Optimization of operation parameters towards sustainable WWTP based on deep reinforcement learning

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Abstract

A large amount of wastewater has been produced nowadays. Wastewater treatment plants (WWTPs) are designed to eliminate pollutants and alleviate environmental pollution resulting from human activities. However, the construction and operation of WWTPs still have negative impacts. WWTPs are complex to control and optimize because of high non-linearity and variation. This study used a novel technique, multi-agent deep reinforcement learning (DRL), to optimize dissolved oxygen (DO) and dosage in a hypothetical WWTP. The reward function is specially designed as LCA-based form to achieve sustainability optimization. Four scenarios: baseline, LCA-oriented, cost-oriented and effluent-oriented are considered. The result shows that optimization based on LCA has lowest environmental impacts. The comparison of different SRT indicates that a proper SRT can reduce negative impacts greatly. It is worth mentioning that the retrofitting of WWTPs should be implemented with the consideration of other environmental impacts except cost. Moreover, the comparison between DRL and genetic algorithm (GA) indicates that DRL can solve optimization problems effectively and has great extendibility. In a nutshell, there are still limits and shortcomings of this work, future studies are required.

Keywords: Wastewater, reinforcement learning, multi-objective optimization, sustainability
1. Introduction

1.1. Motivation

With an increasing population and the acceleration of urbanization and industrialization, a large amount of wastewater has been produced. Wastewater treatment plants (WWTPs) have been designed to eliminate pollutants and alleviate environmental pollution resulting from human activities. Normally, there are four phases in treating wastewater: pretreatment, primary treatment, secondary treatment, and tertiary treatment, each phase has plenty of techniques to choose. From a global scale, WWTPs have positive effects in environment protection [1]. However, the construction and operation of WWTPs consume resources (freshwater, energy, chemicals, etc.), emit greenhouse gases (GHGs) and produce residual sludge. WWTPs are complex to control and optimize because of high non-linearity and variation. At current stage, traditional control strategies driven by Single Objective Optimization (SOO), such as effluent quality, are lack of systematic thinking [2]. Besides, people mainly focus on economic benefits and ignore comprehensive influence caused by WWTPs. For example, setpoints of aeration rate are normally determined by nitrogen and BOD removal efficiency [3]. Nevertheless, the content of dissolved oxygen (DO) can also affect the emission of nitrous oxide ($N_2O$) [4] and energy consumption. With the rise of environmental consciousness, the optimization towards sustainability is imperative.

1.2. Related work and contributions

Multi-objective optimization (MOO) control encompasses more than one variable and factor, and the optimization problem is actually to find a trade-off among several conflicting objectives. There are two strategies solving MOO problems [5]. One is multi-objective to single objective strategy, which is to optimize a scalar with SOO methods. The other one is the Pareto strategy, which presents possible solutions by Pareto front. Jun-Fei Qiao et al. [6, 7] and Rainier Hreiz et al.[8] optimized control system of WWTP by adaptive multi-objective differential evolution algorithm. Effluent quality and energy consumption
were considered as objectives. Compared with other algorithms, novel algorithms achieved better performance. Genetic algorithm (GA) is a meta-heuristic algorithm and can generate high-quality solutions to MOO problems. Recently, GA has been proven as a powerful tool in water engineering. An integrated sewage model was developed with sewer system, wastewater treatment and streams [9], GA was applied to optimize stream quality and energy consumption. Similarly, GA was used to minimize GHG emissions, operational costs and effluent pollutant concentrations in an activated sludge WWTP [10]. The study from Kim et al. [11] also involved GHG emissions, however, they used weighted-sum method and solved the problem with Nelder-Mead simplex method. Rui Zhang et al. [12] introduced Support Vector Machine (SVM) as surrogate model, and combined SVM with GA to speed up computation to optimize Solid Retention Time (SRT) and Hydraulic Retention Time (HRT) based on Activated Sludge Model 2d (ASM2d) [13].

Life Cycle Assessment (LCA) is a cradle-to-grave or cradle-to-cradle analysis technique to assess environmental impacts with the production activity. Basically, there are various midpoint indicators in LCA, such as eutrophication potential, GHG emissions, toxicity-related impacts [14]. Since 1990s, LCA is deemed as an effective tool to evaluate comprehensive performance of water facilities [15]. Nowadays, numerical LCA has been integrated into mathematical optimization as objective functions. ABB de Faria et al.[16], Yi Li et al. [17] and Aras Ahmadi et al. [18] used LCA model to solve Multi-Objective Optimization (MOO) problems, this modification achieved minimization of environmental impacts, which provided more comprehensive guidance on management and design of water facilities.

Since the release of Alpha GO [19], Reinforcement Learning (RL) has received much attention and been used to optimize different processes in WWTPs. RL is a branch of machine learning, an agent learns from interacting with the environment [20]. Hernández-del-Olmo et al. [21] applied value-based RL in WWTP to minimize effluent ammonia and energy consumption simultaneously. The environment was modelled based on Benchmark Simulation Model No.1 (BSM1). In order to communicate accurately, operation cost was used as the metric. The inputs (or states) of the agent were ammonia and oxygen from two sensors, and the agent chose the DO setpoint among 1.5, 1.7 and 2.0 \( mg/L \). This new trial presented a
great potential of RL within water industry. Syafie et al. [22] used Q-learning [23] to con-
trol oxidation process in WWTP according to oxidation-reduction potential measurement.
Temporal abstraction was applied to reduce the amount of non-relevant exploration and
the calculation time. The aim of the agent was to maintain oxidation-reduction potential
(ORP) at specific point. The ORP level was discrete based on measurement noise. The
HRT of anaerobic and aerobic reactions was optimized by Q-learning in activated sludge
process based on ASM2d model. The state was generated according to effluent COD and
TP, and the agent updated the HRT under four different step-lengths. The results showed
that Q-learning could make real-time intelligent strategies [24, 25]. However, Q-learning is
under tabular formulation and can only handle discrete state and action spaces. Different
from value-based algorithms, policy-based algorithms naturally represent state and action
spaces continuously. REINFORCE algorithm was used to control bioprocesses [26]. The
control policy was parameterized by recurrent neural network. The agent was firstly trained
off-line in a simulated environment, after transfer learning, the algorithm was applied on
the true system. A novel policy-based algorithm, proximal policy optimization (PPO), was
applied to optimize the control of pump station in WWTPs [27]. The actions were sampled
from Beta distribution. The authors also used gradient boosting trees (GBT) to predict
inflow rate. The state presentation was a combination of the current environment. Tank
level and pump consumption were integrated as the reward function, therefore, the aim of
the agent was to control tank level within reasonable range and reduce energy consumption.

1.3. Paper overview

This paper focuses on MOO of operation parameters in an activated sludge based
WWTP. An actor-critic algorithm with multi-agents, Multi-Agent Deep Deterministic Pol-
icy Gradient (MADDPG), is applied to achieve optimal control of dissolved oxygen and
chemical dosage in a hypothetical WWTP under continuous action and state spaces. In
order to obtain sustainable control strategies, the reward function is specifically designed
based on Life Cycle Assessment (LCA).
2. Methodology

2.1. WWTP overview

A hypothetical WWTP based on activated sludge is optimized in this study as Fig. 1 shows. The main process includes primary sedimentation, biological treatment, secondary sedimentation, filtration and sludge treatment. The sludge is treated by thickening, chemical dosing, digestion and dewatering. The WWTP is assumed located in Jiangsu Province, China with the population equivalent is around 6,000. The volumes of primary clarifier, anaerobic tank, anoxic tank 1, anoxic tank 2, aerobic tank and secondary clarifier are 300, 200, 400, 600, 800 and 600 $m^3$ respectively. The sludge recycling ratio is set as 150%, and the internal recycling ratio (IRR) between anaerobic tank and anoxic tank 1 is 300%, the IRR between anoxic tank 2 and aerobic tank is 200%. To further eliminate phosphorus, chemical precipitation is implemented in aerobic tank with 25% Polyaluminium Chloride (PAC) solution. For sludge treatment, 40% ferric chloride solution is applied to pre-treat sludge before digestion. Water from thickening and dewatering returns back to primary clarifier. After treatment, sludge is transported for land-filling. The WWTP is simulated with MANTIS model developed by Hydromantis GPS-X. As a comprehensive model, MANTIS model is based on ASM2d, UCTADM1 [28] and Musvoto precipitation model [29].

The mean influent data are shown in Table 1. Dynamic influent data are generated based on literature [30, 31]. The first 60-day simulation are used to reach steady state, while the following 10 days are used for optimization.

| Item    | Value | Unit  |
|---------|-------|-------|
| Flow rate | 2,000 | $m^3/d$ |
| TP      | 9.9   | mg/L  |
| COD     | 332.2 | mg/L  |
| TN      | 43    | mg/L  |
| SS      | 211.8 | mg/L  |
Under baseline scenario, the DO set-point is 2 mg/L, and the dosage is 100 kg/day. The system boundary of LCA is confined within the WWTP.

Figure 1: WWTP layout

2.2. Problem Statement

In this paper, a popular actor-critic algorithm in RL, DDPG, is used [32] as shown in Fig. 2. Considering a standard RL problem, we model the environment \( E \) as Markov decision process with state space \( S \), action space \( A \), an initial state distribution \( p(s_t) \), transition dynamics \( p(s_{t+1} | s_t, a_t) \), and reward function \( r(s_t, a_t) \). When the environment is not fully observable, state space is replaced by observation space \( O \). An agent interacts with the environment by choosing different actions \( a_t \in \mathbb{R}^N \) at timestep \( t \). After each interaction, the environment releases state \( s_t \). An agent’s behaviors are defined by a stochastic policy, \( \pi \), which maps states to actions \( (\pi : S \rightarrow \mathcal{P}(A)) \).

The return is defined as the sum of discounted future reward:

\[
R_t = \sum_{i=t}^{T} \gamma^{(i-t)} r(s_i, a_i)
\]  

in which \( \gamma \in [0, 1] \) is the discount factor.
The aim of RL is to find an optimal policy that maximizes expected return:

$$\max_{\pi(\cdot)} E_{r_t, s_t, a_t \sim \pi}[R_t | s_t, a_t]$$  (2)

Many RL algorithms acquire expected return by calculating action-value functions recursively, e.g. Bellman equation:

$$Q^\pi(s_t, a_t) = E_{r_t, s_{t+1} \sim E}[r(s_t, a_t) + \gamma E_{a_{t+1} \sim \pi}[Q^\pi(s_{t+1}, a_{t+1})]]$$  (3)

In DDPG, a parameterized deterministic policy $\mu(s|\theta^\mu)$ is considered with parameter $\theta^\mu$. The critic $Q(s, a)$ is learned using the Bellman equation, while the actor is updated by the gradient of expected return from initial state with respect to actor parameters $\theta^\mu$:

$$\nabla J_{\theta^\mu} \approx E_{s_t}[\nabla \theta^\mu Q(s, a|\theta^Q)_{s=s_t, a=\mu(s_t|\theta^\mu)}]$$  (4)

$$= E_{s_t}[\nabla_a Q(s, a|\theta^Q)_{s=s_t, a=\mu(s_t)} \nabla \theta^\mu (s|\theta^\mu)_{s=s_t}]$$  (5)

Similar to Deep Q-Network [33], a replay buffer $\mathcal{R}$ is used in DDPG. Transitions are sampled from the environment by an exploration policy, and the tuple $(s_t, a_t, r_t, s_{t+1})$ are stored in the replay buffer. Gaussian noise is used for exploration. When the replay buffer is full, oldest experiences are discarded. Furthermore, soft target updates are applied in order...
to avoid divergence of Q update. Target networks are firstly copied from actor and critic networks, i.e. $\mu'(s_t | \theta^\mu')$ and $Q'(s_t, a_t | \theta^Q')$. Then these target networks update slowly with learned networks:

$$\theta' \leftarrow \tau \theta + (1 - \tau) \theta'$$

(6)

in which, $\tau \ll 1$.

In this study, two agents are deployed in terms of multi-agent paradigm, i.e. MADDPG [34]. In detail, one agent is for DO control and the other is for dosage control. Normally, multi-agent algorithms have decentralized actor and centralized critic, which means each actor receives its own observations and outputs single actions but critic network of each agent receives complete observations (Fig. 3).

![Figure 3: Overview of multi-agent structure](image)

In this paper, the optimization problem is abstracted to a sequential decision problem. The environment is the WWTP model as described in Section 2.1, and the agents try to set dissolved oxygen (DO) and dosage in terms of deterministic policies. The observation of agents are current DO and dosage respectively. After each interaction, a reward signal is released by the environment. The reward function is specially designed based on LCA (see Section 2.4). The aim of the agents is to minimize negative impacts of the studied WWTP.

2.3. Learning process

The MADDPG learning process mainly follows the original paper [34] and is introduced in this section. Different from the original paper, Gaussian noise $\mathcal{N}$ rather than Ornstein-
Uhlenbeck process is used for exploration. Hyperparameters of MADDPG are fine tuned and listed in Table 2, the total sampling quantity is 25,000. Before training, 500 sample data are acquired by Monte Carlo sampling, actions are sampled from uniform distribution. The value of DO ranges from 0 to 5 mg/L, and chemical dosage ranges from 0 to 200 kg/d. The first training is implemented under LCA scenario, with the SRT as 15 days. For other scenarios, transfer learning [35] is applied to narrow down required data size by freezing part of the network.

| Parameter                  | Value       |
|----------------------------|-------------|
| learning rate              | $10^{-3}$   |
| Activation function        | ReLu        |
| Neuron of actor network    | [32, 64, 32]|
| Neuron of critic network   | [64, 128, 64]|
| $\gamma$                  | 0.99        |
| $\tau$                    | 0.005       |
| buffer capacity            | 100         |
| batch size                 | 64          |
| noise mean                 | [0.0, 0.0]  |
| noise variance             | [0.2, 20]   |
| noise decay rate           | 0.2 % per episode |
| update iteration           | 10          |
| episode                    | 500         |
| time step of each epoch    | 50          |

**Step 0, Initialization:** Randomly initialize actor and critic weights $\theta_i^\mu$ and $\theta_i^Q$ for $i$-th agent. Initialize target networks as $\theta_i'^\mu = \theta_i^\mu$, $\theta_i'^Q = \theta_i^Q$. Initialize replay buffer $R$. Calculate the rewards of the sample points, obtain maximum and minimum values of each term for normalization. The initial state $o$ is randomly chosen from the sample points.

**Step 1, Interaction:** The behavior policy $\beta_i$ receives the observation vector and outputs action $a_{t,i}$ to the environment.

$$a_{t,i} = \mu(o_{t,i}|\theta^\mu) + \mathcal{N}_t$$ (7)
The environment then interacts with GPS-X model and the agent receives a new observation $o'$. Reward $r_{t,i}$ is then calculated based on the new state, tuple $(o, a_{t,i}, r_{t,i}, o')$ is stored in the replay buffer $\mathcal{R}$. If the replay buffer is full, oldest samples will be discarded.

**Step 2, Network training:** Randomly sample $N$ transitions ($N=64$ in this study) in the replay buffer as a mini-batch. For critic network, loss $L$ is calculated by mean squared loss (MSE). The critic gradient is thus $\nabla_{\theta_i^Q} L$.

$$L_i = \frac{1}{N} \sum_j \left( y^j - Q_i^\mu(o^j, a_1^j, ..., a_N^j)\theta_i^Q \right)^2$$  \hspace{1cm} (8)

$$y^j = r_i^j + \gamma Q_i^{\mu'}(o^{j+1}, a_1^j, ..., a_N^j)|_{a_k^j = \mu_k(o^j)}$$ \hspace{1cm} (9)

Actor gradient is obtained from the deterministic policy gradient derived from [36].

$$\nabla_{\theta_i^\mu_i} J \approx \frac{1}{N} \sum_j \nabla_{a_k} Q_i^\mu(o^j, a_1^j, ..., a_N^j)|_{a_k = \mu_k(o^j)} \nabla_{\theta_i^\mu_i} Q_i^\mu(o^j)$$ \hspace{1cm} (10)

Each agent $i$ updates parameters in terms of equation 8 - 10. Policy networks are updated by Adam optimizer [37], target networks are updated using soft updating method. After each epoch, the noise will decay 0.2%.

**Step 3, Repetition:** If time-step reaches $T = 500$, stop; otherwise back to Step 1.

For transfer learning, the first layers of the networks are frozen. Buffer capacity, batch size, noise decay rate, episode and time step of each epoch are changed as 50, 32, 5% per episode, 20 and 25 respectively, therefore, the sampling quantity is reduced to 500.

The algorithm is coded with Pytorch version 1.5 [38] under Python 3.7 environment. The environment is achieved with the RL toolkit, Gym, developed by OpenAI [39].

2.4. Reward function based on Life Cycle Assessment

Several LCA mid-point indicators are chosen to form the reward function. Normalization is then applied to ensure a balanced evaluation. For each dynamic simulation, mean values within 10 days are recorded to calculate rewards. Since the DO and dosage mainly affect biological process and sludge production, other environmental impacts are considered as constant hence are ignored in the optimization problem.
2.4.1. Cost

There are 3 components in cost: energy cost, transportation cost and chemicals cost. The prices are acquired from market investigation.

(1) Energy cost $C_e$: unit price of electricity is 0.8 CNY/kWh, and consumption is derived from Section 2.4.2, only direct energy consumption is considered.

(2) Transportation cost $C_t$: unit price is 0.6 CNY/kg, the cost encompasses transportation of chemicals and treated sludge.

(3) Chemical cost $C_c$: ferric chloride solution (40%) is assumed to pre-treat sludge, the price of $FeCl_3(100\%)$ is 1.7 CNY/kg; 25% PAC solution is applied for phosphorus removal, the price of PAC (100%) is 2.5 CNY/kg.

(4) Biogas cost: biogas is generated from digester and the subsidy of renewable energy is 0.25 CNY/kWh [40]. TBD

The total cost is hence the sum of three parts:

$$C_{tot} = C_e + C_t + C_c - C_{bio}$$

where $C_{tot}$ is total cost in unit CNY/day.

2.4.2. Energy Consumption

Since only aeration rate and dosage are controlled, energy consumed by aeration and sludge treatment processes are included in reward function. Energy consumed by mixing, heating or other pumping processes is assumed as constant, thus is ignored. Specifically, three components are consisted of energy consumption.

(1) Dissolved oxygen is controlled by aeration mechanical power, with a fixed set-point, aeration power $p_a$ is controlled in terms of influent quality by a PI controller.

(2) Energy consumption of pumps includes residual sludge pump, thickening pump, de-wathering pump. The energy consumption are calculated by equation 12 and 13.

$$H = H_{static} + H_{dynamic}$$

$$W = \frac{\rho g Q H}{1000 \eta}$$
where $W$ is the pump power, kWh; $\rho$ is water density, 1000 $kg/m^3$; $g$ is acceleration of gravity, 9.8 $m/s^2$; $Q$ is flow rate, $m^3/s$; $H$ is pumping head, m; $\eta$ is pump efficiency, 0.7. The static water head $H_{static}$ is set as 5 m, and the frictional head loss is assumed as constant, 1 m.

(3) WWTPs often use chemicals to remove pollutants or pre-treat sludge. Chemicals also consume energy during production and transportation. According to Stefano Longo et al. [41], chemical energy consumption of iron chloride (40%) and PAC (25%) is 3.4 and 1.94 kWh/kg respectively.

In a nutshell, total energy consumption is:

$$E_{tot} = E_{aer} + E_{tran} + E_{che}$$  \hspace{1cm} (14)

### 2.4.3. Eutrophication potential

Eutrophication potential measures underlying nutrient discharge of the system to recipient streams by emission factors, in unit $kgPO_4^{eq}$. Emission factors from CML database [42] are shown in Table 3:

| Item  | Emission factor $(kgPO_4^{eq}/kg)$ |
|-------|-----------------------------------|
| TP    | 3.07                              |
| COD   | 0.022                             |
| $NH_4^+$ | 0.33                           |
| $NO_3^-$ | 0.095                         |
| $NO_2^-$ | 0.13                          |

Thus, eutrophication potential can be derived as:

$$EP = 3.07 \cdot TP + 0.022 \cdot COD + 0.33 \cdot NH_4^+$$
$$+ 0.095 \cdot NO_3^- + 0.13 \cdot NO_2^-$$  \hspace{1cm} (15)

### 2.4.4. Greenhouse gas

There are three scopes in GHG emissions: process emissions, energy emissions and material emissions. Process emissions are complicated. MANTIS model in GPS-X encompasses
greenhouse gas module and simulates the emission of \( N_2O \) and \( CH_4 \). In detail, \( N_2O \) and \( CH_4 \) emitted by anaerobic tank, anoxic tank, aerobic tank and digester are considered, emissions from clarifiers and other sludge treatment processes are ignored. In addition, we estimate nitrous oxide and methane emission emitted by discharge with emission factors from IPCC [43].

\[
CH_{4eff} = BOD_{eff} \cdot B_o \cdot MCF 
\]

\[
N_2O_{eff} = TN_{eff} \cdot EF \cdot \frac{44}{28} 
\]

in which, \( CH_{4eff} \) is methane emission rate, \( kgCH_4/d \); \( BOD_{eff} \) is effluent BOD concentration, \( kgBOD/d \); \( B_o \) is maximum \( CH_4 \) producing capacity, 0.25 \( kgCH_4/kgBOD \); \( MCF \) is methane correction factor, 0.035 (fraction); \( N_2O_{eff} \) is nitrous oxide emission rate, \( kgN_2O/d \); \( TN_{eff} \) is nitrogen in the effluent discharged to aquatic environments, \( kgN/d \); \( EF \) is emission factor for \( N_2O \) emissions from wastewater discharged to aquatic systems, 0.016 \( kgN_2O-N/kgN \); the factor 44/28 is the conversion factor of \( kgN_2O-N \) into \( kgN_2O \).

Indirect emissions associated to energy consumption can be calculated based on a factor estimated based on the energy mix for China [44]. Emissions are derived based on various emission factors Table 4.

| Item                  | Emission factor |
|-----------------------|-----------------|
| Electricity           | 1.17 \( kgCO_2-eq/kWh \) [44] |
| FeCl\(_3\)(100%)      | 0.986 \( kgCO_2-eq/kg FeCl_3 \) [45] |
| PAC(100%)             | 1.182 \( kgCO_2-eq/kg PAC \) [46] |
| Transportation(road)  | 0.000192 \( kgCO_2-eq/(kg \cdot km) \) [47] |
| Nitrous oxide         | 298 \( kgCO_2-eq/kg N_2O \) [43] |
| Methane               | 25 \( kgCO_2-eq/kg CH_4 N_2O \) [43] |

Here, we assume that all chemicals and sludge are transported by road, with average distance as 200 km. The equation for global GHG estimation is:

\[
GHG_{tot} = GHG_{pro} + GHG_{energy} + GHG_{material} 
\]

(18)
2.4.5. Weighted sum

The reward function is derived by combining above 4 parts. Normalization is required, for which we need maximum and minimum values in advance. Here, maximum and minimum values are obtained by Monte Carlo sampling: sampling data from uniform distribution before training, i.e. internal normalization [48]. Since the distribution of each term is different, first quantile and second quantile are chosen as the maximum values for EP and GHG.

\[
\text{Item}_{\text{norm}} = \left| \frac{\text{Item}_{\text{tot}} - \text{Item}_{\text{min}}}{\text{Item}_{\text{max}} - \text{Item}_{\text{min}}} \right|,
\]

\(\forall \text{Item} \in I = \{C, E, EP, GHG\}\).

Therefore, the reward function is as follows:

\[
\text{Reward} = w_c C_{\text{norm}} + w_E E_{\text{norm}} + w_{EP} EP_{\text{norm}} + w_{GHG} GHG_{\text{norm}}
\]

In this study, each part is treated equally, i.e. each weight is 0.25.

2.4.6. Extra constraints

In order to obtain reasonable results, an extra constraint is added. The constraint is effluent quality with specific limits. If the effluent concentrations exceed the thresholds, an extra penalty +1 will be added to the total reward. In this study, the limits are referenced from Chinese Discharge Standard of Pollutants for Municipal Wastewater Treatment Plant (GB 189182002), Grade I-A: \(NH_4-N \leq 5\text{mg/L}, TN \leq 15\text{mg/L}, COD \leq 50\text{mg/L}, BOD \leq 10\text{mg/L}, TSS \leq 10\text{mg/L},\) and \(TP \leq 0.5\text{mg/L}\).

At last, the reward is multiplied by -1 to keep consistency with the maximization setting. Therefore, considering a reward with \(m\) indicators \(I_i \in \mathcal{I}\) and \(n\) effluent limits \(L_j \in \mathcal{L}\) of pollutants \(P_i \in \mathcal{P}\), the general form of this optimization problem is:

\[
\max \quad \text{Reward} = -\sum_{i=1}^{m} w_i I_i
\]

\(s.t.\) \(P_j \leq L_j, \quad j = 1, 2, 3 \ldots, n\)

\(I_i \sim \text{Model}, \quad i = 1, 2, 3 \ldots, m\)
2.5. Scenario introduction

To present the results with different emphasis, environmental impacts of four scenarios are compared:

(1) Baseline scenario, parameters are determined according to the experience, here, DO is set as 2.0 mg/L and dosage is 100 kg/d.

(2) Effluent scenario, optimization based on effluent quality (i.e. eutrophication potential) is implemented.

(3) Cost scenario, optimization based on cost is implemented.

(4) Global sustainability scenario (LCA), optimization based on LCA reward is implemented.

Besides, three SRT values (10, 15, 20 days) are compared under LCA-based optimization to figure out the influence of sludge disposal.

Nowadays, the stakeholders generally optimize control strategies based on cost under the constraint of discharge standards. Recently, the Chinese government proposed the Action Plan for Water Pollution Prevention and Control [49], which requires all WWTPs in protected areas to meet the Grade I-A standard of effluent discharge. In some areas, the standards are even stricter than Grade I-A [50], i.e. the standard V for surface water. Common standards are listed in Table 5, and the standard V for surface water only covers TP, COD and ammonia. In this paper, LCA-based optimization under four scenarios are implemented: Grade I-A, Grade I-B, Surface Water V and No Limit, and the SRT is 15 days.

| Item      | Grade I-A | Grade I-B | Surface Water V |
|-----------|-----------|-----------|-----------------|
| $TN$      | 15        | 20        | -               |
| $TP$      | 0.5       | 1.0       | 0.4             |
| $COD$     | 50        | 60        | 40              |
| $BOD$     | 10        | 20        | -               |
| $NH_4 - N$| 5         | 8         | 2               |
| $SS$      | 10        | 20        | -               |
3. Results and discussion

3.1. Scenario comparison

In baseline scenario, the total reward is -0.512. Fig. 4 and Fig. 5 show the reward and parameters vary with training steps under LCA scenario. Five paralleled experiments are implemented. At the beginning, the reward is low and the parameters have high variance since the initialization of weights is random and the policies have high noise to explore the action space. At the end stage, the agents learn the optimal policies and exploit the historical information sufficiently. However, since multiple value combinations lead to the similar performance, the variance still exists. Table 7 lists the results of four scenarios and Fig. 6 indicates the LCA impacts of four scenarios.

![Figure 4: Reward variation under LCA scenario, shadow is the standard deviation of 5 experiments.](image)

Under LCA scenario, the agents optimize the system from a comprehensive perspective. Compare to the baseline, DO is increased and dosage is decreased. As a result, the cost and energy consumption change from 208.9 to 181.0 $CHY/d$ and 247.7 to 253.9 $kWh/d$ respec-
Figure 5: Parameter variation under LCA scenario, shadow is the standard deviation of 5 experiments.

This change enhances the removal of ammonia (from 1.87 to 1.76 mg/L) but increases effluent phosphorus (from 0.45 to 0.49 mg/L), which leads to the variation of GHG emissions and eutrophication potential, from 3853.5 to 3764.4 kgCO$_2$-eq/d and 6.89 to 7.10 kgPO$_4$-eq/d. If only cost is considered, the agents reduce both DO and dosage to decrease energy consumption and cost: total cost from 208.9 to 173.7 CHY/d. Under effluent scenario, the concentrations of TP and ammonia are eliminated to an extreme, with the DO as 5.0 mg/L and dosage as 100 kg/d. Therefore, the eutrophication potential reaches 6.51 kgPO$_4$-eq/d by sacrificing cost and energy consumption. Among four scenarios, effluent scenario owns largest negative environmental impacts, while LCA scenario has the best performance. As the most commonly used strategy, cost-oriented strategies can reach reasonable control parameters, but not the optimal. Effluent scenario has the lowest eutrophication potential, but sacrifices energy, GHG emission and cost. In short, the results indicate that the strategy from a comprehensive perspective has better overall performance.
Different control parameters renders the change of flora distribution. Here, four microorganisms, heterotrophic bacteria (XBH), ammonia oxidizing bacteria (AOB), nitrifying bacteria (NOB), polyphosphate accumulating bacteria (PAO), are compared in Fig. 7. The concentrations of AOB and NOB are stable because the growth of AOB and NOB mainly depend on ammonia and nitrate, when the oxygen supply is sufficient, the oxidation of nitrogen can be processed smoothly. The variation of DO and dosage mainly influence XBH and PAO. When dosage is declined, the number of PAOs increases significantly since there is more phosphate, and the competition between XBH and PAO leads to the decline of XBH.

Solid Retention Time (SRT) is another vital parameter influencing system performance significantly. This study does not try to optimize this parameter because the adjustment of SRT normally requires long-time stabilization. However, the optimization under various SRT are implemented based on LCA to present the system variation (Table 6).

Compared to 15 days, long SRT leads to activity decline of XBH but enhance the growth of AOB and NOB (51.39 and 14.59 mgCOD/L respectively), thus the system requires higher
Figure 7: Flora distribution under four scenarios.

DO for degradation and nitrification. As a result, long SRT has higher expenditure and energy consumption. As for 10-day SRT, short SRT renders the reduction of microorganism (from 789 under 15 SRT to 584 $mgCOD/L$), therefore, extra chemicals increases both energy consumption and cost. This comparison demonstrates that an appropriate SRT can decrease negative environmental impacts significantly.

Table 6: Optimal parameters with various SRT

| SRT day | DO mg/L | Dosage kg/d | Cost CNY/d | Energy kWh/d | EP kgPO$_4$ – eq/d | GHG kgCO$_2$ – eq/d |
|---------|---------|-------------|------------|--------------|-------------------|-------------------|
| 10      | 2.6     | 100         | 201.5      | 250.8        | 7.85              | 3799.7            |
| 15      | 2.8     | 70          | 183.7      | 256.2        | 6.89              | 3779.5            |
| 20      | 3.6     | 90          | 203.9      | 291.2        | 6.35              | 3910.5            |

3.2. Impacts under different discharge standards

The experiments under various standards present that the overall impacts under Grade I-A, Grade I-B and No limit discharge standards have the same optimal results, while the
Table 7: Optimal parameters

| Scenario | DO (mg/L) | Dosage (kg/d) | Total reward |
|----------|-----------|---------------|--------------|
|          | RL | GA | RL | GA | RL | GA |
| Baseline | 2.0 | 100 | -0.512 |
| LCA      | 2.8 | 2.9 | 70 | 70 | -0.406 | -0.405 |
| Cost     | 1.4 | 1.5 | 60 | 60 | -0.524 | -0.534 |
| Effluent | 5.0 | 5.0 | 100 | 100 | -0.609 | -0.609 |

Surface Water V standard increase negative impacts on the contrary with DO as 1.8 mg/L and dosage as 200 kg/d (Fig. 8). In the Surface Water V scenario, dosage is increased greatly to reach a low effluent TP and that leads to high GHG emissions, energy consumption and cost. Moreover, the concentration of PAOs under this scenario is close to zero, because biological phosphorus removal cannot satisfy the standard and nearly all phosphorus is removed by chemical precipitation.

![Figure 8: Radar chart of LCA impacts under different standards.](image)

This results show that the retrofitting of WWTPs towards strict standards reduce the
pollutants in water bodies, but renders impact transfer or leakage, i.e. higher GHG emission, energy consumption and cost. Needless to say, the reconstruction consumes extra materials and funds. In short, we recommend that the retrofitting should be implemented in terms of comprehensive influence and realistic situations.

3.3. Comparison with genetic algorithm

As a mature algorithm, GA has been widely applied in optimization problems. Compared with RL, evolutionary methods require a lot of time to search optimal policy especially under large spaces, and have advantages on problems in which the learning agent cannot accurately sense the state of its environment. In addition, evolutionary methods do not use the fact that the policy is actually a function from states to actions and they do not utilize historical information [51]. Table 7 lists optimized parameters derived from Segregated Elite Genetic Algorithm (SEGA) [52] implemented by Geatpy [53]. The basic hyperparameters of SEGA are: the encoding method is binary, the population size is 40, the mutation rate is 0.5, the crossover rate is 0.7 and the length of chromosome is 28. 20 generations are performed, and the fitness is computed according to LCA-based reward. It shows that DRL has comparable performance to GA. Although DRL consumes plenty of time in the first training, subsequent training based on transfer learning only needs 500 sample quantity. However, GA requires at least 800 sample quantity to acquire satisfactory results. In addition, DRL has better extendibility when the action or state spaces are large which means DRL algorithm can optimize more parameters simultaneously and fast.

3.4. Limitation and future work

Multi-objective reinforcement learning is still under initiative stage [54]. In this work, a scalar reward function rather than the Pareto strategy is used. Scalar scheme is easy to understand and optimize, but cannot obtain Pareto front, which causes difficulties to strategy generation. In addition, same values of a scalar reward may indicate multiple action pairs which also brings confusion. Thus, other algorithms using Pareto framework can be applied in future work. Besides, RL algorithm is sensitive to reward function, hence the
reward engineering can impact performance significantly [55]. This study is a trial of LCA based reward engineering and heuristic method such as the extra constraint is imperative to avoid unrealistic results. In addition, the weights and factors impact optimization results dramatically. The determination of these parameters are intuitive. To sum up, future work is required to explore the performance of non-weighted approaches, and look for an efficient reward engineering method for WWTP evaluation.

Most algorithms of RL are model-free. As data-driven algorithms, they normally require a large number of samples from the real world or models. In this study, data is sampled from the model, which means the accuracy of the model concerns about the final performance. Considering that training models requires plenty of time, the size of replay buffer is selected as 100 then 50 during transfer learning. Besides, DRL introduces neural networks as feature representatives, therefore, there are plenty of hyperparameters that create difficulties when acquiring good performance. When the algorithm is deployed in field, the data size is usually limited. In short, the WWTP in this study is hypothetical and lack of validation, in the future, this novel algorithm should be implemented in field to verify the performance.

Last, the system boundary of LCA is limited to the WWTP and merely four mid-point indicators are chosen because these indicators represents the major concerns in WWTPs and the data of these indicators are easy to acquire or calculate by models. A complete system boundary and ample indicators lead to complete results, but also require lots of data and introduce uncertainty.

4. Conclusion

Multi-objective and sustainability optimization have been studies in water industry. This study applied deep reinforcement learning to optimize DO and dosage simultaneously. An LCA-based reward function is designed for sustainability optimization. The result shows that optimization based on LCA has lowest environmental impacts. The comparison of different SRT indicates that a proper SRT can reduce negative impacts greatly. It is worth mentioning that the retrofitting of WWTPs should be implemented with the consideration of other environmental impacts. Besides, the comparison between DRL and GA indicates that
DRL can solve optimization problem effectively and has great extendibility. Nevertheless, there are still limits and shortcomings of this work, future studies are required.

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