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Parameter optimization of environmental technologies using a LCA-based analysis scheme: A bioaugmentation case study

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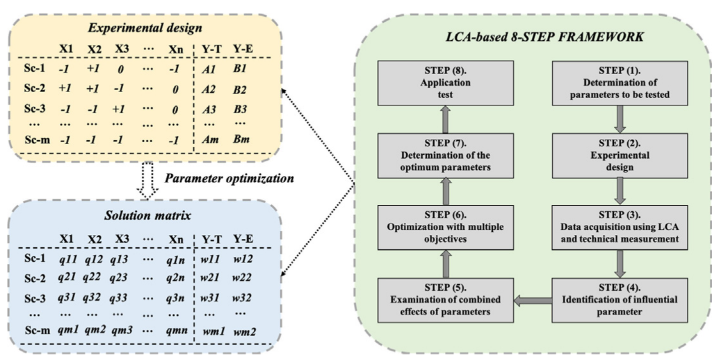
HIGHLIGHTS

- Propose an LCA-based analysis scheme for parameter optimization of environmental technologies
- Integration of LCA into optimization process allows proactive assessment before parameters are predetermined.
- Key parameters that are likely to cause contradictory influences on different objectives can be identified.
- A case study concerning bioaugmentation of constructed wetland was conducted.
- Total environmental impacts of cultivating the strain Arthrobacter sp. ZXY-2 was reduced 13% to 50% via eco-design.

GRAPHICAL ABSTRACT



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ABSTRACT

Life cycle assessment (LCA) has proven to be a useful tool in assessing environmental technologies in a retrospective manner. To fully uncover the environmental improvement potential while advancing technologies under technical and environmental constraints, this study recommended approaching the LCA proactively to assess the progress of parameter optimization before determining critical parameters. To that end, the present work introduced a multimethod eight-step (MMES) analysis scheme, which included an integration of LCA with Plackett-Burman multifactorial design, central composite design, and multi-objective optimization. By creating a large number of scenarios through experimental design, we jointly optimized technical efficiency and environmental sustainability, which allowed for the identification of critical parameters that likely had contradictory influences on different objectives. Through a case study concerning the bioaugmentation of constructed wetland (CW), we applied the MMES scheme to optimize the culture conditions of the strain *Arthrobacter* sp. ZXY-2 for enhanced atrazine removal. The results showed that, by reducing the $Na_2HPO_4 \cdot 12H_2O$ concentration from 6.5 g/L to 6 g/L in the culture condition, we decreased the freshwater ecotoxicity potential and maintained a high level of atrazine removal. Regarding the production process of microbial inocula, the strain ZXY-2 grown at the optimized culture reduced the total environmental impact from 13% to 50% compared with the original culture and helped the CW exhibit more favorable atrazine-removal performance. Taken together, the case study demonstrated the effectiveness of using the MMES scheme for parameter optimization of environmental technologies. For future development, the MMES scheme should extend the application to more fields and refine uncertainty management.

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1. Introduction

With the increasing requirement for global environmental sustainability, the development of environmental technologies not only should enhance the capacity of pollutant removal but also avoid problems shifting from one environmental aspect to others (Golroudbary et al., 2019). It is necessary and significant to consider both technical efficiencies and environmental implications jointly when efforts are made to optimize the technical parameters for practical application (Flores-Alsina et al., 2010; Hakanen et al., 2013). Life cycle assessment (LCA), as a standardized method that strives to capture all of the environmental flows connected to a product or process, has proven to be a feasible approach for generating valuable knowledge to advance the environmental optimization of technical parameters (Foulet et al., 2019; Hauschild et al., 2013; Tsang et al., 2017).

Despite the wide application of LCA, this method has focused mainly on evaluation in which most of the critical parameters have been predetermined. The accomplishment of the parameter optimization has gone beyond the conventional framework of LCA. As guided by ISO 14040–14,044 standards (International Organization for Standardization (ISO, 1997)), a typical application of LCA is to model and assess the environmental impacts of products or processes that have been used commercially with sufficient information and data available from empirical experience (Finnveden et al., 2009; Guinee et al., 2011). In the environmental impact assessment, the technical dimension was not the primary concern, and no specific procedure has been designed within the LCA framework to facilitate parameter optimization.

Optimization of the technical parameters will undergo complicated processes, involving many elements, such as multidimensional objectives and multiple parameters (Rajyalakshmi and Ramaiah, 2013). On one hand, multidimensional objectives that cover both technical and environmental dimensions should be considered jointly during the optimization process. Because of the specific professional requirement of environmental technologies for pollutant removal, the technical efficiency ought to be maintained at favorable levels when efforts are made to decrease the environmental burdens. On the other hand, parameter optimization needs to deal with a large number of parameters. Those parameters usually are kept within specific ranges of values rather than being fixed with absolute values. Interactions exist among parameters, and the combined effects could be over and above the sum of parameters acting on individual levels. Complexity can be exacerbated when considering that the incorporation of LCA will introduce more environmental output variables (e.g., resource consumptions and climate change), although alterations in one parameter may generate conflicting impacts or unexpected variations in results.

To promote the parameter optimization by considering all of the elements mentioned thus far, one option is to integrate and connect LCA with other scientific tools. First, trade-offs between multidimensional objectives are important to determine the optimal parameters, and the application of multi-objective optimization (MOO) could facilitate such a process (Coello, 2006). Second, Plackett-Burman (PB) multifactorial design and central composite design (CCD) are efficient approaches for isolation, investigation, and optimization of the influential factors for products or processes (Almomani, 2020; Levin et al., 2005). These approaches could be used to extend the LCA framework to address all of the parameter-related factors, including relative importance (RI), specific value ranges, parameter interactions, and combined effects. Significant effort has been made to deepen and broaden the LCA methodologies beyond the current ISO framework for extended functions and improved analysis. For instance, Azapagic (1999) proposed a methodological framework called “life-cycle process design” with the inclusion of linear programming to capture the Pareto-optimal sets for optimizing production alternatives. Wernet et al. (2010) applied the artificial neural network to estimate life-cycle inventory and predict characterization results for LCA impact categories based on the molecular structure of the target chemicals. Gavankar et al. (2014) introduced a scheme coupling LCA with the technology and manufacturing readiness levels, which could contextualize a technology's development stage to overcome the lack of large-scale production data. Bai et al. (2018a) integrated LCA with conjoint analysis (CA) to facilitate the involvement of stakeholders in the LCA outcome communication and the decision-making process. To the best of our knowledge, however, no well-established LCA-based scheme exists for guiding the parameter optimization when environmental technologies are developed under the constraints of both technical efficiency and environmental sustainability. In this regard, the present work proposed that the integration of LCA with PB design, CCD, and MOO could enable the establishment of such a scheme. An effort to integrate the four methods appears to be feasible because previous studies had shown successful combinations between PB and CCD (Warda et al., 2016), LCA and MOO (Antipova et al., 2014), as well as PB and LCA (Bai et al., 2019).

In this study, we proposed a multimethod eight-step analysis scheme (MMES) by integrating LCA with MOO, PB, and CCD design. This framework is intended for the parameter optimization of environmental technologies to satisfy multidimensional goals. The following sections start from the descriptions of typical procedures of the MMES framework. To demonstrate how to apply the proposed framework, a case study is conducted concerning the optimization of cultivation parameters of the strain *Arthrobacter* sp. ZXY-2, which is a bioaugmentation candidate for enhanced atrazine removal from wastewater.

2. Methodology

2.1. Assessment framework

Fig. 1 shows the MMES framework consisting of eight steps, which systemically integrates LCA with multiple scientific methods.

Step 1: Selection of parameters to be tested.

We started by determining the parameters to be tested. A list of parameters that will affect the design of emerging technologies was required, with the assigned values having upper and lower limits. Reasonable ranges of parameters were necessary, but they did not need to have identical sizes.

Step 2: Experimental design.

We then used these parameters for experimental design to generate a series of scenarios consisting of parameters ($X_1, X_2, \dots X_n$) and objectives ($Y_1, Y_2, \dots Y_m$). Two options applied to environmental design: complete factorial design and fractional factorial design. Implementing a complete factorial design is a common approach, which would include all of the possible combinations of selected parameters with upper and lower limits (Masetto et al., 2001). When the number of parameters is limited, using such a design can guarantee the maximum information generated to reveal the main effects of various parameters and the interactions between parameters of all orders. Performing a complete factorial design would be inconvenient when a large number of parameters exist, however, because an unmanageable number of scenarios would be required to conduct the experiments and LCA analysis. For example, for an experimental design with 10 parameters, a total of 1024 scenarios (2^{10}) would be generated if each parameter was assigned with high and low values, meaning that 1024 sets of experiments should be conducted. Implementation of the same number of LCA analysis would double the workload, and thus full consideration

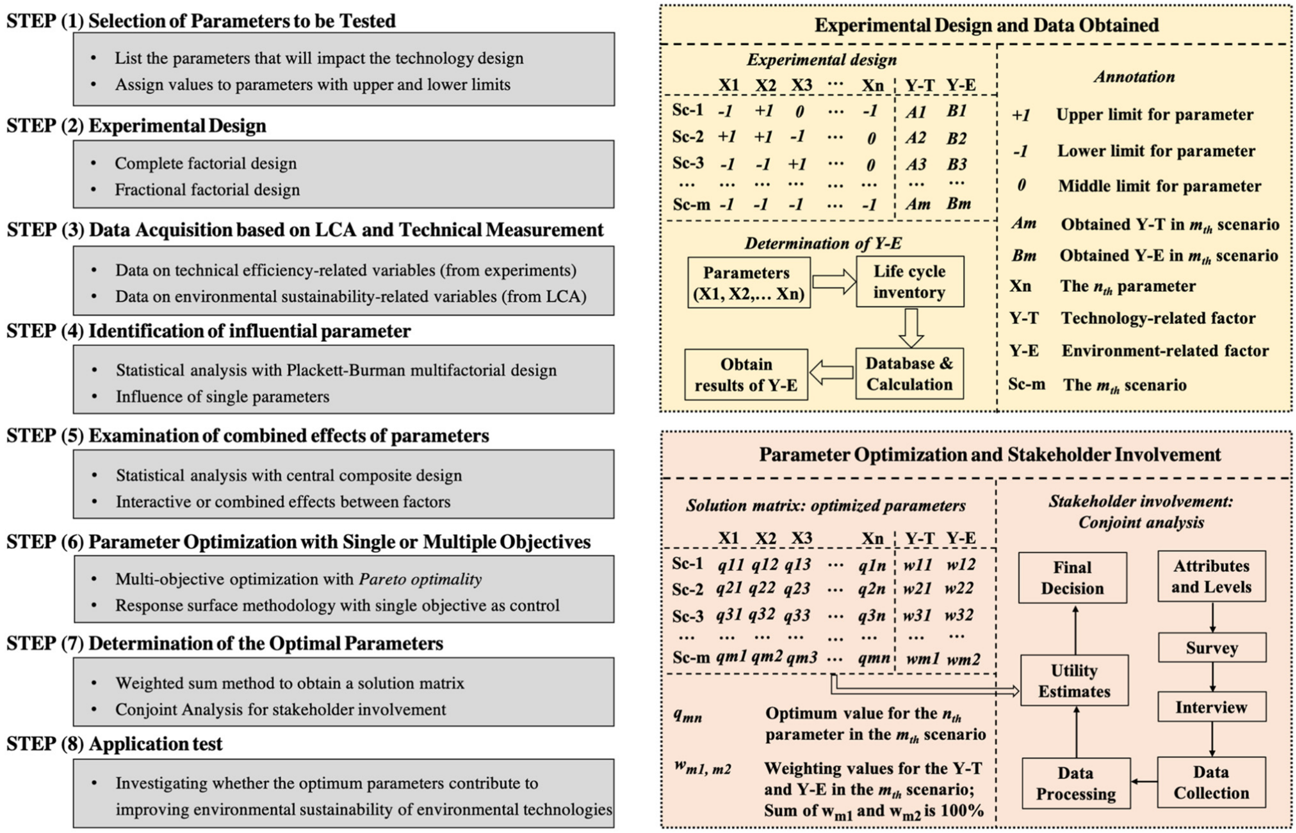

Fig. 1. The multi-method eight-step analysis scheme proposed in this study.

of all scenarios would not be practicable for researchers faced with multiple restraints of time, resources, and finance. In this case, the application of a fractional factorial design using specific methods, e.g., the orthogonal test (Gunst and Mason, 2009), would be recommended to simplify the work.

Step 3: Data acquisition based on LCA and technical measurement.

We next acquired the data. On the basis of the experimental design, we quantified two types of objectives in each scenario: technical efficiency-related objectives (Y_T) and environmental sustainability-related objectives (Y_E). Specifically, we determined Y_T by performing a series of technical measurements that were closely related to the specific technology type. Calculation of Y_E depended on the implementation of LCA, following the standardized procedures defined by the ISO: goal and scope definition, inventory analysis, life-cycle impact assessment, and interpretation (Finkbeiner et al., 2006). We compiled an inventory in each scenario through energy consumption, chemical addition, and environmental emissions from the technical parameters ($X_1, X_2, \ldots X_n$). Quantification of impact-assessment results could use the process LCA model as follows (Heijungs and Suh, 2013):

$$\boldsymbol{Y_E} = \boldsymbol{Qr} = \boldsymbol{QDA}^{-1}\boldsymbol{f}, \tag{1}$$

where $\boldsymbol{Y_E}$ represents the vector of characterization results for all of the impact categories; $\boldsymbol{Q}$ is the matrix of characterization factors for each impact category; and $\boldsymbol{r}$ is the inventory matrix that is calculated by jointly processing $\boldsymbol{D}$, $\boldsymbol{A}$, and $\boldsymbol{f}$, where $\boldsymbol{A}$ is the technology matrix showing inflows and outflows for a certain process, $\boldsymbol{D}$ is the environmental intervention matrix that indicates the resource use and emissions associated with inflows and outflows, and $\boldsymbol{f}$ is a vector of final demands for technological modules.

Step 4: Identification of influential parameter.

Given each scenario (an assembly of parameters) and the associated objectives (the obtained data), we used the PB design to investigate the influence of the parameters on each objective. The PB design, known as a two-level factorial experimental design, can be used to select the most important factor from numerous investigative variables through a few experiments (Vanaja and Shobha Rani, 2007). We recommended that this step focus on the technical efficiency-related objectives (Y_T), to determine the parameters that are significant to ensure the fundamental functions of environmental technologies (e.g., pollutant removal) and to omit the insignificant parameters for a manageable number of parameters in the subsequent step.

For the experimental results obtained by employing the PB design, we defined the impacts of parameters by the first-order polynomial linear equation as follows:

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i X_i \ (i = 1, \ldots, k), \tag{2}$$

where y is the response (Y_T); β_0 denotes the average of all responses; and β_1-β_k represents the coefficients of input parameters X_i calculated by multiple linear regression.

Step 5: Examination of combined effects of parameters.

For the isolated parameters, we used the CCD to detect the combined effects of multiple parameters on multidimensional objectives, with the investigation of interrelationships between parameters. To determine the critical parameters that result in the maximum or minimum output, we fitted the investigative output using the two-order model according to the following equation:

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i X_i + \sum_{i=1}^{k} \beta_{ii} X_i^2 + \sum_{1 \le i \le j}^{k} \beta_{ij} X_i X_j + \varepsilon \ (i, j = 1, \ldots, k), \quad (3)$$

where y is the response (Y_T or Y_E); β_0 is the constant term; β_i, β_{ij}, and β_{ii} represent the coefficients of the linear parameters, interaction parameters and quadratic parameters, respectively; X_i and X_j are input parameters; and ε is the residual associated to the experiments.

Step 6: Parameter optimization employing MOO.

When jointly considering the efficiency dimension (Y_T) and environment dimension (Y_E) for the development of environmental technologies, we identified the optimum parameters to meet the requirement of one dimension without destroying another dimension's need. The use of the MOO satisfied multiple goals simultaneously. Typically, the idea of Pareto optimality is introduced to describe the solutions for MOO problems (Chankong and Haimes, 1993). The general MOO problem is proposed as follows:

$$\begin{aligned} &Minimize: Y(x) = [Y_1(x), Y_2(x), \ldots, Y_k(x)]^T, \text{and} \\ &\quad subject\ to: \varphi_j(x) \le 0; j = 1, 2, \ldots m, \end{aligned} \quad (4)$$

where k is the number of objective functions; m is the number of inequality constraints; $x \in E^n$ is a vector of design variables; and $Y(x) \in E^k$ is a vector of objective functions $Y_i(x): E^n \rightarrow E^1$.

Step 7: Determination of the optimum parameters.

We obtained a group of Pareto optimal solutions using MOO. To determine a single suitable solution, we selectively assigned weights for various objectives using the MMES scheme.

(a) Weighted sum method

This method entailed selecting weights w_i and minimizing the following composite objective function (Marler and Arora, 2010):

$$U = \sum_{i=1}{}^{k} w_i Y_i(x), \text{and} \qquad \sum_{i=1}^{k} w_i = 1. \quad (5)$$

In this way, we artificially assigned the weights of each target, with the sum of all of the targets' weights adding up to 1% or 100%. With a weight matrix that consisted of different sets of weight values, we formed a solution matrix by obtaining various sets of optimal parameters. This optimal parameter matrix can serve as an information pool, which will be helpful for: (1) investigating how the changes of objective importance affect the determination of optimal parameters, and (2) including stakeholders to decide the optimal solution to use for future efforts.

(b) Stakeholder involvement

Incorporating environmental sustainability when performing parameter optimization indicates the integration of new stakeholders (e.g., LCA experts) into the design team of environmental technologies. In this regard, we included CA in the MMES analysis scheme to support the practice of integrating stakeholder's viewpoints into the identification of optimum parameters. Employing CA first required the definition of attributes, levels, and product profiles (Alriksson and Öberg, 2008). In the present work, we divided the attributes of any emerging technology into two classes: technical efficiency and environmental sustainability, which were represented by Y_T and Y_E, respectively. For each attribute, we determined the levels according to the quantitative outcome obtained from either the experimental process or the LCA analysis. On the basis of combinations of attributes and levels, we constructed product profiles to build a bundle of hypothesized alternatives that represented a set of hypothesized decision situations. In these situations, stakeholders could be invited to demonstrate preferences by ranking the hypothesized alternatives.

After collecting preference data from all of the stakeholders involved, the RI of each attribute can be derived using the following statistical analyses:

$$\xi_p = \frac{\max_q\{\xi_{pq}\} - \min_q\{\xi_{pq}\}}{\sum_p \left[\max_q\{\xi_{pq}\} - \min_q\{\xi_{pq}\}\right]} \quad (6)$$

where ξ_p represents the RI value of the p-th attribute, and ξ_{pq} is the utility estimate of the q-th level for the p-th attribute. Detailed processes about the calculation of ξ_{pq} have been presented in our previous studies (Bai et al., 2018a; Bai et al., 2018b). The RI values, to a certain extent, are equated with the intrinsic viewpoints of stakeholders concerning the trade-offs between different objectives. Hence, using the RI values in Eq. (6) helped determine a single Pareto optimal solution for an MOO problem defined as Eq. (5).

Step 8: Application test.

The last step focused on investigating the application performance of optimum parameters, and we preferred a comprehensive analysis covering environment, efficiency, and economy. Application of the optimum parameters at a pilot or industrial scale tests is recommended but not mandatory because designing large-scale experiments may be not available to all environmental technologies.

2.2. Case study: eco-design of bioaugmentation for atrazine removal

To demonstrate how to apply the MMES analysis scheme, we explored an illustrative case of enhanced wastewater treatment through bioaugmentation. This case study focused on the optimization of cultivation conditions of strain *Arthrobacter* sp. ZXY-2, a potential candidate for bioaugmentation in constructed wetland (CW).

2.2.1. Background and objective

In recent years, increased demand for clean aquatic environment has driven rapid development of emerging technologies for wastewater treatment (Ahmed et al., 2017; Grady Jr et al., 2011; Zhou et al., 2018). Bioaugmentation has been intensively investigated to enhance biodegradation and the removal of targeted pollutants with the addition of specialized microbial strains (Liu et al., 2018; Nguyen et al., 2019; Stephenson and Stephenson, 1992; Zang et al., 2020).

In general, determination of the optimum cultivation conditions for making efficient microbial inocula is key to successful application of bioaugmentation. This process commonly takes place in the laboratory, expecting the cultivation conditions with the highest pollutant removal (Zhao et al., 2016; Zhao et al., 2019). When certain microbial strains are employed, the cultural conditions normally serve as predetermined parameters, receiving limited attention in subsequent application. An LCA analysis, however, has revealed that processing and producing microbial strains could occupy a large proportion of negative environmental burdens along with the life cycle of bioaugmentation, accounting for 33.3% and 32.5% in fossil consumptions and global warming, respectively (Zhao et al., 2017). Once such unfavorable environmental influences are formed, they are often difficult to avoid or reduce, because the environmental improvement potential has been locked in the laboratory stage. Thus, the ability to develop sustainable cultivation conditions is both legitimate and necessary to improve the environmental performance along the whole chain of bioaugmentation.

We applied the MMES analysis scheme to a case study concerning the bioaugmentation of CW for enhanced atrazine removal. We selected an atrazine-degrading strain *Arthrobacter* sp. ZXY-2, which has been identified as a potential candidate for bioaugmentation in CW (Zhao et al., 2018), as the research object. This case study first focused on the isolation, evaluation, and optimization of the culture conditions. Then, we built a group of pilot-scale CWs, which were operated in continuous flow with the addition of *Arthrobacter* sp. We implemented a comprehensive technical, environmental, and economic analysis to test whether the optimum culture conditions could contribute to improving the sustainability of bioaugmentation using strain ZXY-2.

2.2.2. Parameter list

Following the MMES analysis scheme, we selected 15 parameters to cultivate ZXY-2, with the value ranges determined according to the basic cultural condition to enrich the medium. The parameters tested included temperature (20 °C–40 °C), pH (5–9), shaking speed (100–200 r/min), inoculum size (1–10%(v/v)), and concentrations of glucose (0–2 g/L), sucrose (0–2 g/L), sodium citrate (0–2 g/L), KNO_3 (0–0.5 g/L), NH_4Cl (0–0.5 g/L), isopropylamine (0–5 mL/L), KH_2PO_4 (1–1.5 g/L), $Na_2HPO_4 \cdot 12H_2O$ (2–12 g/L), $FeSO_4 \cdot 7H_2O$ (0–0.02 g/L), $MgSO_4 \cdot 7H_2O$ (0–0.2 g/L), and atrazine (50–150 mg/L).

2.2.3. First experimental design

We first conducted experimental design to screen the parameters that significantly affected atrazine removal of ZXY-2. We formed a total of 54 scenarios using the fractional factorial design. Coded values for each scenario were given to the independent variables, with +1, −1, and 0 as upper limit, lower limit, and center level, respectively.

2.2.4. First data acquisition: laboratory experiments

We performed only laboratory experiments for all of the scenarios in this phase. We assessed each scenario after 8 h of incubation and tested each in triplicate, using average atrazine-removal percentage (ARP; %) as the response. To assess the ARP, we extracted it with dichloromethane and then filtered it using a sterile filter (Sartorius Stedim, Göttingen, Germany) with a 0.22-μm pore size. We performed the analysis using high-performance liquid chromatography (Shimadzu, Kyoto, Japan) equipped with a C18 column (length 25 cm, internal diameter 4.6 mm, Varian) and an ultraviolet detector at 220 nm wavelength. The mobile phase consisted of acetonitrile/water (6/4, v/v) at a flow rate of 1.0 mL/min. We injected samples with an injection volume of 20 μL. We calculated atrazine concentration by comparison with a standard curve (Li et al., 2008).

2.2.5. PB analysis for significance testing

With the use of PB analysis, we examined the RI of each parameter to screen the factors that could exert significant effects on the response variables. Considering that the fundamental function of the strain ZXY-2 is to remove atrazine, we thus selected the ARP as the single response (technical efficiency-related variable) for the PB design. We employed a Minitab 17.1 (Minitab Inc., State College, PA, USA) to conduct the statistical analysis. We considered parameters that showed a significant effect ($p < .01$) in the regression analysis as the significant factors, which we evaluated in the following investigations.

2.2.6. Second experimental design

We then conducted an experimental design for CCD analysis and parameter optimization. Depending on how many parameters were considered to be significant in the previous phase, we generated a certain number of scenarios using the fractional factorial design. Coded values for each scenario were given to the independent variables, with +1, −1, and 0 as upper limit, lower limit, and center level, respectively.

2.2.7. Second data acquisition: laboratory experiments and environmental impact assessment

We considered both the technical efficiency and environmental sustainability as the response variables. We tested the ARP as the representative of technical output, and the examination of the ARP followed the same experimental processes as described earlier.

For the environmental impact assessment (LCA), we selected global warming, abiotic depletion of fossil fuels, acidification, human toxicity, and freshwater aquatic ecotoxicity as impact categories. The parameters with specific values could be seen as the life-cycle inventory. We defined the functional unit as 1000 L wastewater containing 50 mg/L of atrazine. System boundaries covered all of the energy requirements, substance consumption, and environmental emissions associated with these parameters. By connecting the inventory data with the ecoinvent Database (version 3.5), we performed an impact assessment for each scenario according to the CML method (developed by Leiden University). Both of these indicators have been characterized inside the LCA framework with an integral calculation framework using the openLCA software.

2.2.8. CCD analysis for examining parameter influence

We implemented CCD analysis in this phase to explain the interactive effects between factors on atrazine removal and environmental sustainability. We used Minitab 17.1 for graphic analyses of the interactive effects and to establish regressions between the responses and the parameters.

2.2.9. Determination of optimum cultivation conditions for strain ZXY-2

We implemented an MOO, based on the nondominated sorting genetic algorithm II (Deb et al., 2000), with the simultaneous consideration for the multiple objectives to determine the Pareto solutions. We included three objectives: maximization of ARP, minimization of FAET, and minimization of ADF. We used the weighted sum method to assign weight value to each objective, with a higher value indicating higher RI. The sum of the weight values for the three objectives was 100%. Through trade-offs between objectives (increasing atrazine removal percentage and decreasing environmental burdens as far as possible), we identified a series of optimized cultural conditions, forming a solution matrix.

To determine the final solution, we established a decision group consisting of 10 stakeholders who were familiar with the bioaugmentation techniques. We employed CA to derive the RI value for each objective. The attributes included all of the objectives considered. For each attribute, we specified three levels based on the maximum, minimum, and medium values of experimental results (ARP) and LCA outcome (ADF and FAET). By combining attributes and levels, we formed a bundle of 22 hypothesized decision alternatives for stakeholders to make selections and demonstrate preference. We asked stakeholders to rank the decision alternatives quantitatively with the higher-ranking data representing the more preferred alternatives. After collecting the ranking results from all stakeholders, we used statistical analysis to explore these preference data. Because all of the stakeholders could participate in the process of data collection, no sampling error existed, meaning that the results obtained were statistically representative. On the basis of the utility estimate for each level and each attribute, we determined the RI values of each objective. By associating the RI values with the assigned weights of all objectives in the solution matrix, a final solution (the optimized cultural condition) emerged, which we used for further eco-design analysis to test whether and to what extent the optimized culture could contribute to the eco-design of bioaugmentation. Given that stakeholders may have different or conflicting perspectives about the development directions of novel technologies (Tyl et al., 2015), the process of calculating RI values could be seen as a process in which different perspectives are addressed simultaneously to identify the best compromise.

2.2.10. Bioaugmentation tests with technical and environmental analysis

In this phase, we established and operated a series of microcosm CWs, which were enhanced by the strain ZXY-2 cultivated at the original condition and the optimum condition. The microcosm CWs were in a subsurface flow design using polyvinylchloride columns (25 cm high × 20–30 cm in diameter). Soil samples in CWs were 15 cm deep, which we collected from the topsoil of an atrazine-polluted factory. The calami were approximately 0.66 m in height and were transplanted with a biomass of 1.04 kg fresh weight per/m^2. We used microcosm CWs to treat atrazine wastewater for the average concentration of 5 mg/L. We set up and operated three parallel microcosm CWs under the same conditions as the 5 mg/L atrazine wastewater.

Microcosm (a) was the control group without adding microbial inocula, and microcosm (b) and (c) were dosed with the strain ZXY-2 being cultivated at the original condition and the optimized condition, respectively. We pumped atrazine wastewater into three microcosms under a hydraulic retention time of 4 d during the operation period. When all microcosms reached a steady state, we dosed the strain ZXY-2 to microcosm (b) and (c) to enhance pollutants removal. We tested and compared the ARP for all of the microcosm CWs.

To analyze environmental sustainability, we performed LCA focusing on the cultivation process of strain ZXY-2, with a comparison of environmental impacts between the original condition and optimized condition. System boundaries included the input of chemical substance, cultural medium, and energy consumption, and the output of substance emissions. The analysis of inventory included the nutrient requirement for cultural medium, the chemical substance used to adjust alkalinity of cultural medium, and electricity consumption to maintain cultural temperature. The electricity consumption involved fossil fuel consumption and emissions of carbon dioxide (CO_2) and sulfur dioxide (SO_2). For the LCA impact assessment, we selected global warming, abiotic depletion of fossil fuels, acidification, human toxicity, and freshwater aquatic ecotoxicity as impact categories. We used CML methodology, developed by the Institute of Environmental Sciences at the University of Leiden, to conduct the LCA, and the specific process followed the *Handbook on Life Cycle Assessment* (Guinée, 2002).

For comparison purpose, we obtained a single LCA value that represented total environmental impact using normalization factors and weighting approaches to aggregate the category results. Due to the lack of the appropriate weighting factors designed specifically for bioaugmentation context, all the impact categories are assumed to have the same relative importance with the same weights assigned. This weighting manner in comparison with other weighting approaches, although can result in a different absolute value for one alternative, but will have little influences on comparisons between alternatives (Bai et al., 2017a; Bai et al., 2017b).

3. Results

3.1. Identifying the significant parameters for cultivating strain ZXY-2

On the basis of the first experimental design for the 15 selected parameters (Table S1), we obtained the ARP for all 54 scenarios from laboratory experiments. The ARP ranged from 5% to 98% (Table S2), indicating that those parameters had a significant impact on atrazine removal. By means of PB design, we established a good fit between the observed ARP and model-predicted ARP, with high values of R^2 (0.961) and adjusted R^2 (0.944). According to the p value ($p < .0001$) and a confidence level of 99% set for screening, we identified six parameters as the most influential factors to the growth of strain ZXY-2: temperature, pH, inoculum size, and concentrations of sucrose, atrazine concentration, and $Na_2HPO_4 \cdot 12H_2O$. Among them, temperature and pH had positive effects with higher temperature and pH value resulting in higher ARP within the experimental design region. Relative higher temperature and pH might be beneficial for microorganisms' growth, thus leading to a higher ARP.

3.2. Examining the effect of cultivation factors

On the basis of a further experimental design for the six influential factors (Table S3), we generated another 54 scenarios for the laboratory experiment (obtaining ARP) and the LCA analysis. For the environmental impact assessment (LCA), the chosen responses included freshwater aquatic ecotoxicity (FAET; kg 1,4-DCB eq.) and abiotic depletion of fossil fuels (ADF; MJ). In this study, ADF represented the typical environmental burden that would be caused by all of the tested parameters. In contrast, selection of FAET represented situations in which environmental impacts were determined by two opposite forces. Reduction of the atrazine could reduce the FAET, whereas the life cycle of chemical production or electricity generation along the cultivation of ZXY-2 could increase the FAET. The observed ARP (%) varied from 19.62 to 73.21; the FAET (kg 1,4-DCB eq.) ranged from −3.85 to 32.30; and we obtained the ADF (MJ) between 203.40 and 404.73.

We then employed CCD analysis to investigate how these factors (independently or synthetically) would affect the atrazine degradation and the associated environmental implications. By applying multiple regression analysis, we fitted a predictive quadratic model with the experimental results or LCA outcome. We established a regression relationship between the six influential factors and each response (ARP, FAET, and ADF), with the determination coefficient $R^2 = 0.9738$, 0.9647, and 0.9512, respectively.

Effects of the six influential factors on each response are shown in Table 1. In terms of ARP, we obtained higher coefficient values with 16.65 and −20.12 for the inoculum size and atrazine concentration, indicating a higher significant effect on the atrazine degradation compared with other factors. Of note, $Na_2HPO_4 \cdot 12H_2O$ exerted an insignificant influence on ARP, with the coefficient value being 1.18. For both FAET and ADF, however, $Na_2HPO_4 \cdot 12H_2O$ was the determinant for the generation of environmental burdens, with the highest coefficient values of 19.24 and 20.78.

Interactive effects between $Na_2HPO_4 \cdot 12H_2O$ and other parameters on ARP, FAET, and ADF are shown in Fig. 2. The interactive effects indicated that the variance of $Na_2HPO_4 \cdot 12H_2O$ concentration could not drive the change of ARP but dominated the alteration of FAET and ADF. Taking the pair-wise interaction of $Na_2HPO_4 \cdot 12H_2O$ and pH as an example, the ARP remained 45–50% at 8 (pH) regardless of the fluctuation of $Na_2HPO_4 \cdot 12H_2O$, and only an increase in the pH (to 9) further enhanced the ARP to 50–55%. Increasing the pH from 8 to 9, however, showed little influence on the ADF and FAET, both of which could be raised obviously by a slight increase of $Na_2HPO_4 \cdot 12H_2O$ concentration.

Overall, the different sensitivities of ARP, FAET, and ADF to the $Na_2HPO_4 \cdot 12H_2O$ indicated that decreasing the $Na_2HPO_4 \cdot 12H_2O$ concentration in cultivation conditions could reduce the environmental burdens generated during the production of the strain ZXY-2 while simultaneously keeping the atrazine degradation stable.

3.3. Obtaining cultivation conditions under different objective weights

We derived different optimal cultivation conditions from the multiple objective optimization that assigned diverse weights to the technical efficiency (ARP) and environmental sustainability (ADF, FAET), as shown in Table 2. As a control group, we also performed response surface methodology (RSM) along with the optimization of single objective (ARP). According to the optimal solution obtained from RSM, ARP had an RI of 100%. We obtained the highest atrazine removal rate with the

Table 1
Effects of the six influential factors on each response (obtained from CCD analysis).

Parameters	Coefficient values		
	ARP	FAET	ADF
Temperature	0.88	−0.35	2.59
pH	5.71	−1.51	0.20
Inoculum size	16.64	−5.02	0.07
Sucrose	4.64	−1.26	0.66
Na2HPO4·12H2O	1.17	19.23	197.80
Atrazine	−20.12	−3.947	0.5

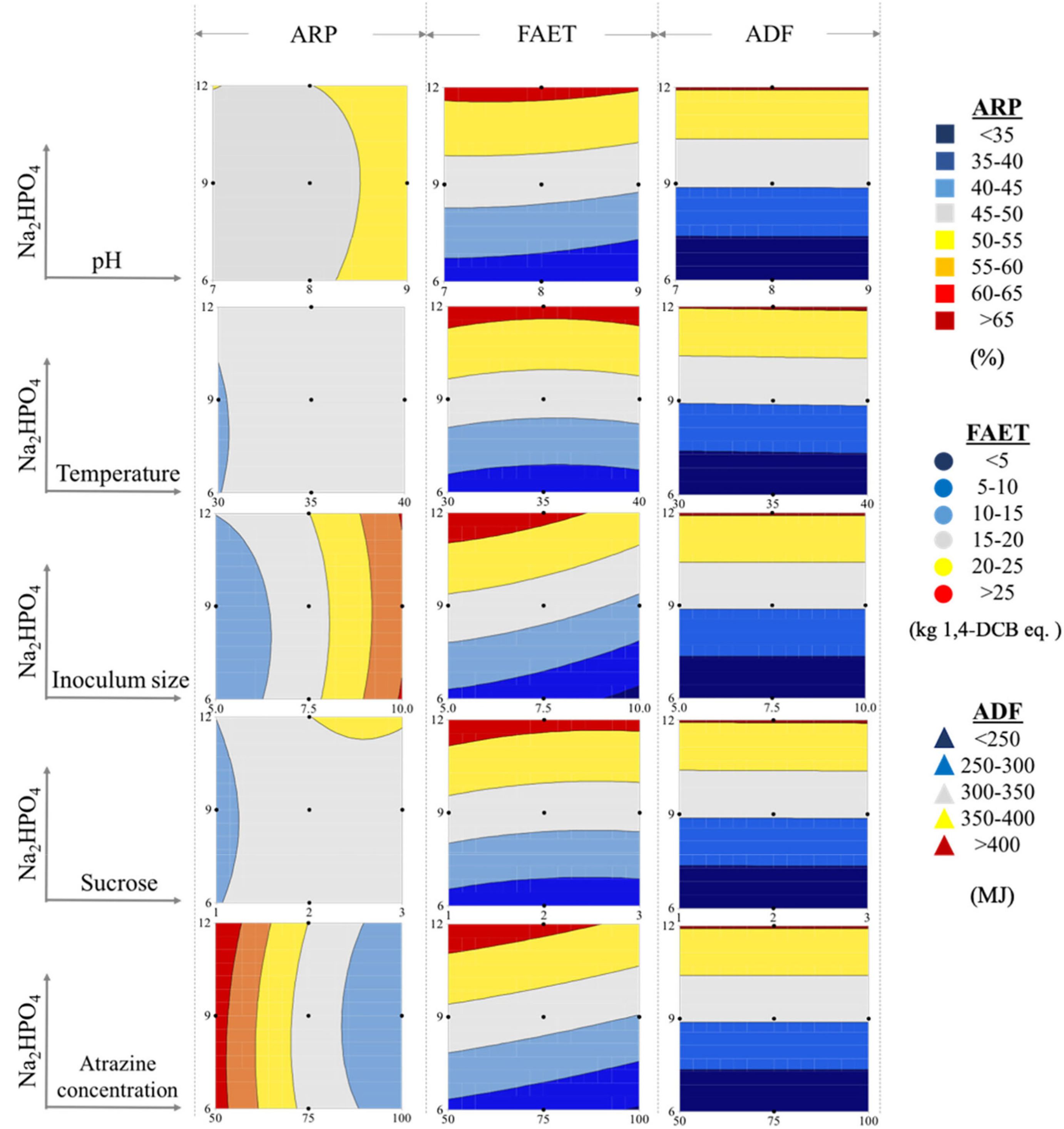

Fig. 2. Interactive effects between $Na_2HPO_4 \cdot 12H_2O$ and other parameters on the ARP, FAET and ADF.

ARP of 76.36% using RSM. Under MOO, however, ARP was only a bit lower, remaining around 75% when it had an RI between 60% and 80%. As the weight of ARP decreased further, the atrazine removal rate reduced accordingly, but it still could be maintained at >60% even at the lowest RI (1%). In addition, ADF was similar under all of the optimal conditions, ranging from 204 MJ to 206 MJ.

Use of RSM produced the highest FAET of 6.87 kg 1,4-DCB eq., although we obtained lower values (from −3.85 to −1.85) using the MOO. When the values of FAET were negative, a net environmental benefit could be obtained in terms of the freshwater ecotoxicity. With special regard to the weight sets that FAET only had a 1% RI, we obtained −3.82 kg 1,4-DCB eq., which was obviously lower than the result using RSM. By comparing the two optimal cultivation conditions, we found that only $Na_2HPO_4 \cdot 12H_2O$ concentration (g/L) changed from 6.5 (RSM) to 6 (1% weight for FAET). Of note, the ARP remained unchanged between these two conditions. Taken together, we concluded that, other cultivation parameters being equal, the decreased $Na_2HPO_4 \cdot 12H_2O$ concentration (from 6.5 g/L to 6 g/L) reduced the

Table 2
Optimized cultivation conditions under different objective weights.

Optimization methods	Single objective optimization cultivation conditions						Environmental impact		Technical efficiency
RSM	Temperature °C	pH	inoculum size% (v/v)	sucrose g/L	Na2HPO4·12H2O g/L	Atrazine mg/L	ADF (MJ)	FAET kg 1,4-DCB eq.	ARP (%)
	34.00	9	10	2.21	6.5	50	204.94	6.87	76.36

Weight values of objectives			Multiple objective optimization cultivation conditions						Environmental impact		Technical efficiency
Weights of ADF	Weights of FAET	Weights of ARP	Temperature °C	pH	Inoculum size% (v/v)	Sucrose g/L	Na2HPO4·12H2O g/L	Atrazine mg/L	ADF (MJ)	FAET kg 1,4-DCB eq.	ARP (%)
49.00%	50.00%	1.00%	34.00	9	10	2.47	6	50	204.16	−1.85	63.91
45.00%	45.00%	10.00%	34.24	9	10	2.58	6	50	205.30	−2.86	67.64
40.00%	40.00%	20.00%	34.85	9	10	2.60	6	50	205.46	−2.91	67.78
35.00%	35.00%	30.00%	35.15	9	10	2.58	6	50	205.53	−2.92	67.81
30.00%	30.00%	40.00%	35.15	9	10	2.60	6	50	205.54	−2.92	67.81
25.00%	25.00%	50.00%	35.25	9	10	2.59	6	50	205.56	−2.92	67.81
20.00%	20.00%	60.00%	34.54	9	10	2.05	6	50	204.94	−3.85	75.01
15.00%	15.00%	70.00%	34.04	9	10	2.05	6	50	204.94	−3.85	75.01
10.00%	10.00%	80.00%	33.54	9	10	2.05	6	50	204.94	−3.85	75.01
1.00%	1.00%	98.00%	33.98	9	10	2.18	6	50	204.95	−3.82	75.02

freshwater ecotoxicity along the life cycle of cultivating the strain ZXY-2, but it maintained the relative higher level of atrazine removal (around 75%). This observation was consistent with our previous findings, and it also indicated that when the decision situation shifted from single objective to multiple objectives, $Na_2HPO_4 \cdot 12H_2O$ concentration could be identified as the factor most likely to be improved, even if the environmental dimension (FAET) was given only a small RI (1%).

3.4. Involvement of stakeholders in determining the final optimized cultural condition

Stakeholder's participation was involved by employing CA to decide the final optimized solution. With the collected preference data serving as input data (Tables S4 and S5), we conducted an estimation to obtain the utility estimate for each attribute's level. In general, a higher estimation value of utility represents a greater extent of respondent's preference.

Table 3
Estimation of utility and relative importance for each attribute in conjoint analysis.

Attributes	Utility estimates				Relative importance
	Levels	Units	Utility values	Std. error	
ARP	64%	Atrazine-removal	0.750	0.023	72%
	71%	Atrazine-removal	1.500	0.13	
	77%	Atrazine-removal	2.250	0.21	
FAET	−1.8	kg 1,4-DCB eq.	−0.182	0.014	17%
	2.6	kg 1,4-DCB eq.	−0.093	0.016	
	7	kg 1,4-DCB eq.	−0.072	0.003	
ADF	204	MJ	0.821	0.034	11%
	205	MJ	0.024	0.002	
	206	MJ	0.011	0.004	

From Table 3, we observed a positive relationship between the ARP and its utility, with the highest atrazine-removal percentage (77%) corresponding to the highest utility estimate (2.250). This indicated that the stakeholders demonstrated increasing preference toward the choices involving the enhanced levels of atrazine degradation.

In contrast, an inverse relationship between FAET and its utility was identified, indicating the decreasing preferences of stakeholders toward the increased levels of freshwater ecotoxicity potential. Significant differences were observed in the utility estimates between positive levels and negative levels of the FAET attribute. We obtained estimation results of 0.024 and 0.011 for the levels of 2.6 and 7.0 (kg 1,4-DCB eq.), whereas the utility was increased by tens of times for the level of −1.8 (kg 1,4-DCB eq.) with the result of 0.82. This meant that the stakeholders demonstrated a higher preference for the level that represented the scenario achieving a net environmental benefit. For the ADF attribute, we also obtained an inverse relationship between levels and its utility, although the difference in utility estimates between different levels was not substantial, which indicated that current levels of fossil fuel consumption did not affect the determination of stakeholders.

We further converted results of utility estimates into the measure of RI for each attribute. The extent of RI values represented how important each attribute was to the overall preferences of stakeholders. Attributes with a higher RI value played a more significant role than those with a lower RI value. As shown in Table 3, the ARP presented the highest RI value (68.8%), implying that the highest priority was atrazine removal for stakeholders to determine the cultural condition. Although FAET and ADF might not be as important as ARP, the aggregated RI values were 31.2%, meaning that the environmental impacts of cultivating the strain ZXY-2 should not be neglected. By associating the RI values with the solution matrix (Table 2), we were able to determine the final optimized cultural condition from the weighting sets that assigned RIs of 70%, 15%, and 15% to ARP, FAET, and ADF. This optimized condition to some extent represented that the solution that could keep a high level of atrazine removal with reduced environmental implications could be used for further bioaugmentation test and eco-design analysis (Fig. 3).

3.5. Bioaugmentation test on the enhanced atrazine removal from constructed wetland

We analyzed atrazine removal during the 65 days' experimental period. As shown in Fig. 4(1), all three microcosm CWs generated the fluctuating removal efficiencies of atrazine (represented by ARP) between 19.6% and 79.3% during the first 25 days' operation. During days 26–35, APR remained stable around 68.2% in each system. We inoculated the strain ZXY-2 into CWs for enhanced removal of atrazine beginning at day 36, with the original and optimized cultivation conditions being adopted for the microcosm (b) and (c), respectively.

Both microcosm (b) and (c) exhibited the increased ARP, indicating that strain ZXY-2 played a role in bioaugmentation. As time passed, the strain and indigenous bacteria might become increasingly competitive for organic matter with the decreased ARP compared with microcosm (a). Additionally, the loss of dosed microbial inocula as a result of being washed out existed for both systems, meaning that reinoculation was necessary to continue the enhanced atrazine removal. We observed similar time periods between inoculations (as one bioaugmentation cycle) for the two systems. As for microcosm (b) and (c), after the second inoculation, ARP resumed rising and gradually increased to 92.1% and 82.9%. We observed the same tread for ARP after the third inoculation.

The microcosm (c), however, achieved more favorable bioaugmentation performance for ARP compared with microcosm (b). The averaged ARP was 88.3% of microcosm (c) in each cycle, which was higher than the microcosm (b) with that of 75.6%. The ARP for each inoculation of microcosm (c) was significantly higher ($p < .01$) than for microcosm (b), which verified that the use of the optimized condition to produce the microbial inocula was applicable to bioaugment atrazine removal in CW microcosm. For the microcosm (a), ARP marked a steady removal of 71.6% showing no enhanced atrazine removal capacity during the entire steady and bioaugmented period.

3.6. Bioaugmentation test: comparisons between optimized condition and original condition

According to this analysis, application of the strain ZXY-2 cultivating at the optimized condition outperformed the original condition in terms of the enhanced atrazine removal from CWs. To further examine whether the optimized condition could contribute to improving environmental sustainability of bioaugmentation, we conducted LCA to investigate the total environmental impacts. When implementing the optimized condition in comparison with the original condition, the environmental impact could be increased because of the pH adjustment from 7 to 9, which could be reduced because of the decreasing utilization of $Na_2HPO_4 \cdot 12H_2O$, sucrose, and other elements. As shown in Fig. 4(2), we observed a reduction of total environmental impacts for the optimized condition, indicating that the adoption of the proposed MMES analysis scheme indeed helped the eco-design of bioaugmentation in this case. Although uncertainty resulting from the choice of LCA methodologies was introduced for the contribution analysis of impact categories, little influence was engaged about the comparisons of total environmental impacts, with the optimized condition being 13–50% lower than the original condition.

4. Discussion

To facilitate the parameter optimization when developing environmental technologies under multidimensional objectives, this study developed an MMES analysis scheme by integrating multiple scientific methods systemically. In this scheme, we integrated LCA into the optimization process as a primary tool for dealing with environmental dimensions. This scheme also allowed for the LCA to be performed before technical parameters were determined. Such proactive assessment distinguishes the present work from other studies in which LCA could be applied only retrospectively to assess the data derived from the finished experiments (Chong et al., 2018; Lardon et al., 2009; Zhang et al., 2019).

Through experimental design, the use of the MMES scheme created a large number of scenarios to investigate how the change of

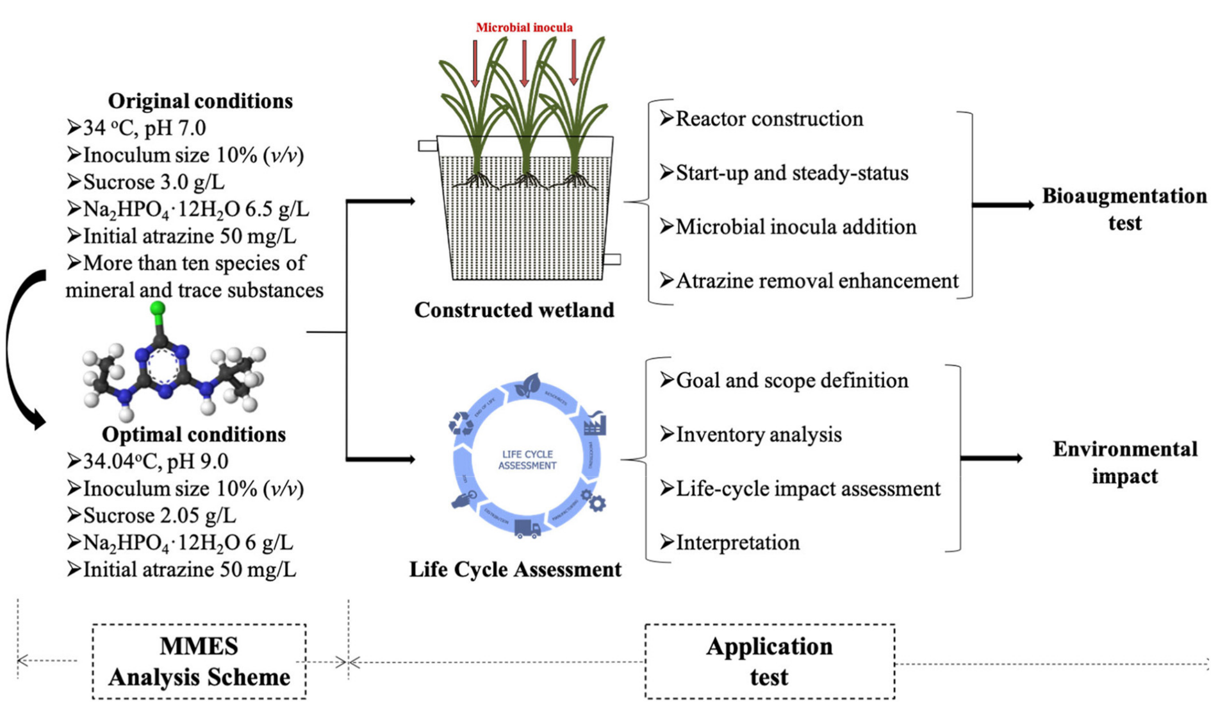

Fig. 3. Scheme diagram of bioaugmentation test and environmental impact analysis for the optimized condition.

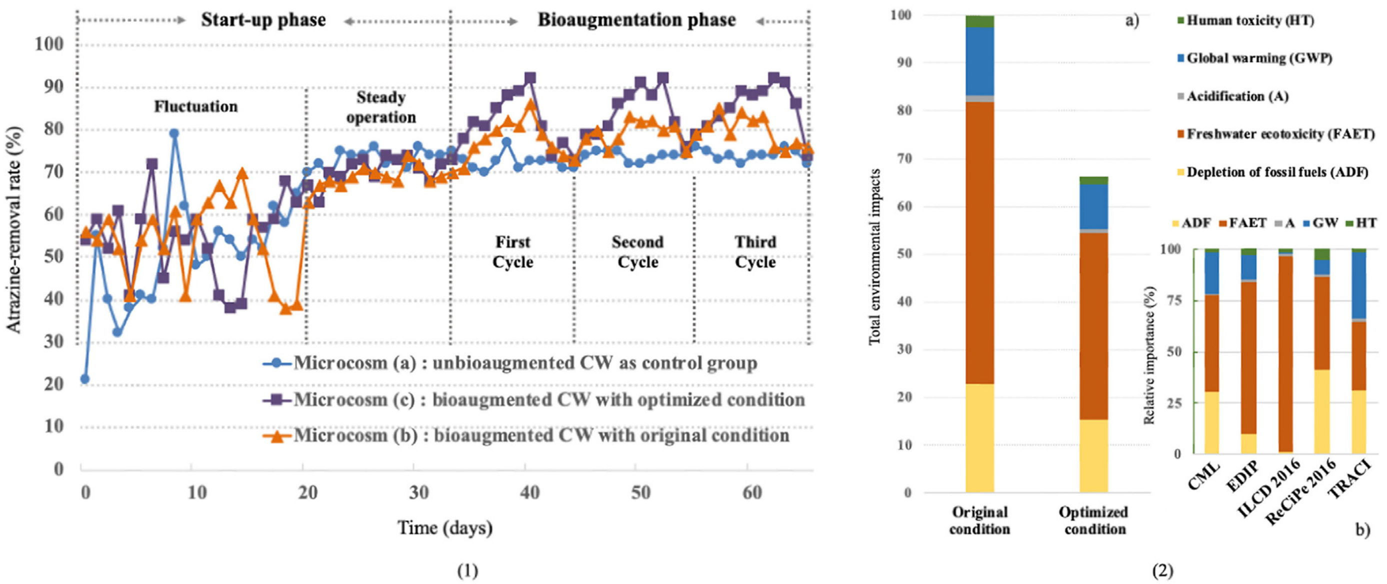

Fig. 4. Atrazine removal of constructed wetland (CW) for bioaugmentation test (1) and comparison of total environmental impacts between original condition and optimized condition for environmental performance analysis (2). *Uncertainty due to the methodological choices was considered in the eco-design analysis, as shown in panel (2)-(b). Different groups of LCA characterization methods (CML, EDIP, ILCD 2016, ReCiPe 2016, and TRACI) were investigated.

parameters would affect both the technical efficiency and environmental sustainability. With consideration of meeting one objective without destroying another's need, we uncovered key parameters that likely caused contradictory influences on different objectives, which contributed to fully revealing the environmental improvement potential by examining the interactive effects between parameters.

By means of a case study concerning the culture optimization of the strain *Arthrobacter* sp. ZXY-2, the MMES analysis scheme proved to be effective for eco-design of bioaugmentation. Indeed, we could extend application of this scheme to a wide range of fields, as long as it is necessary to determine areas where environmental improvement can be made even at low technology readiness levels. Those fields may cover materials production, drug synthesis, and chemical engineering (Galli et al., 2018; Negny et al., 2012). In performing MOO, this MMES analysis scheme could form optimal solutions when diverse weights were assigned to different objectives. Compilation of these optimal solutions created an information pool, which would be helpful if stakeholders are involved in deciding which solution to use for future efforts.

As for future application of the MMES analysis scheme, reducing uncertainty could increase the credibility of evaluation and optimization results. In the existing scheme, two parts caused uncertainty. First, variations in the value ranges assigned to parameters in the use of statistical methods (PB design or CCD) probably contributed to the changed rankings of parameter effects (Bai et al., 2019; Vander Heyden et al., 1995). These variations may have shifted the focus of subsequent optimization from one parameter to another, resulting in different optimized results. Thus, a clarification of reasons, assumptions, and possible changing ranges in the initial value assignment would reduce uncertainty. Second, associated with the integration of LCA into parameter optimization, the conversion of technical parameters into the LCA inventory may have triggered uncertainty. Establishment of an inventory required the compilation of energy flow, material flow, and environmental emissions involved in the technical parameters. Although the required inventory data could be obtained directly from laboratory experiments, data quality was limited when predicting future scale-up events. As a result, the technology scale-up would have different degrees of influence on the flow of input and output. This variable influence could lead to nonlinear scale-up of inventory data. To reduce this uncertainty, future efforts should incorporate the scale-up frameworks of LCA inventory into the analysis scheme to improve the accuracy of predicting environmental performance at industrial scales based on the available laboratory experiment data. Some scale-up frameworks have been proposed, most of which focus on the field of chemical engineering (Piccinno et al., 2016; Piccinno et al., 2018; Simon et al., 2016). Considering that each environmental technology has distinct characteristics, the ability to build a uniform scale-up framework for all technologies is unlikely. Thus, we had to determine which scale-up framework could be integrated into the analysis scheme according to the characteristics of the evaluated technology. Consideration of expert knowledge or estimates on how the technology would behave at a larger scale also would be important.

5. Conclusions

This study presented an MMES analysis scheme in support of the parameter optimization of environmental technologies to satisfy multidimensional goals. By incorporating environmental indicators as the objectives considered during the design and development of technologies, optimization of technical parameters was allowed by balancing the factors that may have caused competing influences on the technical efficiency and environmental sustainability. This proactive optimization contributed to fully uncovering the environmental improvement potential before critical technical parameters were locked for future investigation. We were able to obtain multiple optimal solutions from the MMES scheme, which identified how changing the RI of objectives affected the determination of an optimal solution. An opportunity thus was opened for compromising the ideological profiles of different stakeholders to reveal a final solution. In a demonstrative case study, we optimized the cultivation conditions of the strain *Arthrobacter* sp. ZXY-2 for sustainable enhancement of atrazine removal from CWs. Compared with the original condition, we obtained a reduction in total environmental impacts of 13% to 50% with the optimized condition, mainly as a result of the reduced utilization of $Na_2HPO_4 \cdot 12H_2O$, sucrose, as well as other chemical elements throughout the production process of microbial inocula. Combined with the higher atrazine-removal performance on CW tests, the MMES scheme proved its effectiveness for improving the environmental sustainability of bioaugmentation. Further application and development of the MMES scheme will cover additional research fields and refine the uncertainty management to increase the credibility of evaluation and optimization results.

CRediT authorship contribution statement

Xinyue Zhao: Writing - review & editing.**Shunwen Bai:**Conceptualization, Supervision.**Yinan Tu:**Software, Investigation.**Xuedong Zhang:** Software, Investigation.**Henri Spanjers:**Supervision.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.scitotenv.2020.140284.

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