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An Approach for the Flexibility Design of Activated Sludge Bioreactors Based on the Number-Theoretic Methods for Optimization

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In order to solve the problems, which appear in sewage treatment processes, caused by uncertain parameters, an approach for flexibility design of completely mixed activated sludge bioreactor was proposed based on the number-theoretic method for optimization. The flexibility of a given design can be preliminarily tested by using the number-theoretic net search. The computation points arranged by a number-theoretic net are able to provide comprehensive information for improving process flexibility. By using an operating scheme set generated with the factorial experimental design, the strategy for design improvement can be easily found. Finally, the application of the approach is illustrated with a case study which comes from a design example of a literature.

1. Introduction

It is well known that efficient wastewater treatment technologies are indispensable for the implementation of sustainable development strategy. Traditional design and upgrade concepts for wastewater treatment plants (WWTPs) are based on the forecasting of load parameters over a period of 25 – 40 y. Consequently, WWTPs are typically constructed to be long living and considered as rather static, while future uncertainty is hardly considered during the planning and design of a plant (Dominguez and Gujer, 2006). However, during the operation of a sewage treatment plant, some wastewater parameters such as concentration, flow rate, temperature and kinetic parameters change with higher uncertainty. A survey showed that the average loading rate of the municipal sewage treatment plants in China was 77.48 % (Song et al., 2013).

When the values of the wastewater parameters deviate from the design values in the long term, a series of problems would come, such as the increases in energy consumption and operating costs of treatment facilities (Zhang et al., 2006), the deterioration in the removal rates of the total nitrogen and the total phosphorus (Liu et al., 2013) and sludge bulking (Fan et al., 2008). In order to solve these problems, scholars proposed a transition towards flexibility and additivity of future urban water systems (Hering et al., 2013), that was to say wastewater treatment systems should have certain extent of flexibility. However, the flexibility test model is a kind of highly nonlinear infinite mathematical programming which contains maximum - minimum - maximum constraints (Moon et al., 2008), or involves in high-dimensional space graphics (Lai and Hui, 2008). The concept and the solving process of such model are too complex and require lengthy computation effort (Li and Chang, 2011). Therefore, it is difficult for the general designers and the operators of sewage treatment systems to master them. Spiller et al. (2015) overviewed the status of flexible infrastructure design alternatives for water and wastewater networks and treatment, the results indicate that, with the exception of Net Present Valuation methods, there is little research available on the design and evaluation of technologies that can enable flexibility.

Consequently, it is necessary to develop a new design method that can not only be used to obtain a flexible WWTP, but also be easily used by normal designers. In this paper, a new design approach for designing a flexible completely mixed activated sludge (CMAS) bioreactor, which is merely used to remove organic matter from a wastewater, was proposed based on the number-theoretic methods (NTM) for optimization.

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2. Formulation of flexibility design

2.1 General formulation

The variables of a biochemical process operating at steady state can be divided into 4 categories, which are the vector of the design variables d, the vector of the state variables x, the vector of the control variables z, and the vector of the uncertain parameters θ. The constraint conditions, describing aerobic degradation processes by the 4 kinds of parameters, can be written as the following form:

$$f_i(d, z, \theta) \leq 0 \tag{1}$$

where the equalities are the formulas used in bioreactor design and the inequalities are restrictive requirements for the parameters such as design variables and state variables. For a design scheme d, determining if it can feasibly operate over the range of considered uncertainty,Θ, is equivaluent to analyzing if a proper operating scheme, $z \in Z$, exsits such that (Grossmann et al., 2014).

$$F(d) = \max_{\Theta} \min_{Z} \max_{I} f_i(d, z, \theta) \leq 0 \tag{2}$$

where I is the index set for the inequalities, i = 1, 2, …

Flexibility design in this paper refers to as finding an appropriate design, when the device that is constructed according to such design runs on the domain Θ, there exists an operating scheme z, such that F(d) ≤ 0.

2.2 Selection of the variables

For a CMAS reactor removing only organic matter from a wastewater, the total volume of the bioreactor system, V, and the number of bioreactors, N, are selected as design variables. The parameters such as influent volumetric flow rate, F, readily biodegradable substrate concentration of the influent, $S_{S,0}$, wastewater temperature, T, influent soluble ammonia nitrogen $S_{NH,0}$ and influent slowly biodegradable substrate $X_{S,0}$, are selected as uncertain parameters. The ranges of these uncertain parameters form domain Θ, each point of θ in Θ represents an uncertainty case. If the number of the bioreactors putting into operation is n, then the volume of the bioreactor putting into operation, V_r, is

$$V_r = (V/N) * n \tag{3}$$

The solids retention time (SRT), Θ_c, and V_r are selected as control variables. The variation regions of these two variables form the domain Z. Obviously, when V and N are given, the numbers of the levels of V_r and n all equal N.

3. Design procedure

Step 1 Determination of design and operating schemes at nominal value of uncertain parameters

First, the ranges of V, N and Θ_c of a CMAS bioreactor at the nominal value of uncertain parameters should be determined. And then, calculate the S_S, the mixed liquor suspended solids (MLSS) concentration X, and the oxygen requirement RO.

Step 2 Flexibility test and modification

In order to simplify the solution of Eq. (2), a set of representative points on Θ are used, and the optimal solution among these points is used as an approximate solution of F(d). The flexibility design is an iterative process for improvement. The comprehensiveness of the information of a design scheme over Θ determines if the correct direction, in which the improvements of the flexibility of a design are made, can be found. A number-theoretic net (NT-net) is a uniformly scattered set of points on a certain domain. As a result of the uniformity, the points of an NT-net are a set of representative points on the domain. Just because of the representativeness, the comprehensive flexibility information of a design can be revealed so as to make reasonable and rational engineering decisions to retrofit the design.

For an optimization problem

$$f(x^*) = \max_{D} f(x) \tag{4}$$

where D is a hyperrectangle domain, $f(x^*)$ and x^* are the global maximum and a maximum point on D, respectively.

In order to obtain the global maximum of Eq. (4), Fang and Wang (1994a) proposed the NTM search. The idea of the method is as follows: Take an NT-net $\{x_k, k = 1,2,...,m\}$ on D. It is expected that there is a point x_m^* among $\{x_k\}$ such that $f(x_m^*)$ is close to $f(x^*)$, and x_m^* is close to x^* if m is large. It has been proved that

$x_m^* \rightarrow x^*$ and $f(x_m^*) \rightarrow f(x^*)$ as $m \rightarrow \infty$. Although the global optimum can be obtained by using this method, however, the convergence rate is rather slow. To overcome this shortcoming, the sequential algorithms for optimization with number theoretic nets (SNTO) or RSNTO were proposed (Fang and Wang, 1994a). The methods based on NTM are known as the NTM for optimization.
The above methods do not require that the function f(x) is unimodal and/or differentiable to ensure that the global maximum can be attained, and can contain the expressions "max", "min" or $|x|$, or is defined piecewise. Therefore, the global maximum can be easily obtained.
When computing F(d) with the methods mentioned above, both $\min_Z \max_I f_i(d,z,\theta)$ on domain Z and $\max_\Theta \min_Z \max_I f_i(d,z,\theta)$ on domain Θ can be obtained using the NTM for optimization, where the NT-nets are usually generated by good lattice point (GLP) sets (Fang and Wang, 1994b).
When solving Eq. (2), the point sets $\Theta^{(m)} = \{\theta_k, k = 1,2,...,m\}$ in Θ and $Z^{(r)} = \{z_l, l = 1,2,...,r\}$ in Z, are generated with corresponding NT-nets, respectively. Assign a set $Z^{(r)}$ to each θ_k of $\Theta^{(m)}$, then calculate $f_i(d,z,\theta)$ and find $\max_I f_i(d,z,\theta)$ at each z_l, and then find the minimum, $L_r^m(\theta_k)$, among all $\max_I f_i(d,z,\theta)$ at all points of $Z^{(r)}$

$$L_r^m(\theta_k) = \min_{Z^{(r)}} \max_I f_i(d,z,\theta) \tag{5}$$

$L_r^m(\theta_k)$ is obviously the minimum at θ_k. Finally, calculate all $L_r^m(\theta_k)$ s, and then take the maximium among these $L_r^m(\theta_k)$ s, F_r^m, which is an approximation of F(d) on Θ.

$$F_r^m = \max_{\Theta^{(m)}} L_r^m(\theta_k) \tag{6}$$

In order to find out the directions in which the design scheme can be improved, the computation points of control parameters are generated using the factorial experimental design (FED) , which can also generate NT-nets. There are only 2 control variables, which are V_r and Θ_c, and the numbers of the levels of V_r and Θ_c are generally not too large. Consequently, the number of the points generated with the FED is not too large.

Step 2.1 Generate initial computation point sets
The initial computation point sets include the initial design scheme, the initial computation set on Θ and the initial operating scheme set on Z. The initial value of V can be obtained using the traditional design method, and the initial value of N can be taken to be 2. In this step, if m_1 (the number of the points in $\Theta^{(m_1)}$), and r_1 (the number of the points of $Z^{(r_1)}$) are too large, the workload of analysing modification directions and strategies would be too heavy when the design scheme need to be modified. Therefore, m_1 and r_1 should take small values.

Step 2.2 Preliminarily test flexibility
The main task of this step is to preliminarily judge the feasibility of a design scheme using a small number of points. The test is performed by using the NTM search, that is to say, finding $L_r^m(\theta_k)$ on Z and finding F(d) on Θ are all carried out with the NTM search. $|\delta\Theta_c| \le \varepsilon$ and $L_r^m(\theta_k) > 0$ mean that there exsits no operating sheme at θ_k. Such θ_k is called flexibility bottleneck. Using the values of $f_i(d,z,\theta)$ at flexibility bottlenecks, the modification direction for the infeasible desgns can be easily found.

Step 2.3 Detailed test of the flexibility of a design scheme
To overcome the drawback that the convergence rate of the NTM search is usally slow, RSNTO is used to search F(d). In the calculating process, If F(d) > 0, then return to Step 2.2**;** If F(d) ≤ 0, the design scheme is feasible.

Step 3 Design of the rest parts of CMAS system
After determining the ranges of the values of V, N and Θ_c, the next step is to determine the ranges of the other parameters such as oxygen requirement, and accordingly, the aeration system as well as the other rest parts of the CMAS bioreactor. The procedure of this step is the same as the traditional design method, and therefore not explained here.

4. Case study

This case study was cited from the example appearing in a book (Grady et al., 2011), and calculated with excel 2010.
A CMAS system is to be designed to remove organic matter from a wastewater. Removal of ammonia-N is not required, so the system does not have to nitrify. The average design wastewater flow rate is 40,000 m^3/d and

full equalization will maintain the loading at the average value throughout the day. The oxygen transfer system will be sized to maintain the dissolved oxygen (DO) concentration above 1.5 mg/L under all conditions. The variation ranges of the uncertain parameters involved in this case study are listed in Table 1, and the values of the other parameters that do not vary are the same as those in the original example.

Table 1: The variation ranges of the uncertain parameters

Component	Range	Unit
$X_{S,0}$	40 - 300	mg COD/L
$S_{S,0}$	20 - 250	mg COD/L
$S_{NH,0}$	10 - 100	mg N/L
F	30,000 - 50,000	m^3/d
T	15 - 25	°C

4.1 Constraint conditions

The equality constraints are the design fomulas used in the original example. The inequality constraints used in this exmple originate from the formulas in the refence (Grady et al., 2011).

(1) Volumetric power input

When using diffused aeration systems, volumetric power input, Π*,* is

$$\Pi = 1000 * Q/V_r \tag{7}$$

where Q is in m^3/min, V_r is in m^3。Π must not be greater than the upper limit on volumetric power input, $\Pi_{U,Q}$, which causes excessive shear of the activated sludge floc. Therefore,

$$f_1 = \Pi - \Pi_{U,Q} \le 0 \tag{8}$$

For diffused aeration systems, $\Pi_{U,Q}$ is approximately 90 m^3/min·1,000 m^3.

Π must not be less than the lower limit on the volumetric power input, $\Pi_{L,Q}$, which is determined by the need to maintain solids in suspension. Therefore,

$$f_2 = \Pi_{L,Q} - \Pi \le 0 \tag{9}$$

In this paper, it is considered that $\Pi_{L,Q}$ = 20 m^3/min·1,000 m^3.

(2) Volumetric oxygen transfer rate of an oxygen transfer system

The volumetric oxygen transfer rate, FRO, can be calculated with Eq(10).

$$FRO = RO/V_r \tag{10}$$

where RO is expressed as kg O_2/h, V_r is in m^3.

The maximum volumetric oxygen transfer rate that can be achieved economically on a sustainable basis is around 0.1 kg O_2/m^3·h. Therefore, FRO should satisfy

$$f_3 = FRO - 0.1 \le 0 \tag{11}$$

(3) MLSS concentration

MLSS is generally in the range of 2,000 to 5,000 mg/L (Grady et al., 2011), which means that X should simultaneously satisfy

$$f_4 = 2000 - X \le 0 \tag{12}$$

$$f_5 = X - 5000 \le 0 \tag{13}$$

where X is the MLSS concentration in TSS (total suspended solids) units, mg/L.

4.2 Test of the flexibility of the original designs

In the original example, the bioreactor is designed with the constraints described above. The result of the example is that the volume of feasible bioreactor is in the range of 4,680 – 7,300 m^3 on the premise of not considering the effects of transient loadings, nevertheless, the value of N is not specified.

(1) The original design schemes

Take 5 volume values uniformly scattered in the range of 4,680 to 7,300 m^3. Take N = 2. Then 5 design schemes can be obtained and listed in Table 2.

Table 2: The original design schemes and part results of the flexibility test

Design scheme	V/m^3	N	$F_{r_w}^{10}$	Number of θ$_k$s at which $L_{r_w}^{10}(\theta_k) > 0$
Design scheme 1	4,680	2	978.720	6
Design scheme 2	5,335	2	244.690	5
Design scheme 3	5,990	2	5.060	5
Design scheme 4	6,645	2	0.043	4
Design scheme 5	7,300	2	0.030	4

(2) Computation point sets

The generating vectors for obtaining the NT-net $\Theta^{(m)}$ can be obtained using the GLP method at the minimum of the centered L_2-discrepancy (Hickernell, 1998). The NT-net $\Theta^{(10)}$, used in this paper, was obtained by omitting the last row of the $\Theta^{(11)}$ (Fang and Wang, 1994a). Taking m_1=10, and using $\Theta^{(10)}$ generates the computation point set on the domain Θ. It is recommended that the SRT value is often taken to be at least 3 days for achieving good bioflocculation in activated sludge systems (Grady et al., 2011). As a case study, the range of SRT is set from 3 to 15 days. Because N=2, and V_r has only 2 levels. For SRT, take a level every other day, then 13 levels of SRT can be obtained. On this basis, an operating scheme set $Z^{(26)} = \{z_1, l = 1,2,...,26\}$, can be generated using the FED.

(3) Preliminary test of the flexibility

For each design scheme in Table 2, select ε = 0.1 d, and test the flexibility with the method presented in Step 2.2, part results are summarized in the fourth and fifth columns of Table 2. As shown in Table 2, all the values of $F_{r_w}^{10}$ s of the five design schemes are greater than 0, and the cases in which $L_{r_w}^{10}(\theta_k) > 0$ account for about half of the ten uncertainty cases for the given 5 design schemes; that is to say, in about half uncertainty cases, the design schemes are infeasible.

Above is the analytical results on the condition that N = 2. However, N is not concerned in the original example. Through calculation, it can be concluded that increasing N would not change the values of $F_{r_w}^{10}$ s for the design schemes listed in Table 2.

4.3 Modification on the design scheme

As an example, the Design scheme 5 listed in Table 2 was taken as the initial design scheme. Initially, the flexibility bottlenecks were analyzed and part of the results are shown in Table 3. As can be seen from Table 3, it is at θ_6 (F = 41,111.11 m^3/d, $S_{S,0}$ = 20.00 mg COD/L, T = 21.67 °C, $X_{S,0}$ = 242.22 mg COD/L, $S_{NH,0}$ = 90.00 mg N/L) that $F_{r_w}^{10} = L_{r_w}^{10}(\theta_6) = f_3$ = 0.030 on the condition that V_r takes the maximum value. θ_6 is hereby a flexibility bottleneck. It is can be easily observed, from the relationship between f_3 and V_r indicated in Table 3, that increasing V_r can decrease f_3, which can also be derived from Eq. (10) and Eq. (11). Consequently, to reduce $F_{r_w}^{10}$, V_r should be increased. But the value of V_r is the maximum when $F_{r_w}^{10} = L_{r_w}^{10}(\theta_6)$, so the value of $L_{r_w}^{10}(\theta_6)$ can not be decreased by increasing V_r if the value of V remains unchanged.

Table 3: Part results of the analysis of flexibility bottlenecks of Design scheme 5

	Θ_c /d	V_r /m^3	f_1	f_2	f_3	f_4	f_5	max(f_1, f_2, …f_5)	$L_{r_w}^{10}(\theta_6)$
θ_6	3	3,650	66.009	-136.009	0.160	-2,606.193	-393.807	66.009	0.030
	3	7,300	-11.996	-58.004	0.030	-303.096	-2,696.904	0.030	
	3.1	3,650	66.738	-136.738	0.161	-2,731.757	-268.243	66.738	
	3.1	7,300	-11.631	-58.369	0.031	-365.878	-2,634.122	0.031	

It can be seen from Eq(3) that V_r tends to be larger when V increases. Because increasing N would result in an increase of construction cost, there is no need to change N. Consequently, increasing V while let N unchanged is a strategy for improving Design scheme 5 to decrease $F_{r_w}^{10}$. It can be also found from Table 3 that decreasing SRT can also reduce f_3. However, even though Θ_c is decreased to 3 d, which is the minimum value that SRT can reach, f_3 is still greater than 0. Consequently, it is impossible to make the value of f_3 become negative by reducing Θ_c.

Keep improving untill F(d) ≤ 0, finally, it is found that when V = 16,000 m^3, N = 3 , the desgn scheme is feasible.

5. Conclusions

On the basis of the formulation of the flexibility design, an approach for the design of flexible bioreactor based on the NTM for optimization was proposed. Due to the NTM methods do not require that the corresponding functions are unimodal and/or differentiable to ensure that the global optimum can be attained, and can contain the expressions "max", "min" or $|x|$, or is defined piecewise, the flexibility function F(d) can be easily obtained, thus the proposed approach can test the flexibility of a design scheme precisely. Additionally, the computation points arranged by an NT-net can provide comprehensive information for improving process flexibility, therefore, the appropriate strategy for design improvement can be found easily. The proposed approach can be used for not only the flexibility design of CMAS bioreactors, but also the modification of existing bioreactors.

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