaces. The population is then partitioned into several complexes, each containing 2n+1 points, where n is the number of parameters to be calibrated. After repeated evolution and shuffling steps, all the points are converged into a small space, which is defined by the convergence criteria. Readers could refer to the papers written by Dual et al. (1992, 1993, and 1994) to get further detailed explanation of this algorithm. The variable parameters of MBR were optimized using this method. By using the optimized parameters, the model could achieve the lowest value of the objective function, and this would indicate that the simulation performance of the MBR model was the best.

2.7. Model Implementation and Residual Analysis

After implementing the MBR model using the optimized parameters from SCE-UA, the simulated and observed results were visualized to analyze the effectiveness of the model simulations. In addition, the differences between the simulated and observed results were normalized and plotted over time to analyze the residuals. The ranges of normalized residuals between -0.1 and 0.1 were divided into 11 bins of segments, respectively. Points that fell into each bin were counted. Numbers were then normalized by dividing the total number of data points. Discrete and accumulative distributions of the normalized counts were plotted over the ranges of normalized residuals.

2.8. Impact Analysis of Operating Parameters

The model assisted analysis of operating conditions requires influent COD and ranges of HRT and SRT. During the impact analysis, the HRT and SRT were given a range of 0.1 – 3 and 1 – 300 days, respectively while the influent COD was given a fixed value of 300 mg/L. The model responses of effluent COD and MLSS concentration given the provided HRT and SRT values were plotted to visualize their impacts.

3. RESULTS AND DISCUSSION

3.1. Operation and Sample Analysis of the lab-scale MBR

Fig. 3 shows the influent profile during the experiment. The feed for the MBR collected from the primary effluent of a local wastewater treatment plant was placed in a 15 liter tank. Because of the flow rate of the MBR, which was round 2 L/day most of the time as shown in Fig. 3a, the feed usually stayed for one week before the old tank of feed was replaced. Therefore, the influent COD showed great variety due to the biodegradation. Backwash of membrane was performed when a sharp decline of flow rate or a sudden increase of trans-membrane pressure was observed. It has to be noted that new sludge was added to the MBR when the measured concentration of MLSS was too low. Records showed that the sludge had been added for five times during the experiment, and the days when new sludge was added were 13th (500mg), 22nd (500mg), 29th (2000mg), 45th (2000mg), and 116th (1000mg). The MBR effluent was sampled and analyzed after at least one HRT after the sludge addition. The MBR system was temperature-insensitive, because the temperature did not have much variation, and it was supposed to have negligible impact on biomass since the whole system was placed in a temperature controlled room at 25 °C and the influent usually stayed for a long time in the feed tank. COD was analyzed using the HACH kit. High range [0 – 1500 mg/L] COD digestion vials were used for the influent COD analysis while low range [0 – 40 mg/L] COD digestion vials were used for the effluent COD analysis. This could give the confidence level of the experimental results. According to HACH method, the deviation of results for the MBR influent was 16 mg/L while the deviation for the MBR effluent was 2 mg/L. Standard method 2540B was adopted to analyze the MLSS concentration. The 5% deviation of this method, if converted to mg/L based on an average of 2180 mg/L MLSS, gave the error of 109 mg/L. These deviations need to be taken into account when the observed data points were presented.

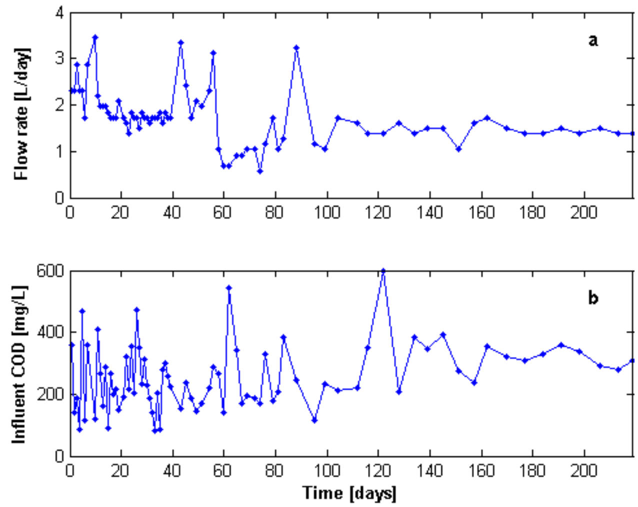

Fig. 3: Data visualization of the influent profile of the lab-scale MBR: a. Profile of the influent flow rate; b. Profile of the influent COD

3.2. Optimized Parameters

The variable parameters for the MBR model can not be considered as random variables. They denote specific conditions of biomass growth and substrate utilization, and they have specific units and distinct ranges of values. For example, the yield Y, which is usually obtained either by stoichiometry based on certain single organic substrate or by experimental data of commonly found bacteria, has a typical value of 0.42 mgVSS/mgBOD$_L$ for aerobic hetertrophs. In this study, the modeling process utilized COD as the basis for yield optimization. Conceptually, the obtained value should be the net yield for all bacteria in the MBR system, such as aerobic hetertrophs, nitrifying autotrophs, sulfide oxidizing autotrophs, and so on. It is shown in Table 1 that yield was given a range between 0 and 1 mgSS/mgCOD. The SCE-UA method would only try values in this range until the model gave the best simulation combined with the choices of other parameter values. Results of optimization showed that yield had a value of 0.325 mgSS/mgCOD. This was lower than 0.42 mgVSS/mgBOD$_L$, which was an empirical value in ASMs. The lower yield could be explained by the net yield of all bacteria in the long-SRT MBR. Typically, bacteria other than aerobic hetertrophs had a true yield much lower than 0.42. Because the SRT is very long for MBR (90 – 300 days in this experiment), the bacteria community in the system is complex and this could result in a net yield of a lower value compared with the yield of aerobic hetertrophs. In addition, complex substrate composition other than carbohydrate BOD present in the MBR influent also resulted in a lower yield. The same way could be explained for the lower maximum specific rate of substrate utilization $\hat{q}$ (9.3 mgCOD/SS·day) compared with the empirically used value (20 mgBODL/VSS·day). The optimized half-saturation substrate concentration K_S was 37.1 mgCOD/L compared with 20 $mgBOD_L$/day, the conventional value for aerobic hetertrophs. This indicated that the net substrate utilization rate of bacteria in the MBR was lower than that of aerobic hetertrophs. The biomass decay rate b in this specific MBR was optimized to be 0.091. Other variable parameters after implementing the SCE-UA method were shown below: f_d, 0.98; $\hat{q}_{UAP}$, 2.24 mgCOD/mgSS·day; K_{UAP}, 199.9 mgCOD/L; k_1, 0.23; $\hat{q}_{BAP}$, 0.028 mgCOD/SS·day; K_{BAP}, 198.3 mgCOD/L; and k_2, 0.92. The RMSE, when the optimized parameters were applied, was 10.431, which was the lowest value using any combination of parameters in the parameter spaces after implementing the SCE-UA algorithm.

3.3. Model Simulation

Fig. 4 shows the simulation results of the MBR model using the optimized parameters by SCE-UA. Fig. 4a shows the simulation of the effluent COD. Compared with the observed result, the model simulation had good capture of the rising limbs and falling limbs. However, it is also observed that the simulated results had obvious under-estimation between 37 and 62 days while over-estimation existed between 63 and 100 days. It is speculated that the discrepancy of under-estimation was caused by the excretion of amounts of SMP after new sludge was added. The simulated data, however, was designed to give an average estimation after the system reached the equilibrium state, and it did not include the impact of sampling a few HRTs after sludge addition on the model output. In addition, the observed data had 2 mg/L of standard deviation using HACH kit. Therefore, it is believed that more confidence should be given to the simulated results in this under-estimated range of discrepancy. The obvious over-estimation range between 63 and 100 days, however, caught the rising and falling limbs well. This indicated that the model explained the general principles well, but the lower values of the observed data were caused by membrane backwashing, which was generally not included in the conceptual model, because there was a sharp increase of flux rate (Fig. 3a) during this period. It was also found that there existed continuous under-estimation after 118 days. Possible explanations could be the accumulation of SMP because the SRT of this period was extended to 300 days.

Fig. 4b shows the simulation of the MLSS concentration in the lab-scale MBR. Same with the other output of effluent COD, the model simulated the rising and falling limbs well. The observed MLSS concentration showed several jumps during the experiment due to external sludge addition. The model included these operation adjustments and demonstrated the same trend of MLSS concentrations after sludge addition. It is also observed that the MBR tended to reach steady-state conditions given the feed substrate concentrations and operating conditions. The observed sharp decline of MLSS concentration at 20th day was caused by solids loss due to improper membrane backwashing. New sludge was added after that. Therefore, more confidence should be given to the simulated results given the MBR was normally operated. Similar to the simulation for effluent COD, continuous under-estimation of MLSS concentrations is observed after 128 days, which could be explained by the accumulation of inert biomass due to the extended SRT.

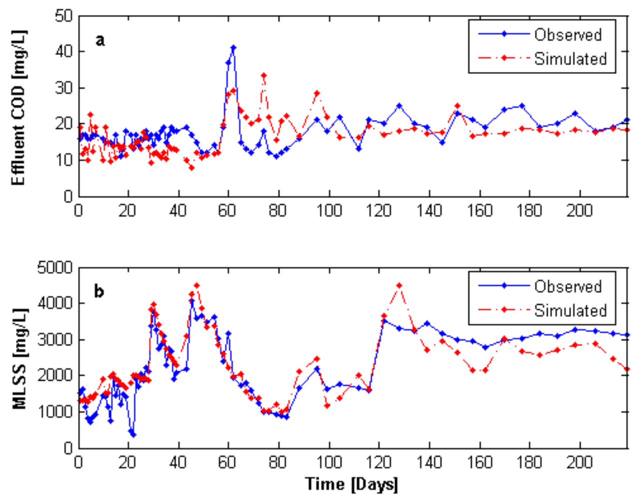

Fig. 4: Simulation by the conceptual MBR model: a. Simulation of the effluent COD; b. Simulation of the MLSS concentration

In general, the conceptual activated sludge based MBR model is shown to be effective in the simulation of effluent COD and MLSS concentration. Noted that the conceptual model only focuses on the COD removal, it did not take into account other removal processes that occurred in the experiment, such as nitrifying activity. Therefore, parameters that were optimized by SCE-UA should be considered as the net values that combined stoichiometric and kinetic characteristics of all processes. Readers could refer to ASMs for detailed descriptions of other bio-processes. The result of focusing on COD removal reduces the number of variable parameters to 11. This makes the optimization of these parameters by a fitting approach computationally possible. In addition, it addresses the most important substrate pathways that occur in wastewater treatment process. The model did not include the impact of temperature change since the temperature variation in this experiment is negligible in the laboratory environment. However, in order to apply the model to the full-scale MBR process that is subject to daily temperature change, it is necessary to make the parameters adaptable by multiplying a temperature adjustment factor. The value of this parameter also could be adjusted by global optimization given the data of annual influent temperature recorded in past years.

3.4. Residual Analysis

Fig. 5 presents the results of residual analysis after implementing the MBR model. It is aimed to give readers a confidence level of model simulations. Fig. 5a shows the normalized residuals for effluent COD over time while Fig. 5c shows the profile of their normalized count over different range of normalized residuals. It is found that more counts are present in the negative regions for effluent COD. This indicated that in more cases the model resulted in under-estimation. Although this could be explained by the low confidence of the observed data that was obtained before the system reached the steady state after sludge addition, it indicates a potential to make further optimization given more field data or a new structure of MBR model. Generally, both the discrete and accumulative distribution for effluent COD roughly demonstrates a pattern of normal distribution, which indicates that readers could give more confidence to the simulation results by the conceptual model.

Fig. 5b shows the normalized residuals for MLSS concentration over time while Fig. 5c shows the profile of their normalized count over different range of normalized residuals. It is observed that the discrete distribution of normalized count shows a clear pattern of normal distribution, which suggests that the conceptual model is effective in the simulation of MLSS concentrations.

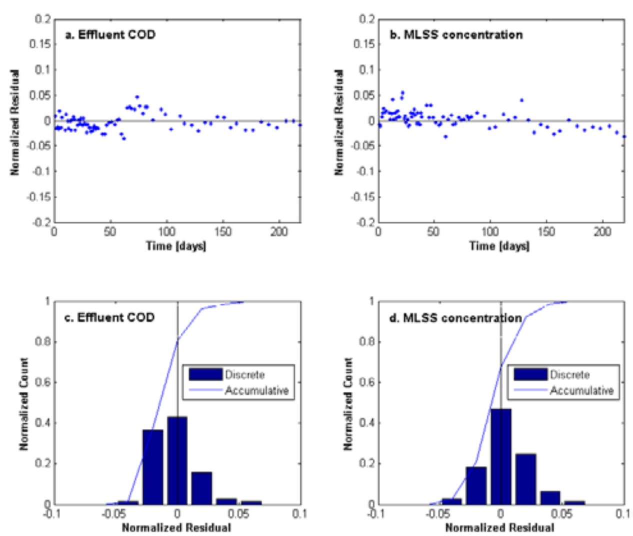

Fig. 5: Residual analysis of the model output: a. Normalized residuals of the effluent COD over time; b. Normalized residuals of the MLSS concentration over time; c. Normalized counts in regions of normalized residuals for effluent COD; d. Normalized counts in regions of normalized residuals for MLSS

Noted that the model calibration is designed to reach a tradeoff of simulation performances between effluent COD and MLSS concentration by using the RMSE shown in Eq. 12 as the objective function value to be optimized, it gives readers an option of adjusting the weight factors to change the confidence of the model outputs. For example, better simulation performances for effluent COD could be achieved by either increasing its corresponding weight factor or decreasing the weight factor of MLSS concentration before implementing the SCE-UA algorithm. However, readers should also be aware that drawbacks might be present after irrational tries, because the resulting parameter sets might be out of rational range and became un-explainable.

3.5. Impact of Operating Conditions

Since the conceptual model using optimized parameters is effective in simulations, it demonstrates great potential to aid in optimizing the performances of the MBR system. Given the constant feed substrate concentration of 300 mgCOD/L, the lab-scale MBR system was evaluated under different operating conditions, and the results were presented in Fig. 6. The HRT was showed to be an insensitive operating parameter for effluent COD in the ranges being evaluated (Fig. 6a). The SRT, however, is very sensitive, because the effluent COD is shown to be proportionally related with the increase of SRT. The results suggest that the decrease of SRT will be helpful to lower the effluent COD while the increase of HRT in this particular MBR system will not show obvious improvement because the potential release of SMP at long SRT is likely to become dominant in this MBR.

Reverse trend is observed in Fig. 6b when analyzing the simulated results for MLSS concentration. The SRT is shown to be a less sensitive parameter than HRT. According to the figure, SRTs higher than 30 days have negligible impact on the MLSS concentration while the increase of HRT from 0.1 to 3 days at 1 day of SRT resulted in a big jump of MLSS concentration from 10 to 16 g/L. Note that HRT is only sensitive when SRT is very low. In most ranges where the SRT is larger than 30 days, the HRT and SRT are both insensitive and the resulting MLSS concentration is 2000 mg/L in average. It could be deduced that the only factor that could affect the MLSS concentration at long SRTs is the feed substrate concentration.

The impact analysis by the simulation studies presents an alternative approach for performance optimization of the MBR. The optimization strategies obtained from the hypothetical studies would suggest an SRT of less than 100 days in order to keep the effluent COD less than 20 mg/L. Adjustment of HRT when the SRT is larger than 30 days is un-necessary for changing the MLSS concentrations.

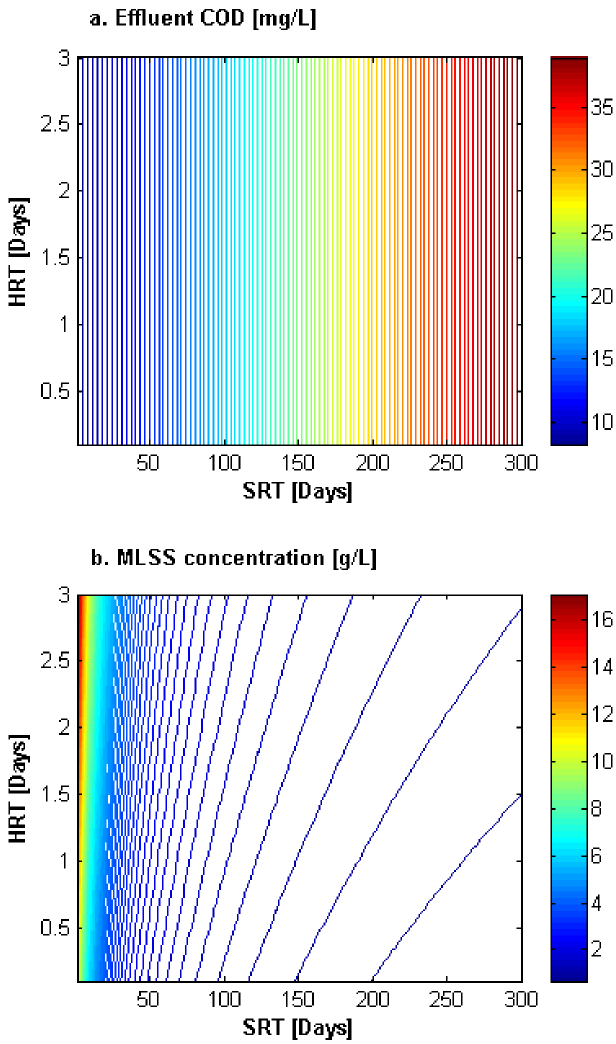

Fig. 6: Impact of operating parameters on the output of the MBR model: a. Visualization of the impacts for effluent COD; b. Visualization of the impacts for MLSS concentration

4. CONCLUDING REMARKS

Other than directly using the published values or the experimental values from batch study, the parameters for MBR models could be obtained by adopting a global optimization method to better describe the biomass growth and substrate utilization conditions. The conceptual activated sludge based MBR model developed by simplifying ASM1 is effective in simulating the effluent COD and MLSS concentration using the optimized parameters. The model assisted analysis of operating conditions presents an alternative approach for performance optimization of MBR systems.

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