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# Multi-Objective Optimization Based on Simulation Integrated Pareto Analysis to Achieve Low-Carbon and Economical Operation of a Wastewater Treatment Plant

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**Abstract:** It is essential to reduce carbon emissions in wastewater treatment plants (WWTPs) to achieve carbon neutrality in society. However, current optimization of WWTPs prioritizes the operation cost index (OCI) and effluent quality index (EQI) over greenhouse gas (GHG) emissions. This study aims to conduct a multi-objective optimization of a WWTP, considering GHG emissions, EQI, and OCI. The anaerobic-anoxic-oxic integrated membrane bioreactor (AAO-MBR) process in an actual WWTP was selected as a typical case, tens of thousands of scenarios with combinations of six operational parameters (dissolved oxygen (DO), external carbon resource (ECR), poly aluminum chloride (PAC), internal reflux ratio (IRR), external reflux ratio (ERR), and sludge discharge (SD)) were simulated by GPS-X software (Hydromantics 8.0.1). It was shown that ECR has the greatest impact on optimization objectives. In the optimal scenario, the main parameters of ATDO, MTDO, IRR, and ERR were 0.1 mg/L, 4 mg/L, 50%, and 100%, respectively. The EQI, OCI, and GHG of the best scenario were 0.046 kg/m$^3$, 0.27 ¥/m$^3$, and 0.51 kg$CO_2$/m$^3$, which were 2.1%, 72.2%, and 34.6% better than the current situation of the case WWTP, respectively. This study provides an effective method for realizing low-carbon and economical operation of WWTPs.

**Keywords:** multi-objective optimization; Pareto analysis; greenhouse gas emissions; AAO-MBR; operational parameters



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## 1. Introduction

Reducing greenhouse gas emissions is of utmost importance in the global fight against climate change. The Paris Agreement, established in 2015, has motivated numerous countries to establish objectives for carbon peaking and carbon neutrality [1]. As a result, industries around the world have adapted their development strategies and implemented emission-reducing measures. According to statistics from major developed countries, the wastewater treatment industry is among the top ten contributors to total carbon emissions, accounting for 1% to 2% [2]. It is expected that the total greenhouse gas emissions (in terms of $CO_2$ equivalent) from China's wastewater treatment industry will be as high as 365 million t by 2030. It accounts for 2.95% of the country's total emissions [3,4]. On 29 December 2023, the Chinese government released the policy entitled "Opinions on the Implementation of Promoting Synergistic Efficiency in Wastewater Treatment for Reducing Pollution and Reducing Carbon". It announced Chinese plans to build 100 green and low-carbon benchmark plants for wastewater treatment in 2025 with high-efficiency recycling in energy and resources. Therefore, measures such as adopting new processes and improving operation levels to achieve carbon reduction in the wastewater treatment industry are of great significance in achieving carbon neutrality.

Due to the diversity of municipal wastewater treatment processes, there is a large level of complexity and uncertainty when it comes to balancing multiple objectives such as operational efficiency and low-carbon emissions. In practice, improving effluent quality and minimizing operating costs are still the primary concerns of operation managers. To attain these objectives, it is crucial to explore avenues for reducing the operation cost index (OCI) and greenhouse gas (GHG) while upholding the standards of the effluent quality index (EQI). This is a problem involving the optimization of multiple objectives in nature.

In terms of single-objective and bi-objective optimization, there have been numerous reports. Wu et al. [5] used WEST 2012® software to simulate and optimize an industrial wastewater effluent plant with complex influent compositions, which led to the reduction in OCI from 6.2 to 5.5 €/m$^3$. Cao et al. [6] screened and analyzed the sensitivity of 61 parameters. They developed a quadratic polynomial response surface model of six key process parameters. Finally, the water quality improvement was achieved by optimizing two process parameters, dissolved oxygen (DO) and solids retention time (SRT). All of the above studies focus on the single-objective optimization problem of wastewater treatment process. However, they have not formed an integrated and comprehensive study. Vega et al. [7] combined real-time optimization and hierarchical control with nonlinear model predictive control, and evaluated the wastewater treatment process EQI and OCI through the control structure. Zhang et al. [8] proposed a multi-objective optimization and control method of BP neural network combined with a genetic algorithm, which effectively solves the problems of EQI and OCI, a pair of mutually constrained optimization objectives. Guerrero et al. [9] used both OCI and EQI as the control optimization objectives, which produced a set of optimal operating setpoints that could be approximated by a Pareto surface. These optimization studies can guide wastewater treatment plants (WWTPs) to effectively reduce OCI without consideration about GHG emissions.

Regarding the tri-objective optimization of EQI, OCI, and GHG, although there are some research reports in recent years, there are still some deficiencies that need to be improved. Lu et al. [10] assessed the effectiveness of gauging a dynamic simulation model in regulating GHG in WWTP. The evaluation puts forth a fresh approach for achieving optimal control of such plants, taking into account EQI, OCI, and GHG. It is important to mention, however, that while the proposed framework is sound in theory, it lacks practical real-world case studies. X. Flores-Alsina et al. [11] found that aerobic tank dissolved oxygen, primary sedimentation tank suspended solid (SS) removal, anaerobic digester temperature, and reflux strategy had effects on the three objectives considered (GHG, EQI, and OCI). But these objectives could not be optimized for all of them. Similar conclusions were obtained in the study of C. Sweetapple et al. [12], where none of the 315 aeration strategies set up could simultaneously achieve the co-optimization of the three objectives. The operation energy consumption, water quality, and carbon emissions of WWTP based on continuous batch reactor were studied, but no collaborative optimization was achieved [13].

Since EQI, OCI, and GHG are three mutually constrained optimization objectives, it is difficult to achieve the optimal solution of the three objectives at the same time. Hence, it is necessary to adopt a nonlinear multi-objective optimization method to determine the overall optimal solution [8]. For this purpose, the study employs Pareto optimization principles and introduces the upstream logic in the NSGA-II algorithm—the Non-dominated Sorting Genetic Algorithms, which has proven effective in optimizing control strategies for WWTPs from prior studies. Chen et al. [14] used NSGA-II to achieve multi-objective optimization of operational energy consumption, effluent quality, total volume of structures, and SS of structures based on the activated sludge method. Beraud et al. [15] coupled NSGA-II with a common wastewater treatment plant model to illustrate how the algorithm can be used to determine the feasibility of Pareto optimality. It is worth noting that researchers use mathematical models to simulate complex process conditions and obtain basic data for optimization evaluation commonly. In this way, as the high input of time and labor decreases apparently, so does the cost of trial and error. Moreover, the issues caused by uncertainty and inefficiency in relying on traditional methods to optimize operational parameters can be avoided efficiently, as well [16].

At present, there are hundreds of domestic and foreign wastewater treatment processes. Among them, the combination of anaerobic-anoxic-oxic (AAO) and membrane bioreactor (MBR) processes (named AAO-MBR) has aroused general attention, because it can achieve high and stable effluent quality, short hydraulic retention time, and low residual sludge volume [17,18]. Due to its high effluent quality, the resulting wastewater can not only be discharged directly into the environment, but also reused for non-potable water applications [19]. Considering the increasing use of AAO-MBR in upgrading projects and underground WWTPs, more than 25% of underground WWTPs use AAO-MBR as the primary process [20], the typical AAO-MBR process was selected as the research object in this study. The nonlinear multi-objective optimization method was explored to achieve low-carbon emission taking into account the effluent quality and operation cost. We established a process model with the help of GPS-X simulation and modeling software to analyze the effects of six typical operational parameters on EQI, OCI, and GHG. A non-dominated sorting method was adopted to search for the Pareto-optimal set of solutions and screen the optimal solution from it. Through the above process, the necessary trade-offs between conflicting control objectives were made, which provided support for enhancing the sustainability of the wastewater treatment system.

## 2. Materials and Methods

### 2.1. A Multi-Objective Optimization Framework

The research framework of the multi-objective optimization comparison method used in this paper is visually depicted in Figure 1. Different from the traditional multi-objective weighted evaluation optimization method, this paper searches for the optimal combination of operational parameters based on the three mutual restraint objectives of EQI, OCI, and GHG by means of Pareto optimal solution set. The optimization process entails three major parts: model construction, multi-parameter evaluation, and optimization comparison.

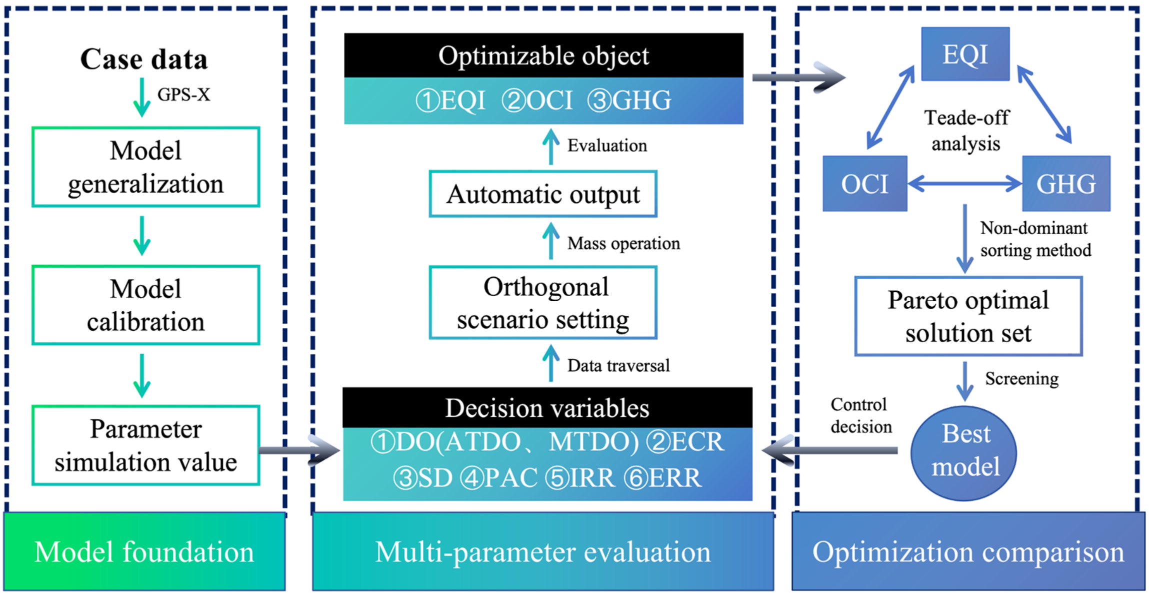


**Figure 1.** The research framework of the multi-objective optimization.

Firstly, the process model was built with the help of GPS-X (Hydromantics 8.0.1) simulation and modeling software. The key operating conditions included six operational parameters, including dissolved oxygen (DO) concentration, external carbon resource (ECR), phosphorus removal agent poly aluminum chloride (PAC), internal reflux ratio (IRR), external reflux ratio (ERR), and sludge discharge (SD). Among these, the DO concentration included the aerobic tank dissolved oxygen (ATDO) concentration and the membrane tank dissolved oxygen (MTDO) concentration. Based on the baseline scenario, the simulated value points of six operational parameters were set.

Secondly, the orthogonal combination of parameter simulation values was carried out through data traversal to form an orthogonal simulation scenario. GPS-X software was used to realize mass simulation calculation and automatic output results.

Finally, based on the simulation results of the orthogonal parameter set, the evaluation values of each scenario were solved by the equal proportion weighting calculation. The optimal scenario was selected to determine the optimal operation parameter combination.

## *2.2. Technological Process Modeling and Scenario Analysis*

### 2.2.1. Construction of Process Model

The case plant is located in Luohu District, Shenzhen, China. It adopts the AAO-MBR treatment process, and the actual treatment scale is 33,500 $m^3/d$, with hydraulic retention time (HRT) of 17.33 h and solid retention time (SRT) of 10.94 d. The influent water quality is shown in Table S1, and the design effluent is required to meet the Class A standard of the China Urban Wastewater Treatment Plant Emission Standard (GB18918-2022) [21].

Based on the actual process and operational parameters of the case WWTP, the model is generalized and the parameters are calibrated according to the standardized procedure [22]. Its actual operational parameters and unit structures are shown in Tables S2 and S3. The generalized model of the case plant is depicted in Figure 2.

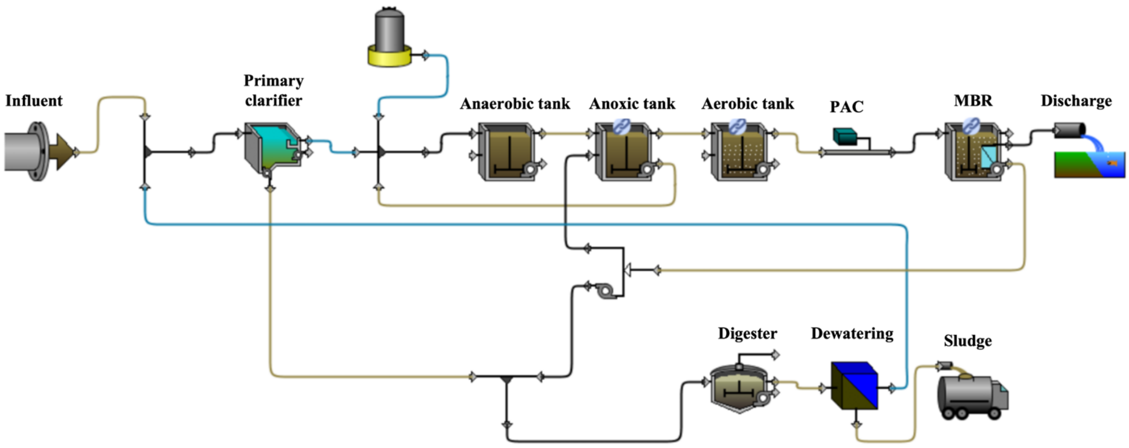


**Figure 2.** Generalized model of the case WWTP established in GPX-S software.

The daily water quality data in 2022 is collected for model calibration of the baseline scenario. Then, the relevant stoichiometric and dynamic parameters in the structure are adjusted to make the simulated effluent water quality the same or close to the actual effluent water quality, with reference to the previous studies [6,23]. The results of the calibration and the baseline simulation scenario of the effluent quality are shown in Table S1. After calibration, the average errors of $BOD_5$, COD, SS, TN, TP, and $NH_4^+$-N were 7.0%, 10%, 8.0%, 0.3%, 18%, and 25%, respectively, and the maximum absolute errors were 0.15, 1.23, 0.02, 0.03, 0.03, and 0.02 mg/L. Almost all the indicators' errors were within acceptable limits [24].

The Python Script Manager attached to the software is used to achieve external control. A large number of exhaustive simulations run within a certain range are completed under the premise of fixed process flow and structure. At the same time, the script is written in Python environment to realize automatic data import and export. The automated operation is implemented through the loop statements of the upper logic. The logical structure of which is shown in Figure S1.

#### 2.2.2. Orthogonal Scenario Settings of Operational Variable

Referring to the basic operational parameters presented in Table S2, we set the optimized values of the six operational parameters, DO (ATDO, MTDO), ECR, PAC, IRR, ERR, and SD of the case WWTP, respectively. These six were chosen from a larger set of operational and design parameters as the set of most likely to be significant to the objective functions [25,26]. These values are combined with the actual operating data of WWTP and the simulative scenario values are shown in Table S4.

Through the way of data traversal, the value points of the operational parameters (Table S4) are arranged and combined successively, forming a total of 80,000 ($4 \times 4 \times 4 \times 5 \times 5 \times 5 \times 10$) groups of parameter combinations, forming orthogonal scenarios. These scenarios are simulated in the construction of the case WWTP model, and the results obtained are used for subsequent analysis. The values of MTDO had no significant effect on the three objectives (Figure S2). Therefore, the effects of six operational parameters, ATDO, ECR, SD, PAC, IRR, and ERR, on EQI, OCI, and GHG were examined separately.

### *2.3. Calculation Method of Three Optimizable Objectives*

#### 2.3.1. Effluent Quality Index (EQI)

The effluent quality is characterized by EQI with a unit of $kg/m^3$, which represents the total amount of pollutants discharged per ton of wastewater treated by the study object. In this study, EQI is characterized by COD, $BOD_5$, TSS, Soluble $PO_4$-P, $NO_x$ ($NO_2 + NO_3$), and TKN. Their weighting factors are used with default values of 1, 2, 2, 2, 2, 1, and 20, respectively. The values are obtained directly from the software, and the reference formula in the software is shown in Equation (1):

$$\mathrm{EQI} = \mathrm{Q}\sum_{i=1}^{6} w_i S_i \tag{1}$$

where Q is the effluent flow of WWTP, $m^3/d$, $w_i$ is the weight of the ith pollutant in the EQI. $S_i$ is the concentration of the ith pollutant in the EQI, mg/L.

#### 2.3.2. Operating Costs Index (OCI)

The operating cost is characterized by OCI with a unit of $\$/m^3$. The OCI includes energy costs, pharmaceutical costs, and sludge disposal costs. The energy costs include aeration energy costs, pumping energy costs, mixing energy costs, heating energy costs, and other energy costs. Similarly, the OCI value can be directly output by GPS-X software, and the OCI calculation formula is shown in Equation (2):

$$\mathrm{OCI} = C_{are} + C_{che} + C_{disp} \tag{2}$$

where $C_{are}$ is electronic energy cost, 0.1 $/kWh. $C_{che}$ is chemical cost, including the carbon source cost of 2.0 $/kg, PAC cost of 0.5 $/kg, and sludge pretreatment chemical cost of 1.0 $/kg. $C_{disp}$ is sludge disposal cost, including the sludge transportation cost of 80 $/t.

Since the associated economic indicators in the software use USD$ as the unit, we convert them to USD$ in the analysis with reference to the USD-RMB exchange rate at the beginning of May 2023, based on 1 USD equals 6.91 RMB.

#### 2.3.3. Greenhouse Gas (GHG)

Operational greenhouse gas emissions are characterized using GHG in units of $tCO_2$ eq/$m^3$. Among the widely used carbon emission accounting methods, the actual-measurement method is not applicable in the simulation and calculation scenarios. This study combines the emission factor method with the mass balance method to slice the carbon emissions of the wastewater treatment plant into multiple parts for separate calculations. The accounting equations are shown in Equations (3) and (4):

$$GHG = Q(C_{in} - C_{out}) \times EF \times GWP \tag{3}$$

$$GHG = AD \times EF \times GWP \tag{4}$$

where AD is the activity data for the emission source and the unit depends on the calculated emission source. EF is the emission factor and the unit depends on the activity data. Q is the effluent flow of WWTP, $m^3/d$. $C_{in}$ is the concentration of the corresponding pollutant in the influent water, mg/L. $C_{out}$ is the concentration of the corresponding pollutant in the effluent water, mg/L. GWP is Global Warming Potential. $GWPCH_4$ is 25 $tCO_2$ eq/$tCH_4$ and $GWPN_2O$ is 298 $tCO_2$ eq/$tN_2O$.

The total carbon emissions are composed of 10 components, which are presented in Table S5. For specific calculations of biochemical processes, power, and chemicals carbon emissions for each structure, refer to Equations (S1)–(S10). Three of the direct emissions (S1), (S2), and (S10) are calculated with the mass balance method (Equation (3)), while the rest of the emission processes are conveniently calculated with the emission factor method (Equation (4)).

### *2.4. Non-Dominated Sorting Method*

Referring to the concept of Pareto optimum, the upstream logic-non-dominated sorting method was introduced in the NSGA-II algorithm to filter out the Pareto optimal solution from tens of thousands of simulation scenarios. It enables us to achieve multi-objective comprehensive optimization of the three objectives, EQI, OCI, and GHG. This method is ideal for optimizing control strategies in WWTPs as it can handle nonlinear optimization problems. Moreover, it is capable of evaluating the objective function with fewer conditions and achieving multi-objective optimization in a single simulation [27].

A cycle-based iterative ranking method is used to achieve the above optimization. For each round of the study objects within the study scope, the "dominance" relationship of each scenario point with other scenario points is examined separately. Then, the optimal scenario in a "non-dominated" state is selected in each round until all the remaining scenarios are not dominated by each other.

In general, the scenarios with Pareto rank 1 obtained by multi-objective sorting are not unique. In order to further complete the screening in "Pareto-optimal" scenarios, this study establishes a ranking method with constraints, focusing on the comprehensive level of objectives under certain weights. By setting the weights, we calculate the composite objective values to complete the final ranking. In this study, the three objectives are considered to be of the same importance, thus the weight factors $K_{i,j}$ of the three objectives were equal. MATLAB (2021B) programming is used to implement the non-dominated sorting and draw the Pareto frontier. The calculation of the integrated objective value for the i'th scenario is shown in Equation (5):

$$S_i = \sum_{j=1}^{3} K_{i,j} \cdot F_{i,j} / F_{0,j} \tag{5}$$

where $S_i$ is the value of the composite objective for the ith scenario. j is the number of the objective. $K_{i,j}$ is the weight of the jth objective ($K_{i,1} = K_{i,2} = K_{i,3} = 1/3$). $F_{i,j}$ is the value of the jth objective for the ith scenario, with units referenced to the objectives. $F_{0,j}$ is the value of the jth objective for the based scenario, with units referenced to the objectives.

## 3. Results and Discussion

### *3.1. Effect of Operational Parameters on Effluent Quality Index (EQI)*

The influence of the six operational parameters on the EQI values is shown in Figure 3. In general, the EQI values increase with the increase in ATDO and SD values, and decrease with the increase in PAC and ERR values. The change in ECR and IRR values does not have a significant effect on the EQI. Among these, the change in PAC values affects the most largely, indicating that PAC is the most influential operational parameter.

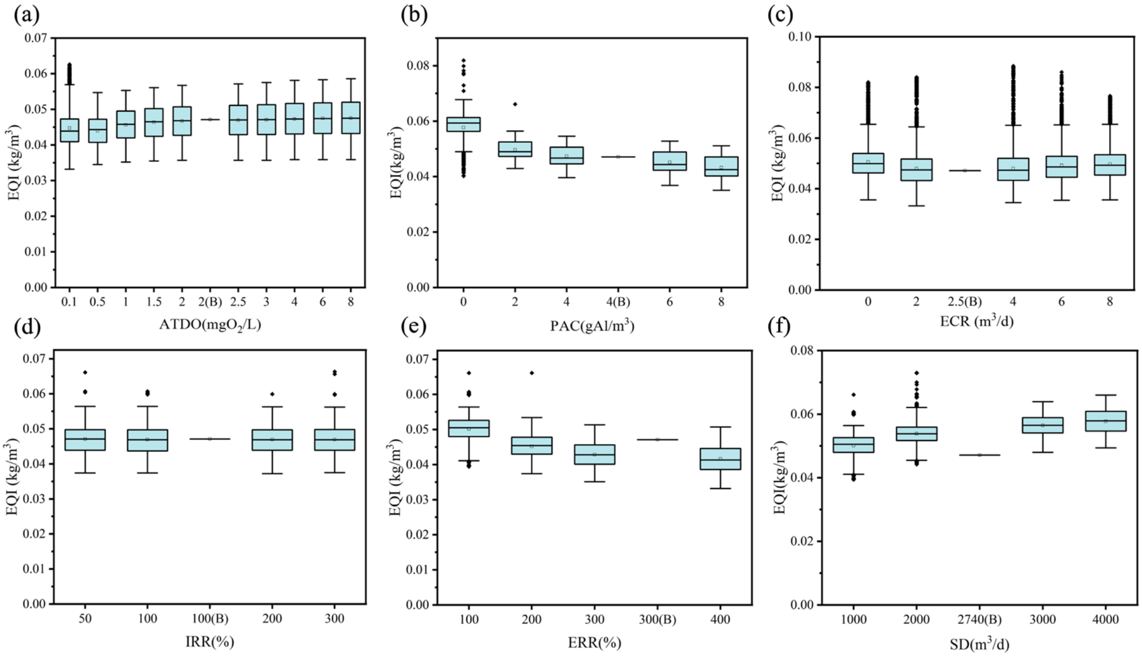


**Figure 3.** The effect of simulated value changes in each operational parameter on EQI for the case plant. (**a**) ATDO; (**b**) PAC; (**c**) ECR; (**d**) IRR; (**e**) ERR; (**f**) SD, and the values of the baseline scenario is denoted by (B) in the abscissa.

The EQI value of the case plant increases slightly with the increase in ATDO, which is shown in Figure 3a, indicating that high ATDO does not enhance the EQI, a similar conclusion was found in the study [28]. Since the subsequent membrane tank is able to share the aerobic tank pressure, the AAO-MBR process allows for extremely low ATDO values to be utilized, resulting in more stable EQI scenarios being met and retained. Jiang et al. [29] demonstrated that the AAO-MBR process improves water quality by efficiently removing nitrogen and phosphorus with limited aeration (DO = 0.5–1.0 mg/L), which is consistent with the simulation results. It is noteworthy that while reducing ATDO to 0.1 mg/L facilitates short-range denitrification, the actual engineering design parameter was set at 2 mg/L. This suggests that an empirical-based design can achieve local optimum values. However, due to insufficient empirical coverage of various scenarios, determining comprehensive and optimal solutions may not always be possible. The results depicted in Figure 3b reveal a noteworthy reduction in the EQI value, as the PAC value rises, which is especially prominent when the PAC value is low. It indicates the significance of PAC in decreasing the integrated water quality index. It also suggests that as the PAC dosage increases, its optimization effect on the EQI dwindles. These two points match with the findings [24,30]. By adding a small amount of ECR, the EQI values have a certain decrease, but with the increase in the dosage, the EQI values will turn to increase (Figure 3c). It indicates that ECR has a limited effect on the overall optimization of effluent water quality as the input of ECR to reduce effluent TN may lead to the increase in COD at the same time, which needs to be analyzed in conjunction with the actual influent C/N ratio. The increases in the C/N ratio in a certain range can enhance the removal of TN and COD [31]. IRR has little effect on the EQI, which is a relatively insensitive parameter, as presented in Figure 3d. Due to the fact that IRR mainly regulates the denitrification process while the carbon source is relatively low, increasing the IRR ratio does not contribute significantly to the effluent quality. The EQI value decreases significantly as the ERR rises (Figure 3e). This is because the rise in ERR increases the concentration of the bicycles, and further improves the EQI. Wang et al. [32] recorded that the $NH_3$-N removal was 98.1%, 98.5%, and 98.9% when the ERR was taken as 100%, 300%, and 500%, respectively. It indicated that the increase in ERR contributes to the water quality, which is in agreement with the simulation results. It has been noted that when the SD increases, the EQI value of the case plant also tends to increase, as depicted in Figure 3f. This is reason that higher SD results in a shorter SRT and lower concentration of mixed liquor suspended solids (MLSS), which are unfavorable conditions for biological treatment [33]. As a result, the effluent quality decreases. Furthermore, the study recommends that this process is better suited for a state of long sludge age.

### *3.2. Effect of Operational Parameters on the Operation Cost Index (OCI)*

The influence of the six operational parameters on the OCI values is shown in Figure 4. It can be seen that IRR and SD do not have a significant effect on the OCI. An increase in the values of the remaining operational parameters causes an increase in the OCI, with a change in the value of ECR causing the largest change in the OCI. It suggests that ECR is the operational parameter with the greatest influence.

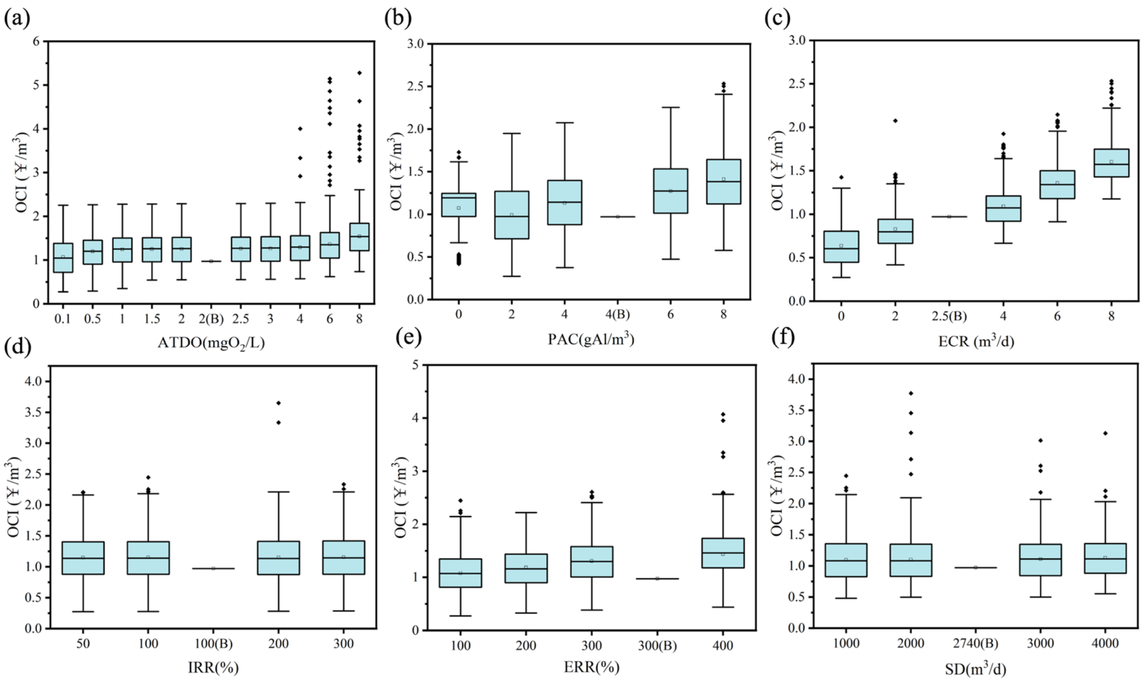


**Figure 4.** The effect of simulated value changes in each operational parameter on OCI for the case plant. (**a**) ATDO; (**b**) PAC; (**c**) ECR; (**d**) IRR; (**e**) ERR; (**f**) SD, and the values of the baseline scenario is denoted by (B) in the abscissa.

As Figure 4a shows, the OCI experiences gradual growth as the ATDO increases. This growth is especially pronounced when the ATDO concentrations are either lower than 0.5 $mgO_2/L$ or higher than 4 $mgO_2/L$. This is the reason that low ATDO reduces energy consumption, and thus OCI in the AAO-MBR process [34,35]. Conversely, higher ATDO levels mean that the water is already saturated with dissolved oxygen, causing a decrease in oxygen transfer rate and utilization. This, in turn, results in an increase in energy consumption and OCI. Other studies have also arrived at similar conclusions [36,37]. Additionally, it has been shown that the aeration process accounts for around 50% of the total power consumption of a WWTP [38] and over 30% of the total OCI [39]. This highlights the crucial role of ATDO in optimizing OCI in wastewater treatment processes. A smooth increase in the OCI with the rise in PAC is presented in Figure 4b. And it matches the traditional concept of the impact of operation. The lower values of OCI for the base scenario demonstrate that the parameter values for the base scenario are relatively better.

The OCI increases dramatically with the increase in ECR (Figure 4c). There is a positive correlation with OCI as the amount of added carbon source is linearly related to the cost of pharmaceuticals as the unit price remains constant. This finding is also well supported by a study that optimizing the dosage rate with a dosing control system can reduce OCI [40]. The effect of ERR is more pronounced on the case plant compared to IRR because the inner return pumps have a lower head than the outer return pumps, and therefore contribute relatively less to OCI, which are shown in Figure 4d,e. Kim et al. [41] analyzed the effect of six decision variables on OCI, in which the effect of IRR on OCI is smaller than ERR, which is consistent with the simulation scenario results. Meanwhile, due to the existence of a multi-stage sludge return line, the number of return pumps and energy consumption are greater compared to other wastewater treatment processes. The change in SD value does not contribute much to OCI (Figure 4f). Improving the OCI of the case plant by adjusting the SD poses a significant challenge. However, utilizing recycled biogas as an energy source can effectively lower electricity consumption. The amount of biogas produced is directly proportional to the SD; therefore, increasing biogas production by raising the SD can help reduce OCI [41]. Yet, this approach has its limitations. Heightening biogas production may increase carbon and nitrogen loads on the environment. Additionally, only the biodegradable portion of the sludge can be transformed into biogas, while the remaining part would require transportation, potentially increasing OCI from 25% to 65% [42]. As a result, further research is necessary to determine the feasibility of this pathway.

### 3.3. Effect of Operational Parameters on Greenhouse Gas (GHG)

The influence of the six operational parameters on the value of GHG is shown in Figure 5. It can be seen that GHG rises with the increase in the values of ECR and ATDO, and the effect of the remaining four operational parameters on GHG is not significant. Among them, the increase in the value of ECR caused a large increase in GHG, which is the same as OCI and is the most influential operational parameter.

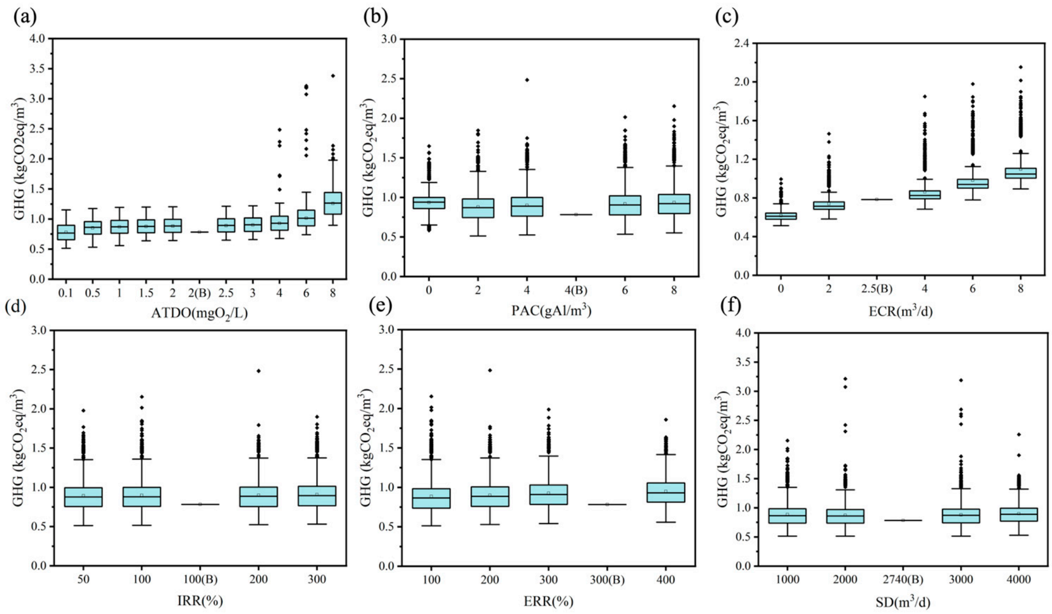


**Figure 5.** The effect of simulated value changes in each operational parameter on GHGI for the case plant. (**a**) ATDO; (**b**) PAC; (**c**) ECR; (**d**) IRR; (**e**) ERR; (**f**) SD, and the values of the baseline scenario is denoted by (B) in the abscissa.

GHG increases with an increase in ATDO which is presented in Figure 5a. This is because higher ATDO increases power consumption and GHG increases with power consumption [43]. A study showed a similar conclusion by demonstrating that electricity consumption is directly related to indirect GHG emissions [44]. The GHG corresponding to the baseline scenario values are lower than the remaining simulated scenario values, indicating that the ATDO design values have been taken to a more optimal level. Huang, F et al. [45] reduced power consumption and GHG emissions by optimizing DO settings through a DO control system using a conventional proportional-integral control strategy. Flores-Alsina et al. [46] investigated the control strategy of WWTP and activated sludge process modeling for GHG emission benchmarking. They used the Benchmark Simulation Model No 2 (BSM2G) to optimize the ATDO values to achieve carbon reduction. According to Figure 5b, GHG levels remain relatively stable as PAC increases. This suggests that carbon emissions from PAC have a minimal impact on the plant's overall GHG levels. However, as shown in Figure 5c, the GHG levels steadily increase with the rise in ECR, indicating a certain degree of linearity. Determining the emission factor reveals a linear relationship between the amount of additional carbon source injection and carbon emissions. When this component accounts for a significant proportion, an increase in added carbon sources can have a significant impact on the GHG emissions of the entire plant. It is worth noting that in practical situations, it is crucial to consider the influent of C/N ratio when making determinations. Kishida et al. [47] found that an appropriate C/N ratio can substantially decrease $N_2O$ emissions during the denitrification stage. IRR and ERR have a small impact on the GHG and the trends are depicted in Figure 5d,e. The power consumption in the sewage treatment process contributes the most to GHG, while the power consumption in the whole process mainly lies in the energy consumption of sewage lifting pump and aeration energy consumption. The energy consumption of reflux pump accounts for a small proportion [48]; therefore, it contributes little to GHG. At the same time, ERR has a more significant influence on GHG than IRR. On the one hand, the internal reflux pump has a lower head than the external reflux pump. On the other hand, the internal reflux mainly controls the effect and process of denitrification. The denitrification process produces $NO_2$, and the emission of $NO_2$ is mainly affected by DO and C/N [49]. Thus, the contribution of IRR to GHG is relatively minor. Figure 5f shows that the change in the value of SD has almost no effect on the GHG of the case plant, which manifests that the optimization of the GHG by changing the value of SD alone is not very effective. In addition, $CH_4$ accounts for a relatively large proportion of the carbon emissions from wastewater treatment processes [50]; therefore, it is possible to generate electricity from the collection of discharged $CH_4$ and realize the recycling of resources, thus effectively reducing GHG [51].

### *3.4. Multi-Objective Optimization of the Anaerobic-Anoxic-Oxic and Membrane Bioreactor (AAO-MBR) Process*

In order to synthesize the interrelationships among the three objectives and screen the strategies to optimize the operational results, a comprehensive comparison of the three objectives was performed using multi-objective optimization. The study involved analyzing 55,460 different optimization scenarios and comparing them to one set of baseline scenarios in the case plant. The relative relationship between these scenarios and their Pareto ratings was determined using a non-dominated ranking method. The data were compared to produce a total of 133 Pareto ratings (Table S6).

Scenarios with high Pareto ratings are better than scenarios with low Pareto ratings for all three objectives (here, lower values for all three metrics are preferred). If all scenarios were plotted in a three-dimensional coordinate system using the three objectives as coordinates, scenarios with high Pareto ratings would be at the more "frontier" position. Plots with Pareto ratings of 1, 50, and 127 in blue, orange, and yellow are depicted in Figure 6a, respectively, in the 3D coordinate system, interpolating the points to construct an envelope with extra data points.

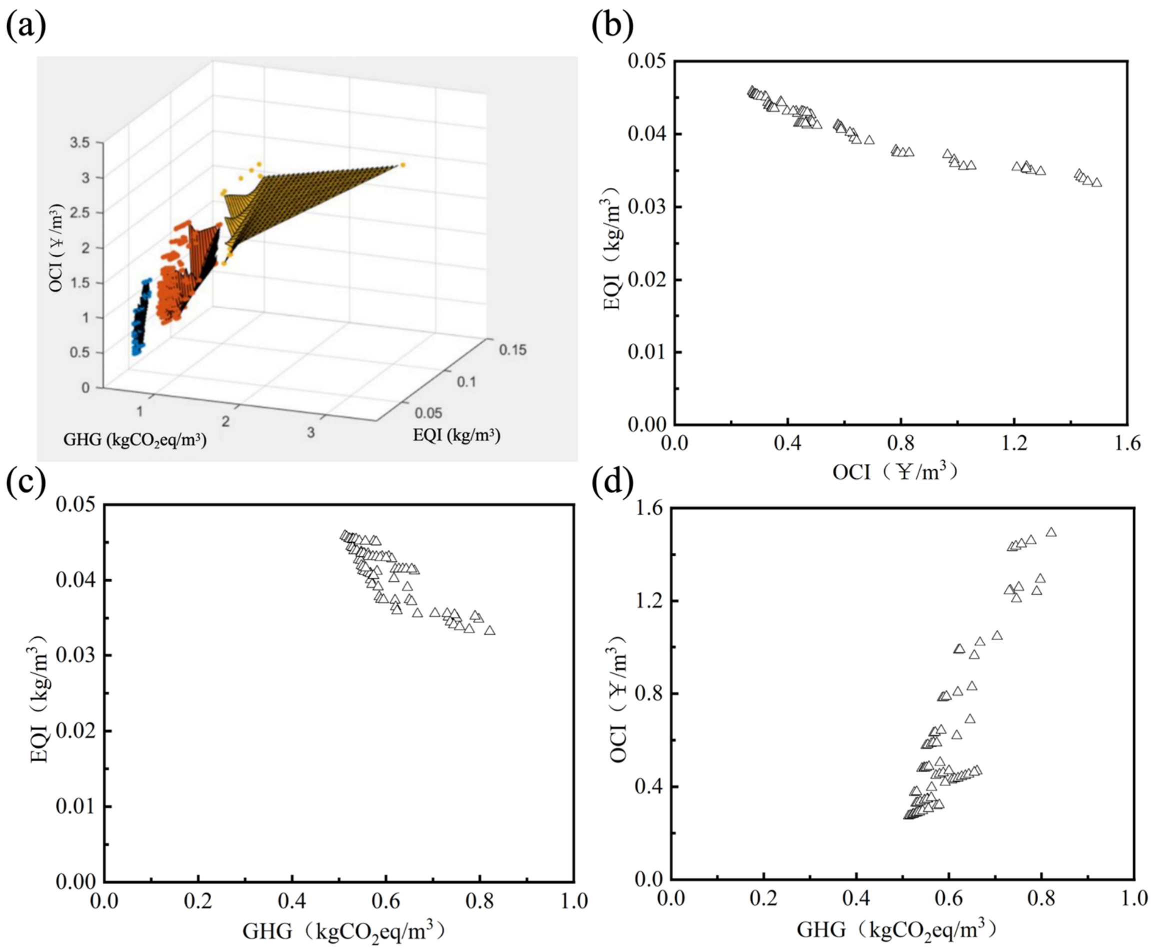


**Figure 6.** Scenarios with different Pareto levels and distribution of optimal scenario indicators. (**a**) Blue, orange, and yellow dots indicated the scenarios with Pareto levels of 1, 50, and 127, respectively; the relationship of OCI and EQI (**b**), GHG and EQI (**c**), and OCI and GHG (**d**) for the "Pareto-optimal" scenarios.

The 75 simulated scenarios with a Pareto rating of 1 can be considered "optimal". Although the data for these scenarios vary and there are even relatively discrete extremes in some of the scenarios, it is not possible to achieve full progress in all three objectives on the basis of these 75 sets of data. The distribution of the values of the three objectives for the "Pareto-optimal" scenario is shown in Figure 6b–d. There is a clear trade-off between the three objectives. In these scenarios, the OCI spans a wide range, indicating that there are still parameter combinations that have a large positive impact on the OCI, but a small negative impact on the other objectives, successfully realizing the "non-dominated" state. In the optimal scenario, with very few outliers removed, the EQI value is concentrated in the range of 0.033–0.046 $kg/m^3$, the OCI value is concentrated in the range of 0.27–1.49 $¥/m^3$, and the GHG value is concentrated in the range of 0.51–0.82 $kgCO_2/m^3$.

After normalizing and weighting the EQI, OCI, and GHG objectives in equal proportions, the top 10 ranked scenarios were calculated as presented in Table 1, where the optimal scenario was 0.046 $kg/m^3$ for EQI, 0.27 $¥/m^3$ for OCI, and 0.51 $kgCO_2/m^3$ for GHG. Compared to the baseline scenario (0.047 $kg/m^3$ for EQI, 0.97 $¥/m^3$ for OCI, and GHG is 0.78 $kgCO_2/m^3$), the optimization is improved by 2.1%, 72.2%, and 34.6%, respectively, which significantly optimizes OCI and GHG under the premise of guaranteeing the EQI. Sweetapple et al. [52] used a non-dominated sorting genetic algorithm to find the Pareto-optimal solution for the three objectives. After the trade-off optimization, EQI is kept basically unchanged, while GHG and OCI are optimized to improve by 17.4% and 3.6%. Santín et al. [53] controlled the whole plant biological wastewater treatment process by the fuzzy controller, EQI, OCI, and GHG were optimized by 1.97%, 14.4%, and 8.24%, respectively. Although the differences in wastewater plant size and influent water quality may affect the optimization effect, it can reflect the advantage of the trade-off objective of the Pareto multi-objective optimization method to a certain extent.

**Table 1.** Multi-objective average weighted optimal ranking of EQI, OCI, and GHG for the case plant.

| Serial Number | ATDO | MTDO | ECR | PAC | IRR | ERR | SD | EQI | OCI | GHG |
|---|---|---|---|---|---|---|---|---|---|---|
| | $mgO_2/L$ | $mgO_2/L$ | $m^3/d$ | $gAl/m^3$ | % | % | $m^3/d$ | $kgCO_2/m^3$ | ¥ $/m^3$ | $kg/m^3$ |
| 251 | 0.1 | 4 | 0 | 2 | 50 | 100 | 1000 | 0.046 | 0.27 | 0.51 |
| 1501 | 0.1 | 4 | 0 | 2 | 100 | 100 | 1000 | 0.046 | 0.28 | 0.52 |
| 1511 | 0.1 | 5 | 0 | 2 | 100 | 100 | 1000 | 0.046 | 0.28 | 0.52 |
| 2751 | 0.1 | 4 | 0 | 2 | 200 | 100 | 1000 | 0.045 | 0.28 | 0.52 |
| 2761 | 0.1 | 5 | 0 | 2 | 200 | 100 | 1000 | 0.045 | 0.29 | 0.53 |
| 1521 | 0.1 | 6 | 0 | 2 | 100 | 100 | 1000 | 0.045 | 0.29 | 0.53 |
| 4001 | 0.1 | 4 | 0 | 2 | 300 | 100 | 1000 | 0.045 | 0.29 | 0.53 |
| 2771 | 0.1 | 6 | 0 | 2 | 200 | 100 | 1000 | 0.045 | 0.29 | 0.54 |
| 4011 | 0.1 | 5 | 0 | 2 | 300 | 100 | 1000 | 0.045 | 0.29 | 0.54 |
| 6501 | 0.1 | 4 | 0 | 2 | 100 | 200 | 1000 | 0.044 | 0.33 | 0.53 |

Focusing on the optimal combination of operational parameters, it can be seen that ATDO maintains a very low concentration of 0.1 mg/L, MTDO is also maintained by pulse aeration and other measures to maintain 4–6 mg/L, IRR is 50–300%, ERR is 100%, a small amount of PAC (2 $gAl/m^3$) is added, the SD is maintained at a low value of 1000 $m^3/d$, and the value of the ECR is taken to be 0, which means that the plant can meet the effluent standard without the addition of the carbon resource. The effluent standard can also be achieved. It can be seen that ERR, SD, and ATDO were taken to low values, which is the same as the results of univariate analysis. IRR and MTDO have a lower impact on the GHG, and therefore were taken to more dispersed values. PAC dosing was not taken to the lowest value, because 0 PAC would result in the effluent TP exceeding the standard, which would lead to a decrease in EQI [54].

To reduce pollution and carbon emissions in an environmentally-conscious and cost-effective manner, the sewage plant should prioritize reducing both ERR and SD. This approach will assist in diminishing the amount of sludge produced during the sewage treatment process and aid in lowering carbon emissions during sludge disposal. One effective way to control ERR is by adjusting the operating frequency of the return pump, while sludge settling time and organic loading rate can also be adjusted to minimize the solid content of the sludge [55]. In addition, the sludge production rate can be lowered by optimizing the operational parameters of the biochemical tank and accurately dosing phosphorus removal chemicals. By implementing these methods, it will further reduce GHG and OCI while still ensuring compliance with the EQI standard.

Based on the results of this study, some issues could be considered in the future. On the one hand, the main parameters for process simulation, such as structure size, stoichiometric parameters, and kinetic parameters, are mainly based on the default values in GPS-X software. It can be calibrated and localized with extensive data from actual wastewater plants if data are available in future studies. On the other hand, equal consideration is given to optimization objectives. When the weights of optimization objectives are not equal, such as carbon reduction as the goal, it is necessary to determine the index weight factor or adopt a fuzzy evaluation method to assist decision-making.

## 4. Conclusions

In this paper, three optimization objectives of WWTP were optimally weighed through a multi-objective optimization method. It demonstrated the potential to reduce GHG emissions cost-effectively while ensuring that the water quality meets the standards, and the following specific conclusions are drawn:

Starting from the idea of Pareto optimization, the GPS-X simulation and modeling software were used to screen 75 scenarios from tens of thousands of orthogonal simulation scenarios to reach the Pareto optimal level. Using the non-dominated sorting method, the optimal solutions were obtained by equal proportional weighting, which guided the attainment of the optimal combinations of operational parameters, as ATDO was kept at a very low concentration of 0.1 mg/L, MTDO was kept at 4 mg/L, IRR was 50%, ERR was 100%, a small amount of PAC (2 gAl/$m^3$) was added, SD was kept at a low value of 1000 $m^3$/d, and ECR was taken to be 0. This paper provides an optimal decision-making solution for this WWTP, which is conducive to the realization of sustainable development in the wastewater treatment industry.

Optimizing the performance of objectives requires a deep understanding of how it responds to operational parameters. Based on simulation results, there appears to be a significant linear relationship between ECR and the three key objectives that operators should prioritize. At the same time, the change in the C/N ratio due to the addition of ECR, thus affecting GHG emissions, is an essential direction for future research.

**Supplementary Materials:** The following supporting information can be downloaded at: https://www.mdpi.com/article/10.3390/w16070995/s1. Figure S1: Batch automation simulation script logic block diagram; Figure S2: Patterns of the effect of simulated value changes in MTDO on three objectives for the case plant; Table S1: The basic situation of influent water quality, actual effluent water quality, and simulated effluent water quality of the case plant; Table S2: Operational parameters of the case plant; Table S3: The parameters of each unit structure of the case plant; Table S4: Optimization scenario orthogonal take point setting of the case plant; Table S5: Summary of carbon emissions of each part; Table S6: Multi-objective optimization of Pareto rank distribution.

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