Optimal synthesis and operation of wastewater treatment process with dynamic influent

Bingxiong Lu,† Simin Huang,† and Ignacio E. Grossmann*,‡

† Department of Industrial Engineering, Tsinghua University, Beijing, 100084, China

‡ Department of Chemical Engineering, Carnegie Mellon University, Pittsburgh, Pennsylvania, 15213, United States

Abstract: This work addresses the problem of optimal synthesis and operation of wastewater treatment process considering dynamic influent streams under different discharge standards and penalty rates of noncompliant emissions. We develop a general disjunctive programming model to address this problem, which is then reformulated as a multi-period mix-integer nonlinear programming model using hull reformulation for the disjunctions. In order to solve the resulting model to global optimality, we propose a Lagrangean-based decomposition algorithm. Numerical studies verify the effectiveness of the algorithm, and comparison studies provide useful management insights for policy makers.

1. Introduction

China is facing a serious water pollution problem. According to a national water quality survey in 2015, water pollution of assessed rivers and lakes is serious. Inferior class V water accounted for 11.7% in rivers and 23.3% in major lakes(1). In addition, the wastewater discharge in China has increased significantly in recent years. Figure 1 shows the discharge of wastewater in China from 2006 to 2014. We can see that the discharge increases from around 50 billion ton in 2006 to more than 70 billion ton in 2014, which is mainly due to the increased discharge of urban sewage. Before discharging into the environment, a large part of wastewater must be treated in order to reduce the contaminant level. Therefore, the design and operation of wastewater treatment plant is crucial, and increased discharge of wastewater has led to higher demand of well-designed and well-operated wastewater treatment plants (WWTPs).

Wastewater treatment process design involves the selection of unit processes and then interconnects units to create the process flow diagram, which is largely determined by the characteristics of contaminants in influent and the discharge limits to be met.

The design of wastewater treatment process is facing major challenges. One such challenge is that regulatory authorities have significantly tightened discharge standards of wastewater. In recent years, the discharge limitation of *COD*, *BOD*, *TSS*, and $NH_3\text{-}n$ of some wastewater discharge standards in China has undergone a tightening of more than 40%, some even more than 80%. In addition to the increasingly stringent discharge standards, WWTPs also face highly dynamic influent flows with variable pollutant concentrations. Consider a WWTP in Shandong Province in China for example, the concentration of *COD* in the influent in 2012 varies between 158 mg/l and 477 mg/l; the concentration of $NH_3\text{-}n$ in the influent varies between 1.8mg/l and 15.3 mg/l.

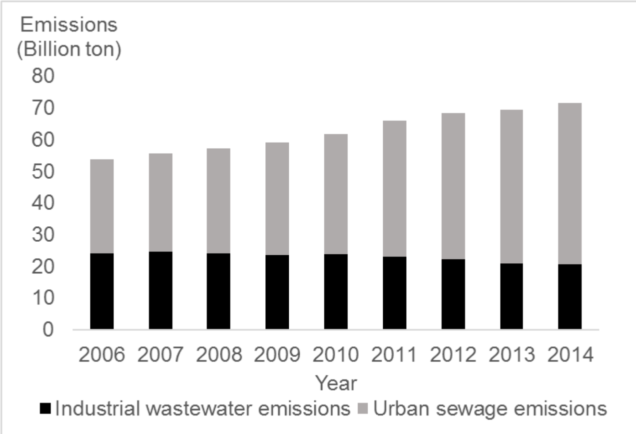

Figure 1 Discharge of wastewater in China from 2006 to 2014, from http://jcs.mep.gov.cn

Facing increasingly stringent discharge standards and highly dynamic influent streams with variable pollutant concentrations, makes it very challenging to design and operate the treatment process. The conventional design of wastewater treatment process has traditionally relied on expert decisions and previous experience[(2)], which requires specific know-how and often involves laboratory and pilot trials[(3),(4)]. While these approaches consider economic and environmental impact of the selected treatment technologies, increasingly stringent discharge standards, highly dynamic influent, and steadily growing alternative technologies, make such decision process more difficult for obtaining optimal design configurations of wastewater treatment processes.

An alternative approach to make decisions about water/wastewater network design is to use optimization-based methods for chemical process synthesis[(5)]. In these methods, the process selection and network design problem is cast as a mathematical optimization problem through the definition of a superstructure in which all possible configurations are include, and of an objective function, typically the minimization of costs. The optimization problem is then solved to determine the optimal network configuration and optimal flows through it[(6)].

The problem of water network optimization has attracted wide attentions for its relevance in industrial applications, starting from the pioneering work of Takama and co-workers[(7)], which solved the planning problem of optimal water allocation in an integrated system including water-using units and wastewater-treating units. Since then, many studies have been published. For a comprehensive review of mathematical programming approaches for water network synthesis, please refer to the work of Bagajewicz[(8)] and Jezowski[(9)]. We classify the literature by category of network, influent, and modelling of treatment units. Table 1 shows a summary of the selected relevant articles. Moreover, the method proposed in this paper is also listed in the table for comparison.

A significant number of papers has been published concerning the total water network (TWN) synthesis problem, and the network consists of water usage network and wastewater treatment network (WWTN). Huang and co-workers[(10)] proposed a mathematical programming model for determining the optimal water usage and treatment network in chemical plant. Karuppiah and Grossmann addressed[(11),(12)] problems for synthesizing the integrated water system consisting of water using and water treating units to minimize total network cost, for which they developed a spatial branch and cut algorithm. Later, Tan et al[13] and Ahmetovic and Grossmann[14] proposed superstructure-based optimization models for the synthesis of water networks. The latter established the tradeoff between cost and complexity of the treatment network. Faria and Bagajewicz[15] presented a planning model for industrial water systems retrofit, which considered the future increase in the load of contaminants in existing units. Water network synthesis problems have been modelled as MINLPs[16]-[18], which are solved using global optimization solvers[16],[17] or algorithms based on parametric disaggregation[18]. Rojas-Torres and co-workers[19] introduced an optimization-based approach for the synthesis of water network accounting for temperature dependence and thermal effects. Yang and co-workers[20] proposed a superstructure model to exploit the trade-offs between treatment cost and removal efficiency of the units. Majozi and co-workers[21],[22] proposed robust water network superstructure optimization approaches for the synthesis of multi-regeneration water network, in which detailed models of regenerators are considered.

Table 1 Summary of literature review[a]

Literature	Type of network		Type of influent			Modelling of treatment unit			
	TWN	WWTN	FW	CIN	DIN	FRR	FOC	SM	MM
Huang et al., 1999	√		√			√			
Karuppiah and Grossmann, 2006	√		√			√			
Karuppiah and Grossmann, 2008	√		√			√			
Tan et al., 2009	√		√			√	√		
Ahmetovic and Grossmann, 2011	√		√			√			
Faria and Bagajewicz, 2011	√		√			√	√		
Khor et al., 2011	√		√	√					√
Khor et al., 2012	√		√	√					√
Teles et al., 2012	√		√			√	√		
Rojas-Torres et al., 2012	√		√			√			
Yang et al., 2014	√				√				√
Abass and Majozi, 2016	√		√						√
Mafukidze and Majozi, 2016	√		√						√
Galan and Grossmann, 1998		√		√		√			
Rigopoulos and Linke, 2002		√		√				√	
Vidal et al., 2002		√		√				√	
Alasino et al., 2007		√		√				√	
Alasino et al., 2010		√		√				√	
Bozkurt et al., 2015		√		√					√
The proposed model		√			√				√

[a] TWN: Total Water Network; WWTN: Wastewater Treatment Network; FW: Freshwater; CI: Constant Influent; DI: Dynamic Influent; FRR: Fixed Removal Ratio; FOC: Fixed Outlet Concentration; SM: Simulation Model; MM: Mechanism Model.

The first use of optimization approach to the wastewater network synthesis problem is the work of Galan and Grossman[23], which addressed the optimum design of distributed wastewater networks where multicomponent streams are considered. Later, some researchers solved the wastewater treatment network optimization problem for either a given treatment process[24] or limited alternative designs[25]. Alasino and co-workers[26],[27] considered problems of optimizing the synthesis and the operating conditions of activated sludge wastewater treatment plants based on superstructure models. These are two of the papers that optimize both the network synthesis and operating conditions. Recently, Bozkurt and co-workers[28] developed a superstructure-based optimization methodology to support optimal treatment process selection, in which treatment process alternatives are mathematically described using a generic process model.

Publications concerning the TWN synthesis mainly use the freshwater as influent[10]-[22]. In these models, freshwater is processed by water using units and then recycled or treated by wastewater treatment units. Some papers about TWN synthesis use both freshwater and constant influent[16],[17]. The influent in papers concerning about WWTN synthesis is usually wastewater with constant pollutant concentrations[23]-[28].

The modelling of wastewater treatment units is of vital importance in the synthesis of TWN and WWTN. There are mainly four methods for wastewater treatment unit modelling: fixed removal ratio, fixed outlet concentration, simulation model, and unit model. Fixed removal ratio and fixed outlet concentration models have been widely used [10]-[15],[18],[19],[23], since it greatly simplifies the water network design, but creates a gap for their applicability to industrial processes. Simulation models have also been employed in some works[24],[27]. Recently, some researchers have also used unit models to represent the wastewater treatment units[16],[17],[20]-[22],[28], which makes these results closer to industrial systems.

There are several important differences between this work and the previous literature. First, this work uses unit models to predict the performance of wastewater treatment units. In addition, the design and operating parameters of the treatment units are both optimized rather than selected according to experience. Second, the conventional WWTN synthesis problem has usually assumed constant influent, which creates a gap for their applicability to industrial processes. This work considers the dynamic influent flow with variable pollutant concentrations, which is closer to practice.

This article is structured as follows: Section 2 provides the problem description; Section 3 describes the complete formulation of the problem; Section 4 presents the computational strategy for optimizing the resulting model; in Section 5, numerical studies are reported to demonstrate the effectiveness of the proposed algorithm, and comparisons are presented to obtain some insights for policy makers. Finally, Section 6 concludes the article.

2. Problem Statement

The problem addressed in this paper can be stated as follows. Given a wastewater treatment process superstructure, a set of dynamic influent data defined over a given number of time periods, and discharge standards for effluent, determine the minimum total annualized wastewater treatment cost, and the optimal wastewater treatment network configuration.

Influent data used in this article is sampled from the predefined dynamic influent data of Benchmark Simulation Model No. 2 (BSM2), which is a benchmarking platform for wastewater treatment that is widely used in the wastewater treatment modelling community. BSM2 defines a simulation model, a plant layout, influent data, and simulation procedures(29). The components of influent are given in Table 2. The contaminants considered in this article are chemical oxygen demand (*COD*), Biochemical Oxygen Demand (*BOD*), total suspended solids (*TSS*), and Ammonia nitrogen (NH_3-*n*). These contaminants are linear combinations of the influent components, and the coefficients are listed in Table 2.

Table 2 The components of influent and their relationship with COD, BOD, TSS, and NH_3-n(30)

Definition	Notation	COD	BOD	TSS	NH_3-n
Soluble inert organic matter	S_I	1			
Readily biodegradable substrate	S_S	1	0.25		
Particulate inert organic matter	X_I	1		0.75	
Slowly biodegradable substrate	X_S	1	0.25	0.75	
Active heterotrophic biomass	X_{BH}	1	0.23	0.75	
Active autotrophic biomass	X_{BA}	1	0.23	0.75	
Particulate products arising from biomass decay	X_P	1		0.75	
Nitrate and nitrite nitrogen	S_{NO}				
$NH_4^+ + NH_3$ nitrogen	S_{NH}				1
Soluble biodegradable organic nitrogen	S_{ND}				
Particulate biodegradable organic nitrogen	X_{ND}				

The discharge standards considered in this article are the discharge limitations for *COD*, *BOD*, *TSS*, and NH_3-*n*. For these standards, the sewage charge for compliant emissions and the penalty charge for noncompliant emissions will be imposed.

With the objective of minimizing total annualized cost (TAC), the decisions are to determine the optimal wastewater treatment network configuration, and the optimal design and operational variables of the treatment units at each time period. To address this problem, we propose a general disjunctive programming (GDP) model, which is first reformulated as a multi-period MINLP model and then solved using a Lagrangean-based decomposition algorithm.

3. Formulation

Based on the problem statement, the wastewater treatment network superstructure in Figure 2 is developed, which is a modification of the work by Bozkurt and co-workers(28). The superstructure is based on the activated sludge plant designed in BSM2(30). In BSM2, the entire treatment plant includes a primary clarifier, an activated sludge unit, a secondary clarifier, a sludge thickener, a sludge digester, and a dewatering unit. The specific description of BSM2 can be found in the literature(29). The discharge standards and operational costs are modified in this article to adjust the wastewater treatment scenario and management policy in China.

The network consists of mixing units (MU), splitting units (SU), and treatment units (TU).

Note that only the treatment units are process units since mixing and splitting units only include converging or diverging pipes. The treatment units can be divided into 3 categories: clarifiers, sludge settlement units, bio-treatment units for wastewater and sludge. Clarifiers are treatment units of type 1 (TU1), including primary clarifier and secondary clarifier. Sludge settlement units are treatment units of type 2 (TU2), including sludge thickening and dewatering units. Bio-treatment units for wastewater and sludge are treatment units of type 3 (TU3). Bio-treatment units for wastewater considered in this article includes Modified Ludzack-Ettinger[(31)] (MLE) and Oxygen ditch[(32)] (OxD), which are activated sludge treatment processes. Bio-treatment units for sludge include anaerobic digestion unit (AnD) and aerobic digestion unit (AeD).

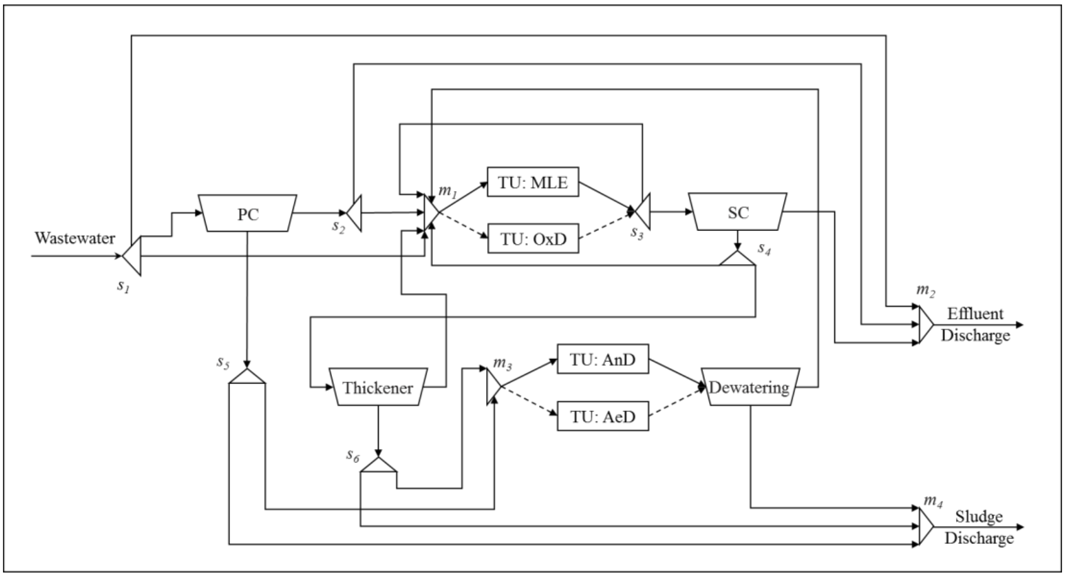

Figure 2 General wastewater network superstructure with multiple units

3.1. Mixing units

The mixing unit $m \in MU$ consists of a set of inlet streams from splitting units and different treatment units. An outlet stream from the mixing unit is directed to treatment unit or discharged into the receiving waterbodies. The overall flow balance for the mixing unit is given by Eq. 1 and the mass balance for each contaminant *j* by Eq. 2, both of which include only linear terms:

$$F_{kn} = \sum_{i \in m_{in}} F_{in} \quad \forall m \in MU, k \in m_{out}, \forall n \in N \tag{1}$$

$$C_{kjn} = \sum_{i \in m_{in}} C_{ijn} \quad \forall m \in MU, k \in m_{out}, \forall n \in N, \forall j \in J \tag{2}$$

In this set of equations, F_{in} and F_{kn} are flowrates (*k(m³)/day*) of stream *i* and *k* in the network respectively, in time period *n*; C_{ijn} and C_{kjn} are flowrates (*ton/day*) of contaminant *j* in stream *i* and *k* respectively, in time period *n*.

3.2. Splitting units

The splitting unit $s \in SU$ consists of an inlet stream from the influent or treatment unit, and a set of outlet streams directed to a treatment unit, another splitting unit, or a mixing unit. The overall flow balance for the splitting unit is expressed by Eq. 3:

$$F_{in} = \sum_{k \in s_{out}} F_{kn} \quad \forall s \in SU, i \in s_{in}, \forall n \in N \tag{3}$$

In this equation, F_{in} and F_{kn} are flowrates (*$k(m^3)/day$*) of stream *i* and *k* respectively, in time period *n*. The contaminant concentration of every stream leaving the splitting unit is equal to that of the inlet stream, which is expressed by

$$\frac{C_{ijn}}{F_{in}} = \frac{C_{kjn}}{F_{kn}} \quad \forall s \in SU, i \in s_{in}, \forall k \in s_{out}, \forall n \in N \tag{4}$$

In this equation, C_{ijn} and C_{kjn} are flowrates (*ton/day*) of contaminant *j* in stream *i* and *k* respectively, in time period *n*. Eq.4 can be rewritten as Eq.4a, which includes bilinear terms:

$$F_{in} \cdot C_{kjn} = F_{kn} \cdot C_{ijn} \quad \forall s \in SU, i \in s_{in}, \forall k \in s_{out}, \forall n \in N \tag{4a}$$

3.3. Treatment units of type 1

Treatment units of type 1 (TU1) include primary clarifier and secondary clarifier. The objective of the treatment by clarifier is to remove floating materials and solids, thus reducing the suspended solids content[(2)]. The treatment unit $t \in TU1$ consists of an inlet from the splitting unit. The inlet and outlet stream flows of treatment *t* are equal and the overall flow balance is given by Eq.5.

$$F_{in} = F_{kn} + F_{ln} \quad \forall t \in TU1, i \in t_{in}, k \in t_{overflow}, l \in t_{underflow}, \forall n \in N \tag{5}$$

In this equation, F_{in}, F_{kn}, and F_{ln} are flowrates (*$k(m^3)/day$*) of inlet stream *i*, overflow stream *k*, and underflow *l* respectively.

The mass balance of each contaminant *j* for treatment unit $t \in TU1$, is given by Eq.6 and Eq.7:

$$C_{ijn} = C_{kjn} + C_{ljn} \quad \forall t \in TU1, i \in t_{in}, k \in t_{overflow}, l \in t_{underflow}, \forall j \in J, \forall n \in N \tag{6}$$

$$C_{kjn} = Rr_j C_{ijn} \quad \forall t \in TU1, i \in t_{in}, k \in t_{overflow}, \forall j \in J, \forall n \in N \tag{7}$$

In this set of equations, C_{ijn}, C_{kjn}, and C_{ljn} are flowrates (*ton/day*) of contaminant *j* of inlet stream *i*, overflow stream *k*, and underflow *l*, respectively; Rr_j is the removal ratio of contaminant *j* by the clarifier, which is a function of hydraulic retention time (*HRT*)[(2)]:

$$\begin{aligned} & Rr_j = 1 - \frac{HRT_n}{a_j + b_j HRT_n} \quad \forall j \in J, \forall n \in N \\ & V_t \geq HRT_n \cdot F_{in} \quad \forall t \in TU1, i \in t_{in}, \forall n \in N \end{aligned} \tag{8}$$

in which a_j and b_j ($j \in J$) are empirical parameters listed in Table 3, and V_t is the volume of treatment unit t.

Table 3 Typical value of empirical parameters related to the removal ratio of clarifiers[(2)]

Contaminant	a	b
BOD	0.018	0.020
TSS	0.0075	0.014

3.4. Treatment units of type 2

Treatment units of type 2 (TU2) include sludge thickening and dewatering units. Sludge thickening unit thickens the sludge wasted from the bottom of the clarifier prior to its digestion, and the dewatering unit dewaters the digested sludge from the digester[(2)]. The overall flow balance of treatment unit $t \in TU2$ is given by Eq.9 and Eq.10.

$$F_{in} = F_{kn} + F_{ln} \quad t \in TU2, i \in t_{in}, k \in t_{overflow}, l \in t_{underflow}, \forall n \in N \tag{9}$$

$$F_{kn} = Rf_t F_{in} \quad \forall t \in TU2, i \in t_{in}, k \in t_{overflow}, \forall n \in N \tag{10}$$

In this set of equations, F_{in}, F_{kn}, and F_{ln} are flowrates (*k(m*[3]*)/day*) of inlet stream *i*, overflow stream *k*, and underflow *l* respectively. In Eq. 10, the recovery ratio of flow (Rf_t) is assumed to be constant.

The mass balance of each contaminant *j* for treatment unit $t \in TU2$ is expressed by Eq.11 and Eq.12.

$$C_{ijn} = C_{kjn} + C_{ljn} \quad \forall t \in TU2, i \in t_{in}, k \in t_{overflow}, l \in t_{underflow}, \forall j \in J, \forall n \in N \tag{11}$$

$$C_{kjn} = Rc_t C_{ijn} \quad \forall t \in TU2, i \in t_{in}, k \in t_{overflow}, \forall j \in J, \forall n \in N \tag{12}$$

In this set of equations, C_{ijn}, C_{kjn}, and C_{ljn} are flowrates (*ton/day*) of contaminant *j* in inlet stream *i*, overflow stream *k*, and underflow *l*, respectively. In Eq. 12, the recovery ratio of contaminant (Rc_t) is assumed to be constant.

3.5. Treatment units of type 3

Treatment units of type 3 include bio-treatment units for wastewater and sludge. Treatment unit $t \in TU3$ consists of an inlet stream from the mixing unit or thickening unit. The flow balance, reaction, capital cost, and operating cost can be formulated as a set of disjunctions given by Eq. 13.

$$\bigvee_{r=1,\dots,RT_t}\left[\begin{array}{c} Y_{rt} \\ F_{kn}=F_{in} \\ C_{kjn}=C_{ijn}+\sum_{react\in J_{tj}}\gamma_{t,react}\cdot\theta_{t,react,j}\cdot C_{i,react,n} \\ h_n\left(d_{rt},F_{in},F_{kn},C_{ijn},C_{kjn}\right)=0 \\ g_n\left(d_{rt},F_{in},F_{kn},C_{ijn},C_{kjn}\right)\le 0 \\ \forall n\in N \\ CAPEX_t=f_1\left(d_{rt}\right) \\ OPEX_{tn}=f_{2n}\left(d_{rt},HRT_{tn},F_{in},F_{kn},C_{ijn},C_{kjn}\right) \end{array}\right] \quad \begin{array}{c} \forall t\in TU3\cup TU4 \\ r=1,\dots,RT_t \\ i\in t_{in} \\ k\in t_{out} \\ \forall j\in J \end{array} \tag{13}$$

$$Y_{rt}\in\{True,False\}$$

In this set of equations, Y_{rt} indicates if technology *r* if selected for treatment unit *t*, d_{rt} is the design variable related to technology *r* and unit *t* that must be accounted for all time periods *n*. F_{in} and F_{kn} are flowrates (*k(m³)/day*) of inlet stream *i* and outlet stream *k* respectively, C_{ijn} and C_{kjn} are flowrates (*ton/day*) of contaminant *j* in inlet stream *i* and outlet stream *k*, respectively. In Eq. 13, the reactant $react\in J$ is removed with the specified conversion efficiency, and other component $j\in J$ is produced or removed according to the conversion efficiency $\gamma_{t,react}$ and reaction stoichiometry $\theta_{t,react,j}$[28]. The constraints related to design and operating conditions are represented by $h_n(\cdot)$ and $g_n(\cdot)$, which are equality and inequality constraints, respectively. HRT_{tn} is the hydraulic retention time of unit *t* in time period *n*. $CAPEX_t$ is the capital cost related to unit *t*, which is the function of design variables represented by $f_1(\cdot)$. $OPEX_{tn}$ is the operating cost of unit *t* in time period *n*, which is the function of design and operating variables represented by $f_{2n}(\cdot)$.

3.5.1. Modified Ludzack-Ettinger

Modified Ludzack-Ettinger (MLE) is one of the most widely used processes to remove nitrogen from wastewater, which involves an anoxic zone and aerobic zone where nitrification occurs in the aerobic zone and nitrate is then recycled back to the anoxic zone for denitrification reaction[31]. In the main reaction of MLE, the key reactant is converted to the other components with a given conversion efficiency, which is given by Eq. 14, and the conversion efficiency and reaction stoichiometry are shown in Table 4 (See Table 2 for the specific notation).

$$\begin{aligned} &C_{kjn}=C_{ijn}+\gamma_{j,react}\cdot\theta_{react}\cdot C_{i,react,n} \quad j\in\{S_S,X_I,X_{BH},X_{BA},X_P\},rr=S_S \\ &C_{kjn}=C_{ijn}+\gamma_{j,react}\cdot\theta_{react}\cdot C_{i,react,n} \quad j\in\{S_{NH},S_{NO},X_{ND}\},rr=S_{NH} \\ &C_{kjn}=C_{ijn}+\gamma_{j,react}\cdot\theta_{react}\cdot C_{i,react,n} \quad j=X_S,rr=X_S \\ &C_{kjn}=C_{ijn} \quad j\in\{S_I,S_{ND}\} \end{aligned} \tag{14}$$

$$\forall n\in N, i\in MLE_{in}, k\in MLE_{out}$$

The design and operating constraints of MLE are given by Eq. 15.

$$
\begin{aligned}
&V_{MLE,ae} = HRT_n^{MLE,ae} F_{in} \quad i \in MLE_{in}, \forall n \in N \\
&V_{MLE,an} = HRT_n^{MLE,an} F_{in} \quad i \in MLE_{in}, \forall n \in N \\
&HRT_n^{MLE,ae} = 0.6 HRT_n^{MLE,an} \quad \forall n \in N \\
&HRT_n^{MLE} = HRT_n^{MLE,ae} + HRT_n^{MLE,an} \quad \forall n \in N \\
&V_{MLE,ae} = 0.6 V_{MLE,an} \\
&V_{MLE} = V_{MLE,ae} + V_{MLE,an} \\
&V_{MLE} \geq SRT_n^{MLE} \cdot F_n^{w} \quad \forall n \in N \\
&\frac{25}{192} d \leq HRT_n^{MLE,an} \leq \frac{25}{64} d \quad \forall n \in N \\
&\frac{15}{192} d \leq HRT_n^{MLE,ae} \leq \frac{15}{64} d \quad \forall n \in N \\
&\frac{5}{24} d \leq HRT_n^{MLE} \leq \frac{5}{8} d \quad \forall n \in N \\
&7d \leq SRT_n^{MLE} \leq 12d \quad \forall n \in N
\end{aligned} \tag{15}
$$

In this set of equations, $V_{MLE,ae}$ and $V_{MLE,an}$ denote the volume of aerobic and anaerobic part of MLE respectively, and V_{MLE} is the total volume of MLE. $HRT_n^{MLE,ae}$ and $HRT_n^{MLE,an}$ are the hydraulic retention time of the aerobic and anaerobic part of MLE in time period *n* respectively. HRT_n^{MLE} and SRT_n^{MLE} are the hydraulic retention time and sludge retention time of MLE respectively.

The capital and operating costs of MLE are given by Eq. 16.

$$
\begin{aligned}
&CAPEX_{MLE} = IC_{ae} \left(V_{MLE,ae}\right)^{\alpha} + IC_{an} \left(V_{MLE,an}\right)^{\alpha} \\
&OPEX_{MLE,n} = p_{elec} \cdot \frac{1}{E_c} \cdot \left(\begin{array}{l} \left(0.94 - \dfrac{0.34}{1 + 0.12 SRT_n^{MLE}}\right)\left(BOD_n^{MLE} - BOD_n^{MLE,out}\right) \\ +4.33\left(TKN_n^{MLE} - NH_n^{MLE,out}\right) - \dfrac{0.096}{1 + 0.08 SRT_n^{MLE}} TKN_n^{MLE} \end{array} \right) \\
&\qquad + 24 \cdot M_e \cdot V_{MLE} + p_{elec} \cdot PF_{int} \cdot F_n^{int} \\
&BOD_n^{MLE} = 0.25\left(C_{i,S_S,n} + C_{i,X_S,n}\right) + 0.23\left(C_{i,X_{BH},n} + C_{i,X_{BA},n}\right) \\
&BOD_n^{MLE,out} = C_{k,S_I,n} + C_{i,S_S,n} + C_{k,X_I,n} + C_{k,X_S,n} + C_{k,X_{BH},n} + C_{k,X_{BA},n} + C_{k,X_P,n} \\
&TKN_n^{MLE} = 0.06\left(C_{i,X_I,n} + C_{i,X_P,n}\right) + 0.08\left(C_{i,X_{BH},n} + C_{i,X_{BA},n}\right) + C_{i,S_{NO},n} + C_{i,S_{ND},n} + C_{i,X_{ND},n} \\
&NH_n^{MLE,out} = C_{k,S_{NH},n}
\end{aligned} \tag{16}
$$

$$
i \in MLE_{in}, k \in MLE_{out}, \forall n \in N
$$

in which IC_{ae} and IC_{an} are unit capital cost of aerobic tank and anaerobic tank, respectively; p_{elec} is the price of electricity, E_c is the electricity consumption rate of oxygen transfer, M_e is the mixing energy consumption rate, and PF_{int} is the pumping energy factor for internal recycle. BOD_n^{MLE}, $BOD_n^{MLE,out}$, TKN_n^{MLE}, and $NH_n^{MLE,out}$ are the inlet flowrate of *BOD*, outlet flowrate of *BOD*, inlet flowrate of *BOD*, the inlet flowrate of total Kjeldahl nitrogen (*TKN*), and outlet flowrate of NH_3-*n*, respectively. We can see that $OPEX_{MLE,n}$ includes linear fractional terms.

Table 4 The conversion efficiency and reaction stoichiometry of different treatment process

Treatment unit	Key reactant	Reaction stoichiometry ($\gamma_{t,react}$)	Conversion (θ_{react})
MLE	S_S, S_{NH}, X_S	With respect to S_S:	100% S_S removal
		S_S = -1, X_I = 0.77, X_{BH} = 0.6	96% S_{NH} removal
		X_{BA} = 0.19, X_P = 0.87	97% X_S removal
		With respect to S_{NH}:	
		S_{NH} = -1, S_{NO} = 0.25, X_{ND} = 0.03	
		With respect to X_S:	
		X_S = -1	
OxD	S_S, S_{NH}, X_S	With respect to S_S:	100% S_S removal
		S_S = -1, X_I = 0.77, X_{BH} = 0.15	98% S_{NH} removal
		X_{BA} = 0.14, X_P = 0.97	97% X_S removal
		With respect to S_{NH}:	
		S_{NH} = -1, S_{NO} = 0.20, X_{ND} = -0.03	
		With respect to X_S:	
		X_S = -1	
AnD	X_{BH}, X_{BA}, X_S	With respect to X_{BH}:	100% X_{BH} removal
		X_{BH} = -1, S_{NH} = 0.07, X_P = 0.02	100% X_{BA} removal
		With respect to X_{BA}:	80% X_S removal
		X_{BA} = -1	
		With respect to X_S:	
		X_S = -1	
AeD	X_{BH}, X_{BA}	With respect to X_{BH}:	100% X_{BH} removal
		X_{BH} = -1, S_{NO} = 0.07, X_P = 0.27	100% X_{BA} removal
		With respect to X_{BA}:	
		X_{BA} = -1	

3.5.2. Oxidation Ditch

An Oxidation Ditch (OxD) is a modified activated sludge treatment process providing anaerobic and aerobic treatment in the same circular basin[32], which is similar to the treatment unit in a sequential batch reactor. In the main reaction of OxD, the key reactant is converted to other components with a given conversion, which is given by Eq. 17. The conversion and reaction stoichiometry are shown in Table 4.

$$\begin{aligned}
&C_{kjn} = C_{ijn} + \gamma_{j,react} \cdot \theta_{react} \cdot C_{i,react,n} \quad j \in \{S_S, X_I, X_{BH}, X_{BA}, X_P\}, rr = S_S \\
&C_{kjn} = C_{ijn} + \gamma_{j,react} \cdot \theta_{react} \cdot C_{i,react,n} \quad j \in \{S_{NH}, S_{NO}, X_{ND}\}, rr = S_{NH} \\
&C_{kjn} = C_{ijn} + \gamma_{j,react} \cdot \theta_{react} \cdot C_{i,react,n} \quad j = X_S, rr = X_S \\
&C_{kjn} = C_{ijn} \quad j \in \{S_I, S_{ND}\}
\end{aligned} \tag{17}$$

$$\forall n \in N, i \in OxD_{in}, k \in OxD_{out}$$

The design and operating constraints of OxD are given by Eq. 18.

$$
\begin{aligned}
&V_{OxD,ae} = HRT_n^{OxD,ae} F_{in} \quad i \in OxD_{in}, \forall n \in N \\
&V_{OxD,an} = HRT_n^{OxD,an} F_{in} \quad i \in OxD_{in}, \forall n \in N \\
&HRT_n^{OxD,ae} = 0.6 HRT_n^{OxD,an} \quad \forall n \in N \\
&HRT_n^{OxD} = HRT_n^{OxD,ae} + HRT_n^{OxD,an} \quad \forall n \in N \\
&V_{OxD,ae} = 0.6 V_{OxD,an} \\
&V_{OxD} = V_{OxD,ae} + V_{OxD,an} \\
&V_{OxD} \geq SRT_n^{OxD} \cdot F_n^w \quad \forall n \in N \\
&\frac{25}{48} d \leq HRT_n^{OxD,an} \leq \frac{25}{32} d \quad \forall n \in N \\
&\frac{15}{48} d \leq HRT_n^{OxD,ae} \leq \frac{15}{32} d \quad \forall n \in N \\
&\frac{5}{4} d \leq HRT_n^{OxD} \leq \frac{5}{6} d \quad \forall n \in N \\
&20d \leq SRT_n^{OxD} \leq 30d \quad \forall n \in N
\end{aligned} \tag{18}
$$

In this set of equations, $V_{OxD,ae}$ and $V_{OxD,an}$ denote the volume of aerobic and anaerobic part of OxD respectively, and V_{OxD} is the total volume of OxD. $HRT_n^{OxD,ae}$ and $HRT_n^{OxD,an}$ are the hydraulic retention time of the aerobic and anaerobic part of OxD in time period n, respectively. HRT_n^{OxD} and SRT_n^{OxD} are the hydraulic retention time and sludge retention time of OxD respectively.

The capital cost and operating cost of OxD are given by Eq. 19:

$$
\begin{aligned}
&CAPEX_{OxD} = IC_{ae}\left(V_{OxD,ae}\right)^{\alpha} + IC_{an}\left(V_{OxD,an}\right)^{\alpha} \\
&OPEX_{OxD,n} = p_{elec} \cdot \frac{1}{E_c} \cdot \left(\begin{array}{l} \left(0.94 - \dfrac{0.34}{1+0.12 SRT_n^{OxD}}\right)\left(BOD_n^{OxD} - BOD_n^{OxD,out}\right) \\ +4.33\left(TKN_n^{OxD} - NH_n^{OxD,out}\right) - \dfrac{0.096}{1+0.08 SRT_n^{OxD}} TKN_n^{OxD} \end{array} \right) \\
&\qquad + 24 \cdot M_e \cdot V_{OxD} \\
&BOD_n^{OxD} = 0.25\left(C_{i,S_S,n} + C_{i,X_S,n}\right) + 0.23\left(C_{i,X_{BH},n} + C_{i,X_{BA},n}\right) \\
&BOD_n^{OxD,out} = C_{k,S_I,n} + C_{k,S_S,n} + C_{k,X_I,n} + C_{k,X_S,n} + C_{k,X_{BH},n} + C_{k,X_{BA},n} + C_{k,X_P,n} \\
&TKN_n^{OxD} = 0.06\left(C_{i,X_I,n} + C_{i,X_P,n}\right) + 0.08\left(C_{i,X_{BH},n} + C_{i,X_{BA},n}\right) + C_{i,S_{NO},n} + C_{i,S_{ND},n} + C_{i,X_{ND},n} \\
&NH_n^{OxD,out} = C_{k,S_{NH},n}
\end{aligned} \tag{19}
$$

$$
i \in OxD_{in}, k \in OxD_{out}, \forall n \in N
$$

in which BOD_n^{OxD}, $BOD_n^{OxD,out}$, TKN_n^{OxD}, and $NH_n^{OxD,out}$ are the inlet flowrate of *BOD*, outlet flowrate of *BOD*, inlet flowrate of *BOD*, the inlet flowrate of total Kjeldahl nitrogen (*TKN*), and outlet flowrate of NH_3-n, respectively. We can see that $OPEX_{OxD,n}$ includes linear fractional terms.

3.5.3. Anaerobic digestion unit

Anaerobic digestion is among the oldest processes for the stabilization of solids and biosolids, and the decomposition of organic and inorganic matter. The major applications of anaerobic digestion are in the stabilization of concentrated sludge produced from the treatment of municipal and industrial wastewater. The main reaction can be described by Eq. 20.

$$\begin{aligned} &C_{kjn} = C_{ijn} + \gamma_{j,react} \cdot \theta_{react} \cdot C_{i,react,n} \quad j \in \{X_{BH}, S_{NH}, X_P\}, rr = X_{BH} \\ &C_{kjn} = C_{ijn} + \gamma_{j,react} \cdot \theta_{react} \cdot C_{i,react,n} \quad j = X_{BA}, rr = X_{BA} \\ &C_{kjn} = C_{ijn} + \gamma_{j,react} \cdot \theta_{react} \cdot C_{i,react,n} \quad j = X_S, rr = X_S \\ &C_{kjn} = C_{ijn} \quad j \in \{S_I, S_S, X_I, S_{NO}, S_{ND}, X_{ND}\} \\ &\forall n \in N, i \in AnD_{in}, k \in AnD_{out} \end{aligned} \tag{20}$$

The related conversion and reaction stoichiometry are presented in Table 4.

The design and operating constraints and capital cost of AnD are given by Eq. 21.

$$\begin{aligned} &V_{AnD} = SRT_n^{AnD} F_{in} \quad i \in AnD_{in}, \forall n \in N \\ &4d \le SRT_n^{AnD} \le 30d \quad \forall n \in N \\ &CAPEX_{AnD} = cc_{an} \cdot V_{AnD} \end{aligned} \tag{21}$$

where V_{AnD} is the volume of AnD, SRT_n^{AnD} is the sludge retention time of AnD in time period n, $CAPEX_{AnD}$ is the capital cost of AnD.

3.5.4. Aerobic digestion unit

Aerobic digestion has been used in several different processes, ranging from conventional to autothermal sludge treatment[33]. The main reaction can be described by Eq. 22, and the related conversion and reaction stoichiometry are also shown in Table 4.

$$\begin{aligned} &C_{kjn} = C_{ijn} + \gamma_{j,react} \cdot \theta_{react} \cdot C_{i,react,n} \quad j \in \{X_{BH}, S_{NH}, X_P\}, rr = X_{BH} \\ &C_{kjn} = C_{ijn} + \gamma_{j,react} \cdot \theta_{react} \cdot C_{i,react,n} \quad j = X_{BA}, rr = X_{BA} \\ &C_{kjn} = C_{ijn} + \gamma_{j,react} \cdot \theta_{react} \cdot C_{i,react,n} \quad j = X_S, rr = X_S \\ &C_{kjn} = C_{ijn} \quad j \in \{S_I, S_S, X_I, S_{NO}, S_{ND}, X_{ND}\} \\ &\forall n \in N, i \in AeD_{in}, k \in AeD_{out} \end{aligned} \tag{22}$$

The design and operating constraints and capital cost of AeD are given by Eq. 23.

$$\begin{aligned} &V_{AeD} = SRT_n^{AeD} F_{in} \quad i \in AeD_{in}, \forall n \in N \\ &4d \le SRT_n^{AeD} \le 30d \quad \forall n \in N \\ &CAPEX_{AeD} = cc_{ae} \cdot V_{AeD} \end{aligned} \tag{23}$$

where V_{AeD} is the volume of AeD, SRT_n^{AeD} is the sludge retention time of AeD in time period n, $CAPEX_{AeD}$ is the capital cost of AeD.

3.6. Objective function

The objective function addressed in this article is total annualized cost (TAC), which is widely used in many articles to solve water network problems[(14)]. TAC consists of annualized capital cost and operating cost. Capital cost includes capital cost for primary clarifier, secondary clarifier, wastewater bio-treatment units, and sludge bio-treatment units. Operating cost consists of cost for clarifiers, wastewater bio-treatment units operating cost, thickening unit operating cost, dewatering unit operating cost, sewage charge cost, and penalty cost. We define: $CAPEX$ as the total capital cost; $OPEX_n$ as the total operating cost in period *n*; $CAPEX_{pc}$ as primary clarifier capital cost; $CAPEX_{sc}$ as secondary clarifier capital cost; $CAPEX_{bio}$ as wastewater bio-treatment units capital cost; $CAPEX_{ad}$ as sludge bio-treatment units operating cost; $OPEX_{n,clarifier}$ as operating cost of clarifiers in time period *n*; $OPEX_{n,bio}$ as operating cost of wastewater bio-treatment unit in time period *n*; $OPEX_{n,thick}$ as operating cost of thickening unit in time period *n*; $OPEX_{n,dewat}$ as operating cost of dewatering unit in time period *n*; $OPEX_{n,charge}$ as the sewage charge for compliant emission in time period *n*; $OPEX_{n,penalty}$ as the penalty charge for noncompliant emission in time period n. TAC, $CAPEX$, and $OPEX$ are given by Eq. 24.

$$\begin{aligned} &TAC = AR \cdot CAPEX + H \cdot \sum\nolimits_{n \in N} OPEX_n \\ &CAPEX = CAPEX_{pc} + CAPEX_{sc} + CAPEX_{bio} + CAPEX_{ad} \\ &OPEX_n = OPEX_{n,clarifier} + OPEX_{n,bio} + OPEX_{n,thick} \\ &\qquad + OPEX_{n,dewat} + OPEX_{n,charge} + OPEX_{n,penalty} \end{aligned} \tag{24}$$

where AR is the annualized factor for investment cost, and H is the annualized factor for operating cost.

The specific formulations of each capital cost are given by Eq.25.

$$\begin{aligned} &CAPEX_{pc} = IC_{pc} \cdot \left(V_{pc}\right)^{\alpha} \\ &CAPEX_{sc} = IC_{sc} \cdot \left(V_{sc}\right)^{\alpha} \\ &CAPEX_{bio} = CAPEX_{MLE} + CAPEX_{OxD} \\ &CAPEX_{ad} = CAPEX_{AnD} + CAPEX_{AeD} \end{aligned} \tag{25}$$

where IC_{pc} and IC_{sc} are capital cost parameter of primary and secondary clarifier, respectively. $CAPEX_{MLE}$, $CAPEX_{OxD}$, $CAPEX_{AnD}$, and $CAPEX_{AeD}$ are given by Eq. 16, Eq. 19, Eq. 21, and Eq. 23, respectively. The capital cost includes concave terms in Eq. 25.

Different categories of operating cost are given by Eq. 26

$$\begin{aligned} &OPEX_{n,clarifier} = \sum\nolimits_{t \in TU1} \sum\nolimits_{l \in t_{underflow}} PF_t \cdot F_{l,n} \\ &OPEX_{n,bio} = OPEX_{n,MLE} + OPEX_{n,OxD} \\ &OPEX_{n,thick} = p_{elec} \cdot PF_{tu} \cdot F_n^{tu} \\ &OPEX_{n,dewat} = p_{elec} \cdot PF_{du} \cdot F_n^{du} \end{aligned} \tag{26}$$

where PF_t, PF_{tu}, and PF_{du} are the pumping energy factor for underflow of clarifier, thickening, and dewatering unit, respectively. F_{tu} and F_{du} are the underflow of thickening, and dewatering unit respectively. $OPEX_{n,MLE}$ and $OPEX_{n,OxD}$ are given in Eq. 16 and Eq. 19, respectively.

According to the water pollutant discharge standards and charge system in China[34], sewage charge and penalty charge are imposed on pollutants. We consider four main pollutants in this article: *COD*, *BOD*, *TSS*, and NH_3-*n*. The sewage charge and penalty charge are given by Eq. 27:

$$\begin{aligned} OPEX_{n,charge} &= OPEX_{COD,n}^{charge} + OPEX_{COD,n}^{charge} + OPEX_{TSS,n}^{charge} + OPEX_{NH_3-n,n}^{charge} \\ OPEX_{n,penalty} &= OPEX_{COD,n}^{penalty} + OPEX_{COD,n}^{penalty} + OPEX_{TSS,n}^{penalty} + OPEX_{NH_3-n,n}^{penalty} \end{aligned} \tag{27}$$

As for each pollutant, the sewage charge and penalty charge are modeled using disjunctions, which are given by Eq. 28 to Eq. 31.

$$\begin{bmatrix} Y_{COD,n}^{compli} \\ COD_n^{eff} \le lim_{COD} F_n^{eff} \\ OPEX_{COD,n}^{charge} = \dfrac{cr \cdot COD_n^{eff}}{load_{COD}} \\ OPEX_{COD,n}^{penalty} = 0 \end{bmatrix} \vee \begin{bmatrix} Y_{COD,n}^{exceed} \\ COD_n^{eff} \ge lim_{COD} F_n^{eff} + \varepsilon \\ OPEX_{COD,n}^{charge} = 0 \\ OPEX_{COD,n}^{penalty} = \dfrac{pr \cdot COD_n^{eff}}{load_{COD}} \end{bmatrix} \tag{28}$$

$$Y_{COD,n}^{compli} \in \{True, False\}, Y_{COD,n}^{exceed} \in \{True, False\}, \forall n \in N$$

$$\begin{bmatrix} Y_{BOD,n}^{compli} \\ BOD_n^{eff} \le lim_{BOD} F_n^{eff} \\ OPEX_{BOD,n}^{charge} = \dfrac{cr \cdot BOD_n^{eff}}{load_{BOD}} \\ OPEX_{BOD,n}^{penalty} = 0 \end{bmatrix} \vee \begin{bmatrix} Y_{BOD,n}^{exceed} \\ BOD_n^{eff} \ge lim_{BOD} F_n^{eff} + \varepsilon \\ OPEX_{BOD,n}^{charge} = 0 \\ OPEX_{BOD,n}^{penalty} = \dfrac{pr \cdot BOD_n^{eff}}{load_{BOD}} \end{bmatrix} \tag{29}$$

$$Y_{BOD,n}^{compli} \in \{True, False\}, Y_{BOD,n}^{exceed} \in \{True, False\}, \forall n \in N$$

$$\begin{bmatrix} Y_{TSS,n}^{compli} \\ TSS_n^{eff} \le lim_{TSS} F_n^{eff} \\ OPEX_{TSS,n}^{charge} = \dfrac{cr \cdot TSS_n^{eff}}{load_{TSS}} \\ OPEX_{TSS,n}^{penalty} = 0 \end{bmatrix} \vee \begin{bmatrix} Y_{TSS,n}^{exceed} \\ TSS_n^{eff} \ge lim_{TSS} F_n^{eff} + \varepsilon \\ OPEX_{TSS,n}^{charge} = 0 \\ OPEX_{TSS,n}^{penalty} = \dfrac{pr \cdot TSS_n^{eff}}{load_{TSS}} \end{bmatrix} \tag{30}$$

$$Y_{TSS,n}^{compli} \in \{True, False\}, Y_{TSS,n}^{exceed} \in \{True, False\}, \forall n \in N$$

$$\begin{bmatrix} Y_{NH_3-n,n}^{compli} \\ NH_3-n_n^{eff} \le lim_{NH_3-n} F_n^{eff} \\ OPEX_{NH_3-n,n}^{charge} = \dfrac{cr \cdot NH_3-n_n^{eff}}{load_{NH_3-n}} \\ OPEX_{NH_3-n,n}^{penalty} = 0 \end{bmatrix} \vee \begin{bmatrix} Y_{NH_3-n,n}^{exceed} \\ NH_3-n_n^{eff} \ge lim_{NH_3-n} F_n^{eff} + \varepsilon \\ OPEX_{NH_3-n,n}^{charge} = 0 \\ OPEX_{NH_3-n,n}^{penalty} = \dfrac{pr \cdot NH_3-n_n^{eff}}{load_{NH_3-n}} \end{bmatrix} \quad (31)$$

$$Y_{NH_3-n,n}^{compli} \in \{True, False\}, Y_{NH_3-n,n}^{exceed} \in \{True, False\}, \forall n \in N$$

Consider the discharge of *COD* given by Eq. 28 for example, $Y_{COD,n}^{compli}$ and $Y_{COD,n}^{exceed}$ are Boolean variables indicating if *COD* discharge violates the discharge limitation lim_{COD}. COD_n^{eff} is the flowrate of *COD* in effluent in time period *n*, F_n^{eff} is the flowrate of effluent in time period *n*, cr is the sewage charge rate, pr is the penalty rate, and $load_{COD}$ is the load factor of *COD*. The load factors of *COD*, *BOD*, *TSS*, and *NH_3-n* are presented in Table 5.

Table 5 Load factors of different pollutants[34]

Pollutant	Load factor
COD	0.5
BOD	1
TSS	4
NH_3-n	0.8

4. Computational strategies

4.1. Strategy for Global Optimization

The problem given by equations in 1-31, includes several bilinear, linear fractional, and concave terms. Therefore, the resulting problem is a multi-period nonconvex generalized disjunctive programming (GDP-m), which is reformulated as an MINLP using the hull reformulation for the disjunctions[35]. Due to the nonconvexity of the problem, we may obtain suboptimal solutions if using non-global solvers. Therefore, a more efficient global optimization strategy is needed if we want to solve this nonconvex GDP model to global optimality.

In the multi-period model (GDP-m), the design variable (d_{rt}) are complicating variables which need to be accounted for in all periods. We can define copy variables d_{rt}^n for each period, then the complicating variables can be reformulated as complicating constraints as shown in Eq. 32

$$d_{rt}^1 = d_{rt}^n \quad \forall t \in TU3 \cup TU4, r = 1,...,RT_t, n = 2,...,|N| \quad (32)$$

This allows decomposing the problem by relaxing the complicating constraints.

We propose a Lagrangean-based decomposition algorithm shown in Figure 3, which is inspired by the work of Yang and co-workers[20]. The proposed algorithm consists of an outer problem and an inner problem. We first obtain a global upper bound (GUB) by solving problem (*P*) using a non-global MINLP solver and then fix the technology selection binary variables. The outer problem determines a global lower bound (GLB) by solving the relaxation problem (*RP*). For each technology selection combination, the inner problem is solved using Lagrangean decomposition algorithm. The decomposed subproblems (SP_1)-(SP_N) determine the local lower bound (LLB), and the local solution of *P* with fixed discharge related binary variables determines the local upper bound (LUB).

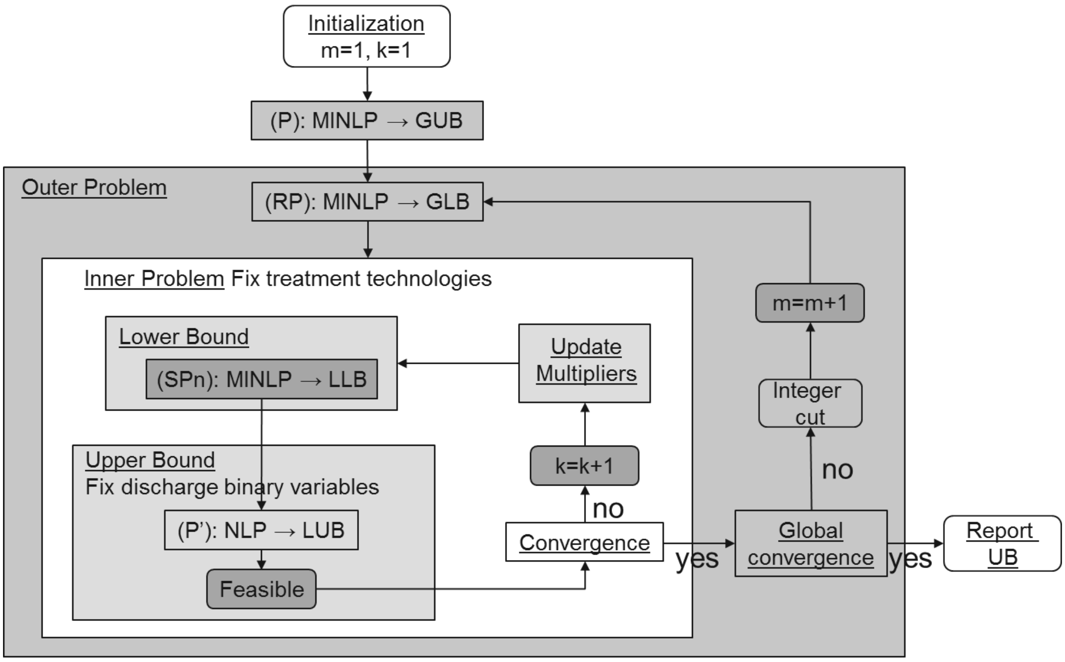

Figure 3 Block diagram of decomposition algorithm

4.2. Subproblem Descriptions

The original problem (GDP-m) is a multi-period nonconvex GDP. Problem (*P*) is a multi-period nonconvex MINLP (mixed-integer nonlinear programming) that results from reformulating problem (GDP-m) using the hull reformulation[35]. The relevant hull reformulation can be found in the Appendix A. Problem (*RP*) is the convex relaxation of problem (*P*), which is obtained by replacing all nonconvex terms in (*P*) with their convex underestimators. Therefore, the solution of problem (*RP*) provides a valid lower bound of problem (*P*). The relevant nonconvex terms and related convex underestimators can be found in the Appendix B. Problems (SP_n) are nonconvex MINLPs obtained from decomposing problem (*P*) into |*N*| single-period problem by dualizing complicating constraints related to design variables given by Eq. 32. The objective function of problem (SP_n) is given by Eq. 33.

$$\begin{aligned} &min \quad TAC_1 = \frac{1}{|N|} AR \cdot CAPEX + H \cdot OPEX_1 + \sum_{n=2}^{|N|} \lambda_n d_{rt}^1 \\ &min \quad TAC_n = \frac{1}{|N|} AR \cdot CAPEX + H \cdot OPEX_n - \lambda_n d_{rt}^n \quad n = 2,\ldots,|N| \end{aligned} \tag{33}$$

Problem (*P'*) is the resulting NLP (Nonlinear Programming) upper bounding problem by fixing all binary variables in problem (*P*), in which Y_{rt} are determined by the solution of problem (*P*), and discharge binary variables ($Y_{COD,n}^{compli}$, $Y_{COD,n}^{exceed}$, $Y_{BOD,n}^{compli}$, $Y_{BOD,n}^{exceed}$, $Y_{TSS,n}^{compli}$, $Y_{TSS,n}^{exceed}$, $Y_{NH_n-n}^{compli}$, and $Y_{NH_n-n}^{exceed}$) are determined by the solution of problem (SP_n).

4.3. Algorithm

The specific steps of the proposed decomposition algorithm are as follows:

Step 1: Initialization:

Set the GUB to ∞ and GLB to $-\infty$. Set outer iteration count m to 1 and inner iteration count k to 1. Set the initial Lagrangean multiplier λ_n as the dual values of dualized constraints from the linear relaxation of the problem (*P*).

Step 2: Global Upper Bound:

Solve the MINLP problem (*P*) using non-global MINLP solvers such as DICOPT or SBB. Fix the technology selection binary variables for the inner problem according to the solution of problem (*P*).

Step 3: Global Lower Bound:

Solve problem (*RP*) to global optimality to determine the global lower bound.

Step 4: Inner Problem:

i. Solve problem (SP_n) for each period $n \epsilon N$ to global optimality for the fixed binary variables (technology selection). The local lower bound is obtained by summing the subproblems' objective $TAC_n^*(n \in N)$. Once the (SP_n) problems are solved, fix the discharge related binary variables.

ii. Solve problem (*P'*) to local optimality with fixed binary variables (technology selection and discharge), then update Z^{LUB}.

iii. Check for convergence of the inner problem. If $Z^{LUB} \leq Z^{GUB}$, then replace Z^{GUB} with Z^{LUB}; if $(Z^{LUB} - Z^{LLB})/Z^{LUB} \leq \epsilon_1$ or $Z^{LLB} \geq Z^{GUB}$, end the inner loop.

iv. Update the Lagrangean multipliers[36], and set $k = k + 1$.

Step 5: Convergence test:

Check if the global convergence criteria is satisfied: $(Z^{GUB} - Z^{GLB})/Z^{GUB} < \epsilon$. If the criteria is not satisfied, add the integer cut shown in Eq.34. Set $m = m + 1$.

$$\sum_{(r,t)\in S_{rt}^1} (1 - Y_{rt}) + \sum_{(r,t)\in S_{rt}^0} Y_{rt} \geq 1$$
$$S_{rt}^1 = \{(r,t) \mid Y_{rt} = 1\} \quad S_{rt}^0 = \{(r,t) \mid Y_{rt} = 0\} \tag{34}$$

5. Numerical examples

In this section, we present results of several numerical examples. First, we provide an illustrative example to show the optimal treatment network under the given discharge standard and penalty rate. Second, we present the computational performance to demonstrate the effectiveness and efficiency of the proposed method. The impacts of discharge limitation for contaminants and penalty rates for noncompliant discharge are then studied in detail to provide useful insights for relevant policy makers to improve the policy-making process.

In this article, we consider the wastewater management policy scenarios in China, which include discharge standard, charge rate for compliant discharge, and penalty rate for noncompliant discharge. The discharge standard considered here is the discharge standard for Xiaoqinghe in the Shandong province in China shown in Table 6, which has changed 3 times since it was established in 2007. We take the value of charge rate for compliant discharge as 1.4 yuan per load according to the regulation of National Development and Reform Commission in 2014(34). The penalty rate for noncompliant discharge in China used to be 2.8 yuan per load(37). A consecutive daily penalty has been implemented since January 1, 2015 (according to the Environmental Protection Law of the People's Republic of China), which may result in a significantly increased penalty for noncompliant discharge. We consider a penalty rate of 28 and 280 yuan per load for comparison in this article.

Table 6 The discharge standard for Xiaoqinghe in Shandong province (http://www.mep.gov.cn)

Standard	Time	COD (mg/L)	BOD (mg/L)	TSS (mg/L)	NH_3-n (mg/L)
Standard 1	2007.04-2008.06	100	40	70	15
Standard 2	2008.07-2009.06	80	30	70	15
Standard 3	2009.07-2012.12	60	20	70	10
Standard 4	2013.01-	50	10	20	5

The influent data used in this article is sampled from the predefined dynamic influent of BSM2, which is shown in Figure 4. In all 12 time periods, influent data in period 1 is the influent with largest contaminant concentration, and influent data in period 3 is the influent with the smallest contaminant concentration.

Problem (GDP-m) is reformulated as a multi-period MINLP using the hull reformulation(35). The MINLP models are implemented with GAMS 24.7(38) and solved on an Intel Core i5 2.30 GHz CPU and RAM 4.0 GB. DICOPT(39) and SBB(40) are used as the local solver of MINLP, and BARON 15.6.5(41) is used as the global solver of MINLP.

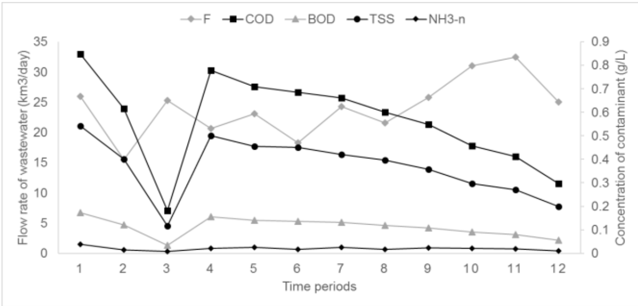

Figure 4 Flowrate of influent and concentration of COD, BOD, TSS, and NH_3-n

5.1. Illustrative example

We consider the network whose superstructure is shown in Figure 2 as the illustrative example. The environmental discharge limitation for the contaminants is standard 4 (*COD*≤50 mg/L, *BOD*≤10 mg/L; *TSS*≤20 mg/L; *NH3-n*≤5 mg/L), and the penalty rate is taken to be 280 yuan/load. We apply the proposed algorithm to solve this problem, and the resulted optimal network structure and flows with a total cost of 192, 457.20 yuan are shown in Figure 5. For each flow, there are three numbers, which represent streams in three periods. We can see that Oxidation Ditch is chosen as the wastewater treatment technology and Aerobic Digestion is chosen as the sludge treatment technology. In the optimal treatment network, wastewater is first treated by the primary clarifier, and all the flow is then guided to the biotreatment unit and no flow is bypassed. After the separation of the secondary clarifier, the overflow is discharged and the underflow is then treated. The overflows of the thickener and dewatering units are all recycled to the biotreatment unit.

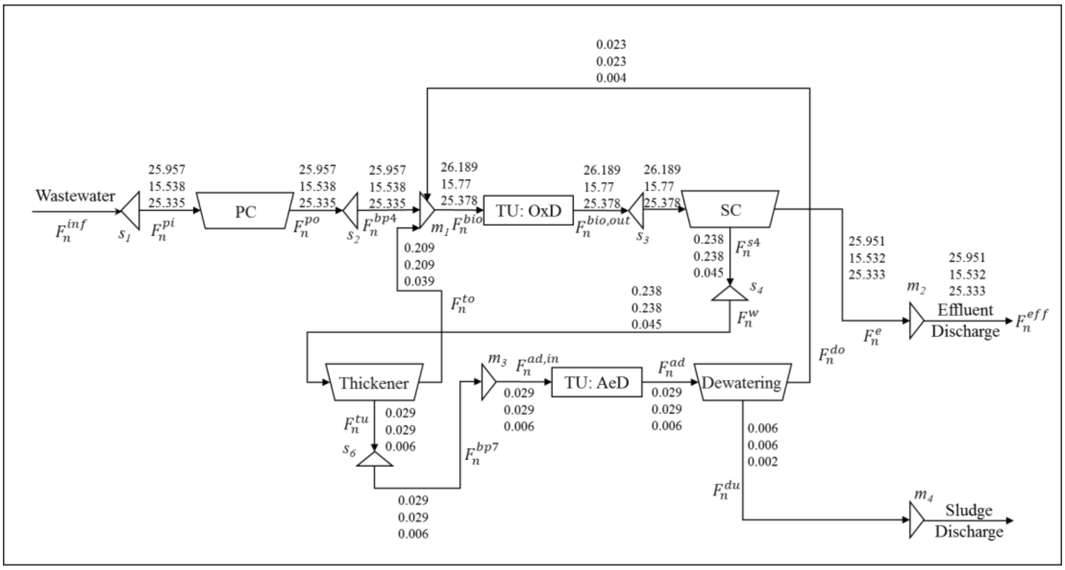

Figure 5 Optimal network structure for the illustrative example

The concentrations of contaminants in the main streams in the optimal network are presented in Table 7. We can see that contaminants are mainly removed by the primary clarifier, the biotreatment unit, and the secondary clarifier. Specifically, particulate matters are first separated by the primary clarifier, nitrogen is digested in the biotreatment unit, and the resulted particulate matters are then separated by secondary clarifier. We can see that the discharges of *BOD* and NH_3-*n* are within the discharge limitation in all 3 periods, while the discharges of *COD* and *TSS* are in excess of the discharge limitation in period 1 and 2.

Table 7 Concentrations of main streams in the optimal network

	Concentration (mg/L)											
	COD			BOD			TSS			NH_3-n		
Stream	n1	n2	n3	n1	n2	n3	n1	n2	n3	n1	n2	n3
F_n^{pi}	849	615	181	172	121	34	542	401	117	39	22	8.9
F_n^{po}	288	210	65	56	38	10	158	116	34	39	22	8.9
F_n^{bio}	359	251	76	59	40	11.1	212	147	42	40	23	9.1
$F_n^{bio,out}$	262	171	50	12	8.51	2.34	177	106	27	0.8	0.44	0.2
F_n^{eff}	99	74	26	3.81	2.64	0.73	55	33	8.35	0.8	0.45	0.2
Discharge limitation	50			10			20			5		

5.2. Computational performance

We consider the problem of *n*-period influent, in which the influent data is period 1 to period *n* (*n*=3, 5, 8, 10, 12) in Figure 4. The wastewater management policy scenarios are the combination of 3 different penalty rates (2.8 yuan/load, 28 yuan/load, and 280 yuan/load) and 4 discharge standards (standard 1, standard 2, standard 3, and standard 4 shown in Table 6). The problem size of the tested cases is given in Table 8, which shows the number of variables, number of equations, number of nonlinear variables, and number of binary variables. We can see that the problem size increases with the number of periods in the case.

The tested cases are first solved using the proposed method, and then compared with the results solved by BARON. The CPU time limitation is 7200 seconds. We compare the scaled TAC, gap, and CPUs of the proposed method and BARON solver, and the specific results are shown in Appendix C. For the scaled TAC, BARON performs better than the proposed algorithm in some instances, but the gaps are very close. For the gap, the proposed method dominates BARON in most instances. For the CPU time, the proposed method dominates BARON in most instances.

The CPU time statistics are shown in Figure 6. For every 4 tested cases with the same penalty rate, we do the average of their CPU times. For example, “1.4-2.8” is the average of scenario 1.4-2.8-Standard 1, 1.4-2.8-Standard 2, 1.4-2.8-Standard 3, and 1.4-2.8-Standard 4. For the same penalty rate, the CPU time increases with the number of periods of tested cases, which is resulting from the increased size of problem. For the same problem size, CPU time decreases with increased penalty rate. The reason that the problems with large penalty rate can be solved more efficiently can be explained as follows. When the penalty rate is large, the value of binary variables relevant to technology selection and discharge in decomposed single-period problems are the same with that of the corresponding multi-period problem, which yields a tight lower bound for the multi-period problem.

Table 8 Problem size of tested cases

Case	Number of variables	Number of equations	Number of nonlinear variables	Number of binary variables
3-period	1,381	1,133	399	28
5-period	2,299	1,883	661	44
8-period	3,676	3,008	1,054	68
10-period	4,594	3,758	1,316	84
12-period	5,512	4,508	1,578	100

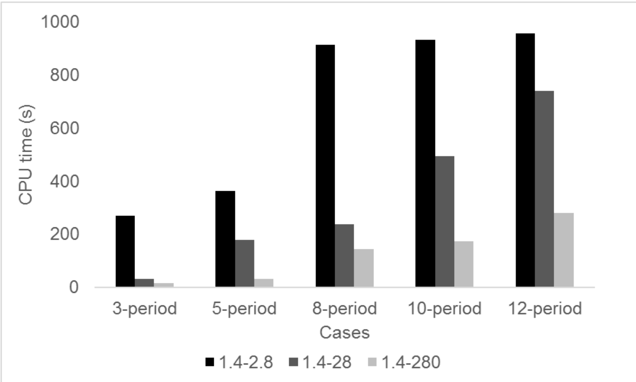

Figure 6 Average CPU time of tested cases

5.3. Impact of discharge standard

In this section, the 12-period problem is used to study the impact of discharge standard on total annualized cost (TAC) under different penalty rates. Figure 7 shows the results of TAC and its components under each discharge standard when penalty rate is 2.8 yuan per load. As can be seen, the main contributions to TAC are capital cost, treatment cost, emission charge, and penalty cost. In addition, TAC increases with more stringent discharge standard, which is mainly due to the increase of the penalty cost. The decrease of emission charge offsets the sharp increase of penalty rate, which results in the slow increase of TAC. Therefore, WWTP tends to pay higher penalty cost to handle more stringent discharge standard in this case.

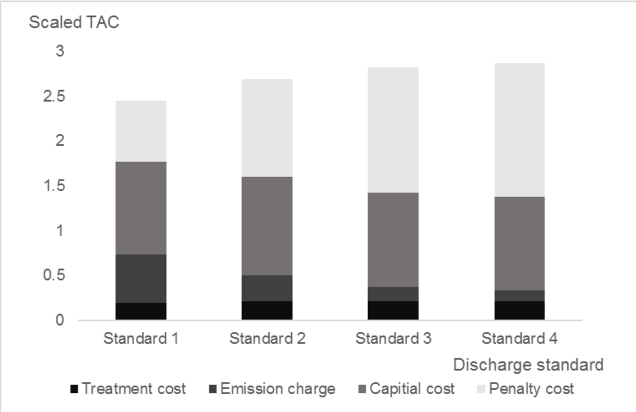

Figure 7 Comparison analysis of discharge standard on total annualized cost when penalty rate is 2.8 yuan per load

Figure 8 shows the results of TAC and its components under each discharge standard when the penalty rate is 28 yuan per load. We can see from Figure 8 that the main contributions to TAC are capital cost, treatment cost, emission charge, and penalty cost. The increase of the TAC is mainly caused by the sharp increase of the penalty cost. In addition, the treatment cost also increases significantly (more than 100%), which means WWTP tends to increase the investement on wastewater treatment in this case.

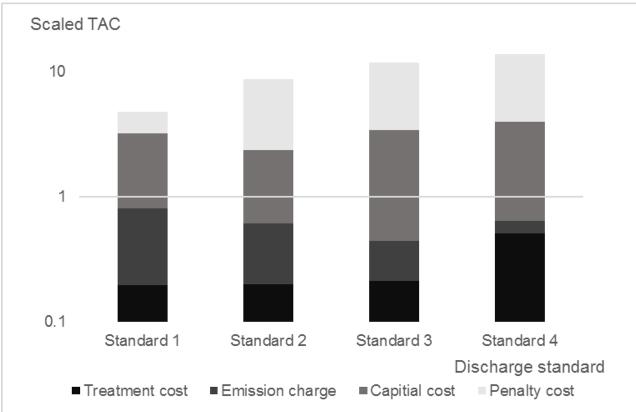

Figure 8 Comparison analysis of discharge standard on total annualized cost when penalty rate is 28 yuan per load

Figure 9 shows the results of TAC and its components under each discharge standard when the penalty rate is 280 yuan per load. As can be seen, the TAC increases significanly with more stringent discharge standard, which results from the sharp increase of the penalty cost. Besides, penalty cost dominates other components of TAC in standard 2, 3, and 4. In other words, WWTP has to pay a huge penalty cost for noncompliant discharge when discharge standard is stringent in this case.

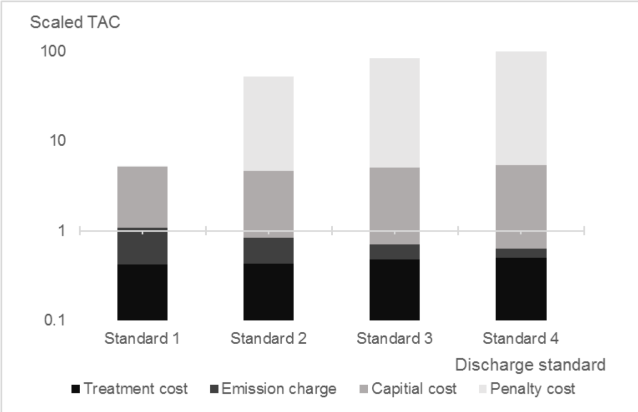

Figure 9 Senstive analysis of discharge standard on total annualized cost when penalty rate is 280 yuan per load

In conclusion, the impact of the discharge rate on the total annualized cost varies with different penalty rates. When the penalty rate is small, WWTP tends to increase the investment on wastewater treatment to handle more stringent discharge standards; when the penalty rate is large (i.e., 200 times of sewage charge rate), WWTP has to pay a large penalty cost for noncompliant discharge when the discharge standard is stringent.

5.4. Impact of penalty rate

In this section, the 12-period problem is used the study the impact of penalty rate on total annualized cost under different discharge standards. Figure 10 shows the results of TAC and its components under each penalty rate. When the discharge standard is standard 1 (shown in Figure 10a), the TAC increases with larger penalty rate, which is mainly due to the significant increase of capital cost and treatment cost. This means that WWTP tends to increase the investment on wastewater treatment to improve the effluent quality in this case.

Shown in Figure 10b are the results of the TAC and its components under each penalty rate when discharge standard is standard 2. As can be seen, TAC increases significantly with larger penalty rate. Specifically, capital cost and treatment cost increase significantly (more than 200% for capital cost and around 100% for biotreatment cost). The most important increase for the TAC comes from the sharp increase of the penalty cost. This means the WWTP has to pay more penalty cost when penalty rate is large in this case, although it has increased the investment on wastewater treatment.

Figure 10c shows the results of TAC and its components under each penalty rate when discharge standard is standard 3. We can see that the results are quite similar with the case when discharge standard is standard 2. TAC increases significantly with larger penalty rate, which is mainly due to the sharp increase of penalty cost. Simultaneously, capital cost and treatment cost also increase significantly (more than 300% for capital cost and more than 120% for biotreatment cost). This means that although WWTP tends to increase the investment on wastewater treatment, it has to pay a large penalty cost when penalty rate is large in this case.

Shown in Figure 10d are the results of TAC and its components under each penalty rate when the discharge standard is standard 4. We can see that the results in this case are quite similar with the case when the discharge standard is standard 3. Capital cost, treatment cost, and penalty cost all increase significantly when the penalty rate increases, which leads to the sharp increase of TAC. Therefore, the WWTP also has to pay a large penalty cost when penalty rate is large in this case.

In conclusion, the impact of penalty rate on total annualized cost varies with different discharge standards. When discharge standards are loose, the WWTP tends to improve the effluent quality; when the discharge standard becomes stringent, the WWTP has to pay both high penalty cost and wastewater treatment cost to handle large penalty rate.

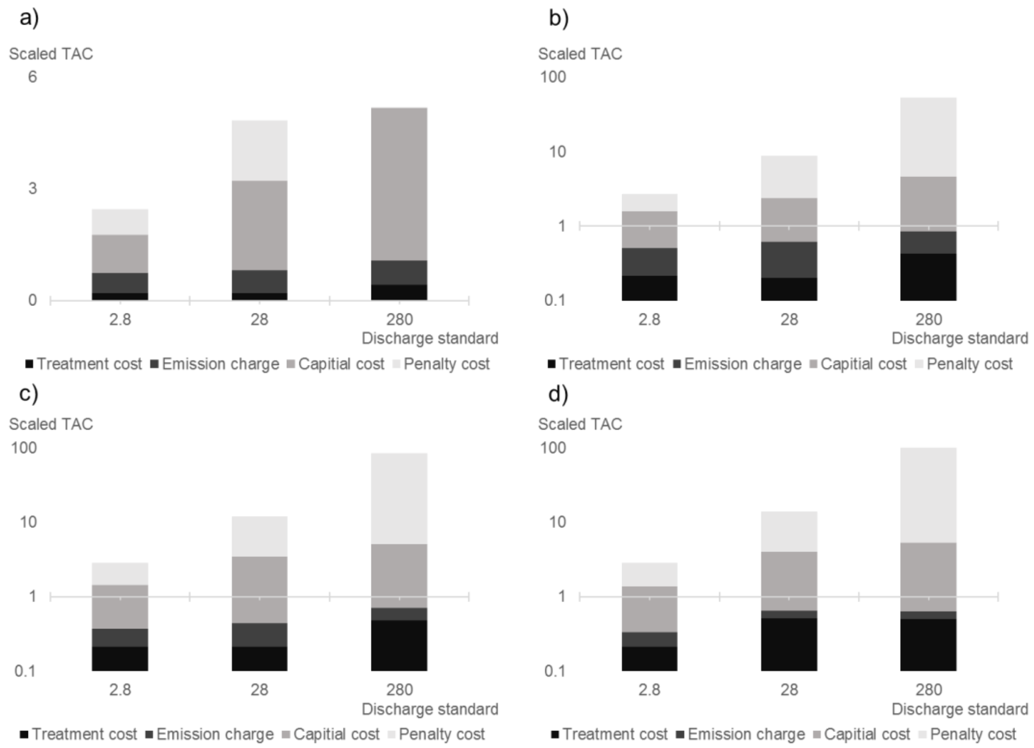

Figure 10 Senstive analysis of penalty rate on total annualized cost: (a) standard 1; (b) standard 2; (3) standard 3; (d) standard 4

6. Conclusion

This article has addressed the problem of optimal synthesis and operation of wastewater treatment process considering dynamic influent under different discharge standards and penalty rates of noncompliant emissions. To do this, we developed a comprehensive model (GDP-m), in which unit models are used for the wastewater treatment units, and the selection of treatment technology and the discharge of wastewater are modeled using disjunctions. In order to solve the resulting multi-period MINLP model to global optimality, we proposed a Lagrangean-based decomposition algorithm. Numerical studies have verified the effectiveness of the algorithm, and comparison studies also provided policy insights for policy makers. Moreover, experiments on the total annualized cost show that the impacts of discharge standard and penalty rate interact with each other, which motivates policy makers that different policy instruments should cooperate with each other.

Appendix A: Hull reformulation

Table A1 Reformulation of Disjunctions with Linear Constraints[35]

(GDP) Disjunctions		(Hull Reformulation) Constraints	
		$x = \sum_{i \in D_k} \nu^{ki}$	$k \in K$
$\vee_{i \in D_k} \begin{bmatrix} Y_{ki} \\ A^{ki} x \le a^{ki} \end{bmatrix}$	$k \in K$	$A^{ki} \nu^{ki} \le a^{ki} y_{ki}$	$k \in K, i \in D_k$
$\underline{\vee}_{i \in D_k} Y_{ki}$	$k \in K$	$x^{lo} y_{ki} \le \nu^{ki} \le x^{up} y_{ki}$	$k \in K, i \in D_k$
		$\sum_{i \in D_k} y_{ki} = 1$	$k \in K$

Table A2 Reformulation of Disjunctions with Nonlinear Constraints[35]

(GDP) Disjunctions		(Hull Reformulation) Constraints	
		$x = \sum_{i \in D_k} \nu^{ki}$	$k \in K$
$\vee_{i \in D_k} \begin{bmatrix} Y_{ki} \\ r_{ki}(x) \le 0 \end{bmatrix}$	$k \in K$	$y_{ki} r_{ki} \left(\nu^{ki} / y_{ki} \right) \le 0$	$k \in K, i \in D_k$
$\underline{\vee}_{i \in D_k} Y_{ki}$	$k \in K$	$x^{lo} y_{ki} \le \nu^{ki} \le x^{up} y_{ki}$	$k \in K, i \in D_k$
		$\sum_{i \in D_k} y_{ki} = 1$	$k \in K$

Appendix B: Convex envelopes

- Bilinear terms[42]: $F \cdot C \rightarrow fc$; $F \cdot HRT \rightarrow fh$

$$\left. \begin{aligned} fc &\ge F^{min} \times C + F \times C^{min} - F^{min} \times C^{min} \\ fc &\ge F^{max} \times C + F \times C^{max} - F^{max} \times C^{max} \\ fc &\le F^{min} \times C + F \times C^{max} - F^{min} \times C^{max} \\ fc &\le F^{max} \times C + F \times C^{min} - F^{max} \times C^{min} \end{aligned} \right\} \tag{32}$$

$$\left. \begin{aligned} fh &\ge F^{min} \times HRT + F \times HRT^{min} - F^{min} \times HRT^{min} \\ fh &\ge F^{max} \times HRT + F \times HRT^{max} - F^{max} \times HRT^{max} \\ fh &\le F^{min} \times HRT + F \times HRT^{max} - F^{min} \times HRT^{max} \\ fh &\le F^{max} \times HRT + F \times HRT^{min} - F^{max} \times HRT^{min} \end{aligned} \right\} \tag{33}$$

- Concave term[20]: $V^{\alpha} \rightarrow \Theta$

$$\Theta \geq \left(V^{min}\right)^{\alpha} + \left(\frac{\left(V^{max}\right)^{\alpha} - \left(V^{min}\right)^{\alpha}}{V^{max} - V^{min}}\right)\left(V - V^{min}\right) \tag{34}$$

Appendix C: Comparison of computational results

Table C1 The comparison of scaled total annualized cost, gap, and CPUs between the proposed method and BARON for 3-period case

Policy scenario	Scaled TAC		Gap		CPUs	
	Proposed	BARON	Proposed	BARON	Proposed	BARON
1.4-2.8-Standard 1	0.613	0.613	**0.049**	0.050	**95.569**	1057.56
1.4-2.8-Standard 2	0.654	0.654	**0.046**	0.050	**214.3**	1487.85
1.4-2.8-Standard 3	0.654	0.654	0.050	0.050	**87.704**	3757.84
1.4-2.8-Standard 4	0.659	**0.657**	**0.049**	0.050	**683.52**	5145.21
1.4-28-Standard 1	1.273	1.273	0.049	0.049	61.237	**21.2**
1.4-28-Standard 2	2.276	**2.268**	**0.049**	0.050	**42.586**	73.54
1.4-28-Standard 3	2.929	2.929	**0.043**	0.050	**13.416**	106.76
1.4-28-Standard 4	3.084	3.084	**0.046**	0.048	**13.714**	41.28
1.4-280-Standard 1	1.278	1.278	**0.041**	0. 048	**22.381**	25.7
1.4-280-Standard 2	15.739	15.739	**0.037**	0. 048	**9.183**	15.04
1.4-280-Standard 3	22.113	22.113	**0.017**	0. 048	**14.702**	17.73
1.4-280-Standard 4	23.467	23.467	**0.016**	0. 048	16.338	**13.46**

Table C2 The comparison of scaled total annualized cost, gap, and CPUs between the proposed method and BARON for 5-period case

Policy scenario	Scaled TAC		Gap		CPUs	
	Proposed	BARON	Proposed	BARON	Proposed	BARON
1.4-2.8-Standard 1	**1.143**	1.145	**0.049**	0.186	**771.853**	7200
1.4-2.8-Standard 2	1.183	1.183	**0.047**	0.206	**23.249**	7200
1.4-2.8-Standard 3	**1.183**	1.188	**0.05**	0.206	**627.155**	7200
1.4-2.8-Standard 4	1.196	1.196	**0.05**	0.194	**30.679**	7200
1.4-28-Standard 1	**2.158**	2.161	**0.049**	0.05	**432.33**	2263.75
1.4-28-Standard 2	5.097	5.097	**0.027**	0.05	**31.138**	2690.94
1.4-28-Standard 3	5.755	5.755	**0.049**	0.05	**228.06**	4792.76
1.4-28-Standard 4	6.056	6.056	**0.023**	0.05	**20.576**	6171.64
1.4-280-Standard 1	2.163	2.163	**0.024**	0.048	**60.32**	85.64

1.4-280-Standard 2	38.534	**38.532**	**0.015**	0.048	**17.24**	60.46
1.4-280-Standard 3	44.895	44.895	**0.01**	0.048	37.65	**36.45**
1.4-280-Standard 4	47.559	47.559	**0.008**	0.048	**16.65**	52.23

Table C3 The comparison of scaled total annualized cost, gap, and CPUs between the proposed method and BARON for 8-period case

Policy scenario	Scaled TAC		Gap		CPUs	
	Proposed	BARON	Proposed	BARON	Proposed	BARON
1.4-2.8-Standard 1	**1.745**	1.820	**0.05**	0.355	**1121.138**	7200
1.4-2.8-Standard 2	**1.886**	1.919	**0.049**	0.295	**1037.972**	7200
1.4-2.8-Standard 3	1.886	1.886	**0.049**	0.254	**764.089**	7200
1.4-2.8-Standard 4	1.92	**1.912**	**0.05**	0.274	**728.746**	7200
1.4-28-Standard 1	3.449	3.449	**0.05**	0.124	**421.352**	7200
1.4-28-Standard 2	7.494	7.494	**0.05**	0.112	**337.112**	7200
1.4-28-Standard 3	9.361	9.361	**0.016**	0.098	**72.338**	7200
1.4-28-Standard 4	9.84	9.84	**0.018**	0.05	**119.527**	2172.21
1.4-280-Standard 1	3.454	3.454	0.049	0.049	**351.324**	483.57
1.4-280-Standard 2	51.248	51.248	**0.023**	0.048	**177.523**	185.67
1.4-280-Standard 3	**73.698**	74.391	**0.007**	0.048	**20.857**	134.9
1.4-280-Standard 4	77.948	77.948	**0.006**	0.048	**27.743**	191.04

Table C4 The comparison of scaled total annualized cost, gap, and CPUs between the proposed method and BARON for 10-period case

Policy scenario	Scaled TAC		Gap		CPUs	
	Proposed	BARON	Proposed	BARON	Proposed	BARON
1.4-2.8-Standard 1	**2.122**	2.161	**0.05**	0.366	**1325.312**	7200
1.4-2.8-Standard 2	2.365	**2.36**	**0.05**	0.316	**1123.828**	7200
1.4-2.8-Standard 3	**2.417**	2.449	**0.049**	0.282	**839.522**	7200
1.4-2.8-Standard 4	2.464	**2.453**	**0.049**	0.274	**445.821**	7200
1.4-28-Standard 1	4.301	4.301	**0.049**	0.272	**932.871**	7200
1.4-28-Standard 2	8.211	8.211	**0.049**	0.118	**783.284**	7200
1.4-28-Standard 3	11.306	11.306	**0.042**	0.144	**131.156**	7200
1.4-28-Standard 4	12.594	**12.547**	**0.042**	0.109	**127.541**	7200
1.4-280-Standard 1	4.335	4.335	**0.049**	0.057	**362.684**	7200

1.4-280-Standard 2	52.156	52.126	**0.025**	0.048	154.839	**137.06**
1.4-280-Standard 3	84.248	**84.18**	**0.009**	0.048	**30.459**	162.95
1.4-280-Standard 4	99.346	**99.294**	**0.013**	0.048	**134.73**	185.7

Table C5 The comparison of scaled total annualized cost, gap, and CPUs between the proposed method and BARON for 12-period case

Policy scenario	Scaled TAC		Gap		CPUs	
	Proposed	BARON	Proposed	BARON	Proposed	BARON
1.4-2.8-Standard 1	**2.454**	2.742	**0.05**	0.435	**1970.459**	7200
1.4-2.8-Standard 2	**2.695**	2.941	**0.029**	0.392	**1184.89**	7200
1.4-2.8-Standard 3	**2.827**	2.947	**0.041**	0.329	**272.524**	7200
1.4-2.8-Standard 4	**2.868**	2.875	**0.034**	0.295	**394.725**	7200
1.4-28-Standard 1	**4.831**	4.832	**0.05**	0.294	**923.125**	7200
1.4-28-Standard 2	8.755	8.755	**0.05**	0.153	**750.387**	7200
1.4-28-Standard 3	11.922	11.922	**0.049**	0.168	**695.535**	7200
1.4-28-Standard 4	13.839	13.839	**0.049**	0.137	**591.91**	7200
1.4-280-Standard 1	5.18	5.18	0.05	0.05	**468.281**	497.09
1.4-280-Standard 2	53.32	**52.932**	0.049	**0.048**	**232.53**	498.9
1.4-280-Standard 3	85.086	**85.083**	**0.017**	0.049	**209.371**	650.17
1.4-280-Standard 4	100.823	**100.781**	**0.01**	0.048	**209.213**	541.68

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