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Fertilizer or pollutant: analyzing the effects of biochar on soil organisms using machine learning

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Abstract

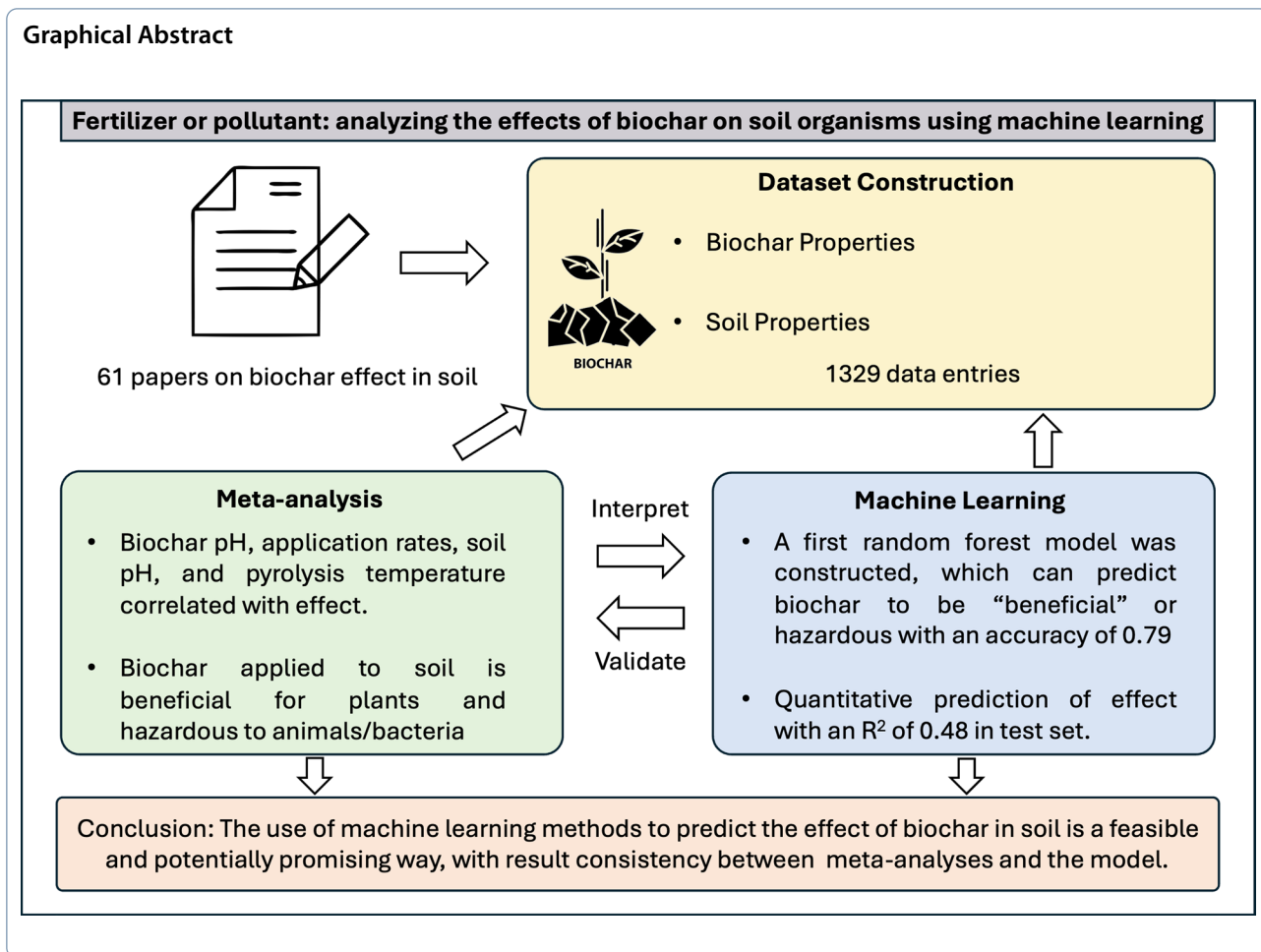
In the context of carbon neutrality targets, biochar is widely promoted as a soil amendment to sequester organic carbon in soils. Although a wealth of research has illustrated the benefits of biochar to plants, its potential toxicity to soil fauna and microbes requires serious consideration. The aim of this study was to perform a meta-analysis of experimental data on biochar effects (i.e. percentage change in endpoints after biochar application compared to the control group) on plants, animals, and microorganisms. The experimental data were extracted from 61 papers and consists of 1329 data points. In a next step, machine learning was used to develop a classifier to predict, whether biochar has positive or negative consequences on soil organisms based on biochar and soil properties. The meta-analysis shows that the effect of biochar is negatively correlated with the biochar application rate, biochar pH, pyrolysis temperature, and soil pH. A random forest classifier was then developed to classify whether biochar was “beneficial” or “hazardous” based on four types of descriptors: biochar properties, soil properties, test organism, and endpoint type. The accuracy of the best model achieved an R^2 of 0.79. In the next step, a quantitative model was developed to predict the effect with an R^2 of 0.48. The model is of great significance for understanding the role of biochar in soil and improving the quality control strategy for biochar production.

Highlights

- Positive and negative effects of biochar on soil biota were extracted from 61 studies
- A model was developed to predict whether biochar has positive or negative consequences
- 4 types of descriptors: biochar properties, soil properties, test organism, endpoint type
- The accuracy of the best model achieved an R^2 of 0.79

Keywords Biochar, Soil, Machine learning, Toxic effects, Beneficial effects

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1 Introduction

Can a single soil amendment simultaneously serve as a fertilizer, a carbon sink, and a pollutant? Biochar, a carbon-rich material derived from biomass pyrolysis, has sparked intense scientific interest due to its dual nature in soil ecosystems. While widely promoted for improving soil fertility and storing carbon, other studies suggest that biochar may also disrupt microbial communities or harm soil fauna under certain conditions (Crombie et al. 2015). These contradictory findings raise urgent questions about how biochar truly functions in diverse soil environments (Crombie et al. 2015).

Biochar’s annual global production volume was higher than 350,000 metric tonnes in 2023 (International Biochar Initiative 2015). The annual growth rate of biochar was more than 90% between 2021 and 2023. Biochar is a carbon-rich material obtained from heating biomass with little or no oxygen (Lehmann & Joseph 2015). The difference between conventional charcoal and biochar is that charcoal is mainly used as fuel, while biochar is mainly used for environmental management in soils (Hagemann

et al. 2018; Reichle 2015). Biochar is produced from various biomass feedstocks such as straw and wheat (Meng et al. 2019; Pawar & Panwar 2022). Other mixed biomass, such as agricultural waste or sludge, can also be adopted as raw materials for biochar.

Biochar has beneficial properties such as high specific surface area, high nutrient content, and low density. Because of its outstanding physical and chemical properties, biochar is widely applied for soil fertilization and remediation (Chen et al. 2019). Besides impacting plants, the microbial structure of the soil is also positively influenced by biochar. For example, Liu et al. concluded that with the addition of biochar, the microbial biomass increased by 18% in total (Liu et al. 2016).

However, with the booming trend of biochar application, the focus should not only be on its advantages but also on its possible negative effects because biochar can also be a pollutant. For example, heating biomass can produce polycyclic aromatic hydrocarbons (PAHs) and enrich heavy metals in the material (Hilber et al. 2017) and potential harm to soil and groundwater from these

pollutants has been reported (Brtnicky et al. 2021). As classified by IBI, biochar would be defined as “not recommended” with a PAHs content higher than 300 mg/kg for minimizing potential hazards (International Biochar Initiative 2015). Some researchers pointed out that biochar application could reduce crop yields (Deb et al. 2016). For instance, as shown by Baronti et al., with an application rate of 33 g/kg, a 20% reduction in ryegrass biomass was observed (Baronti et al. 2010). High-pH biochar can also be toxic to soil fauna, such as earthworms (Liesch et al. 2010). At an application rate of 55 g/kg, the average earthworm survival rate decreased by more than 70% (Malev et al. 2016).

The available studies show that the effect of biochar varies because of the different biochar properties (Albuquerque et al. 2014), soil properties (Dai et al. 2020), and test species (Baronti et al. 2010). It is, therefore, difficult to reach a consensus on whether applying biochar to soils is beneficial or hazardous. For example, Noguera et al. found that biochar has a positive effect on rice growth in fertile soils but has no impact in nutrient-poor soils (Noguera et al. 2010). The variable experimental conditions illustrate that studying the effects of biochar in natural environments is a complex and challenging topic. For synthesizing results from different experiments and identifying patterns between the biochar effect and environmental conditions, meta-analysis is a powerful tool. Whereas several meta-analyses have dealt with biochar, only a few have also included the potential negative impacts of biochar (see Table S1 for a complete overview). Only two studies suggested that biochar can have adverse effects on soil productivity under specific conditions, such as in alkaline soil (Zhang et al. 2018). Some studies have also drawn conclusions about the impact that biochar and soil properties have on the observed effect. For example, Dai et al. found that biochar with $\text{pH} < 6$ positively affected plant productivity on average, while biochar with $\text{pH} \geq 6$ showed the opposite effect (Dai et al. 2020). All meta-analyses so far have only investigated the effects of biochar on plants (soil productivity), and some also included soil microorganisms. However, no meta-analysis has included the effects of biochar on all soil organisms including soil fauna.

Machine learning (ML) is another tool for analyzing complex datasets. Currently, there is no model available to predict the effects of biochar on soil organisms. However, there has been recent progress in adopting models to predict the toxicity of materials that vary in their composition and characteristics (Zhou et al. 2023; Zhang et al. 2023). However, a significant difference compared to predicting adverse effects of other materials is that biochar has not just toxic but also positive effects. Parameters such as the effective concentration 50 (EC_{50})

or the lethal concentration 50 (LC_{50}) cannot be used for biochar modeling, which poses additional challenges.

Consequently, the aim of our work was to address the following research questions: Can we collect enough biochar ecotoxicological data on soil fauna and conduct a meta-analysis? Can we make a prediction tool based on machine learning for the biochar effect? For answering these questions, we compiled a dataset capturing both positive and negative effects of biochar on soil organisms, including plants, microbes, and animals, and analyzed correlations with biochar properties, soil conditions, test organisms, and toxicity endpoints. Based on this, we performed subgroup meta-analyses and developed three machine learning models to compare classification performance. Our final goal was to build a quantitative predictive model capable of estimating biochar effects under given environmental and material conditions. Notably, this is the first study to integrate a meta-analysis with machine-learning across the entire soil biota spectrum—including plants, microbes, and soil fauna—thus bridging methodological gaps left by previous analyses. This integrative approach not only improves mechanistic understanding but also provides practical guidance for standardized and safer biochar application.

2 Methods

2.1 Literature selection and data extraction

To collect the database, a search was performed according to the following steps in the Web of Science (WOS) with two different search terms. One was “Topic=‘biochar’ AND ‘effect’ AND ‘organisms’” and the other was “Topic=‘biochar’ AND ‘ecotoxicity’.” The combination of the two research terms covers both agricultural studies and toxicity tests. Given the timelines of the studies and the fact that most studies on biochar toxicology have appeared after 2010, the time frame of the search was set from January 1st, 2010, to December 31st, 2023. The first search term provided 226 studies, and the second provided 166. In the end, a total of 368 papers were found after removing duplicates.

For quality control, the exclusion criteria given in Table S2 were adopted to filter the results. The details about the paper collection process can be found in the PRISMA flowchart in Figure S1. For example, papers about aquatic toxicity effect were removed. The aim of the exclusion criteria was to define the scope of the paper and remove studies about environment remediation. Biochar addition to contaminated soil is usually considered to be beneficial, which would have added a bias in this study which targets biochar addition to agricultural soils. After applying the exclusion criteria, 30 papers remained. To extend the search, the cited references of the 30 papers were checked to see if additional articles would

also provide useful data. After checking an additional 264 papers using the same criteria, another 31 papers were added to our database.

Characterization and effects data was extracted from all 61 papers. The “effect” represents the difference between the experimental group to which biochar was applied and the control group to which no biochar was applied for a given endpoint, expressed as a percentage. Some studies did not contain the numerical values that could be used directly to calculate the effect but only recorded the results in the figures. In this case the values were extracted using the online tool Plotdigitizer 2.6.8 (Huwaldt & Steinhorst 2015).

When the experiments in one study used the same type of biochar, soil, and organism at different concentrations, this data series was defined as one experimental group. Experiments targeting growth, reproduction, and survival of organisms were considered. The following criteria were adopted to ensure uniformity in the data extraction process: (1) For growth inhibition/stimulation, the effects on crop yield, productivity, root growth, and shoot growth before and after biochar application were considered to belong to the endpoint type “growth.” For an identical experimental group, the above tests were selected in the priority order of crop yield > productivity > root growth > shoot growth when they were all reported. (2) If for the same experimental group results of several experiments with different time durations were presented, the one with the longest duration was selected. (3) For the pH of soil and biochar, the pH of the biochar and the soil in the control group was recorded. The pH of the mixed soil after the addition of biochar was not recorded, nor were the changes in pH over time assessed. Such information was only available for a very small number of studies and thus was excluded. Regarding the recorded descriptors, the details of the four categories of descriptors can be found in Table S3.

2.2 Meta analysis

For the meta-analysis the data were grouped into subgroups: three subgroups based on endpoint type, biochar type, and test organisms, three subgroups based on biochar properties (biochar pH, pyrolysis temperature, application rate), and one subgroup on soil pH. Details of the subgroups are listed in Table S4.

The meta-analysis in the research was carried out based on the effect. Here, the value in the control group is X_c , and the value in the experimental group is X_e (for example, in the control group, the crop growth is 10 cm while in the experimental group with biochar the crop growth is 11 cm). The response ratio is calculated with Eq. 1 according to Luo et al. (Luo et al. 2006):

$$ResponseRatio = \ln\left(\frac{X_e}{X_c}\right) \quad (1)$$

Regarding the number of studies, no studies were discarded because of the lack of replicates. Adopting standard deviation and variance as weighting functions would cause difficulty since some studies did not provide any control group. Besides, standard deviation as a weighting function was also reported to be unreliable because of various experimental conditions. Sometimes, the weight given by estimation from standard deviation would be extremely low or high. In our case, the dataset for biochar contains many different types of studies and a variety of endpoints. To avoid underestimating or overestimating effects, the number of replicates in the experiment was adopted as the weight function according to Li et al. (2020). The number of replicates for control groups is N_c , the number of replicates for experimental groups is N_e , then the equation of weight is shown in Eq. 2:

$$Weight = \frac{N_c \times N_e}{N_c + N_e} \quad (2)$$

When visualizing the results, the response ratio was converted to an effect with Eq. 3 to make the graph tangible:

$$Effect = \left(e^{RR} - 1\right) \times 100\% \quad (3)$$

When calculating the weighted average effect of the subgroup, the 95% confidence interval (CI) was calculated for the statistical analysis. For generating the 95% CI, the ‘confint’ function in the ‘boot’ package in R was adopted (Canty & Ripley 2022). An effect was considered significantly different from zero if the 95% intervals did not overlap with zero (Luo et al. 2006). In addition, the Wilcoxon signed-rank test was used to compare whether there was a significant difference between groups and the difference between the effect with biochar applied and zero. This test does not need to satisfy the normal distribution and homogeneity of variance test. It is more robust in the face of extreme values, which is more in line with the characteristics of the data in this study than the analysis of variance test.

2.3 Machine learning

The dataset for training the machine learning model was constructed from the dataset with numerical and categorical descriptors. For training the model, the data were processed by the following steps: (1) Columns with more than half of the values missing were deleted from the dataset. The 50% threshold was adopted following best practices in environmental data modeling to ensure sufficient data representation without introducing imputation

bias. (2) For the remaining numeric descriptors, missing values were replaced with the median value of the column for training. This method was chosen because the distributions of many descriptors (e.g., pH, temperature) are skewed, and using the median helps to reduce the influence of extreme values. The replacement was only applied to descriptors where missing values accounted for less than 50% of total entries. Parameters with more than 50% missing values were excluded from model training. (3) One-hot encoding was adopted to convert variables into binary vectors for categorical descriptors (biochar type, endpoint type, and tested organisms). In the first step, 10 descriptors were removed because they contained more than 50% missing values. After one-hot coding, the number of descriptors used for modeling was 23 and can be found in Table S5.

This z-score normalization was applied to ensure all numerical descriptors contribute comparably to model learning, especially since the descriptors vary in scale (e.g., EC in mS/cm vs pH in unitless values). The normalization for numerical descriptors was applied to prevent overcontribution and biases, as shown in Eq. 4:

$$X_i' = \frac{(X_i - \mu_i)}{\theta_i} \quad (4)$$

where X_i is the observed value, X_i' is the normalized value, μ_i is the mean value for the descriptor, and θ_i is the standard deviation for the descriptor. After preprocessing, 23 descriptors were left for model training. The details of the processing can be found in Table S5.

The models developed in this study were of three categories. The first one was the binary classification model, which predicted if the biochar was “beneficial”, or “hazardous”. If the recorded effect was greater than zero, the biochar was categorized as “beneficial”, if it was not, then the biochar was categorized as “hazardous”. The second model category was the ternary classification model, which predicted if the biochar was “beneficial”, “neutral”, or “hazardous”. For generating three categories, if the recorded effect was greater than 10%, the biochar was categorized as “beneficial”; if it was less than -10%, the biochar was categorized as “hazardous”, and the rest was categorized as “neutral”. The category “neutral” was created specifically because, given the uncertainty of the effect, biochar in the range of -10% to 10% often cannot be categorized with certainty as “beneficial” or “hazardous”. Such data points are expected to cause large errors in the binary classification. The “neutral” category was designed to see if such points caused large biases and if achieving a ternary classification with good accuracy through the model was possible. The third model type was the quantitative model, which quantitatively predicts the effect of biochar from the chosen descriptors.

For the qualitative classification model, three different machine-learning models were adopted: supporting vector machine (SVM), random forest (RF), neural network (NN). SVM was included to provide a perspective on whether complex but primarily linear relationships exist between descriptors and biochar effects. Random Forest was selected as a representative tree-based method known for its robustness and suitability for medium-sized datasets with many descriptors and moderate missingness. Compared to more complex ensemble methods like XGBoost, RF offers a balance between performance and interpretability. NN was chosen for its capacity to capture highly non-linear and multi-dimensional relationships, particularly useful when modeling interactions among many features. For the quantitative prediction modeling, RF was selected as the method because it performed best in the classification. The modeling was carried out with the help of the R packages “Keras”, “e1071”, “randomForest” and “nnet” (Allaire & Chollet 2023; Meyer et al. 2023; Rigatti 2017; Venables & Ripley 2002). For the details about the parameter settings of the models in the code, see Table S6.

For training the models, the dataset was divided into a training set and a test set with a 75:25 ratio. To improve the performance of the model, the training set was further split into training and validation sets with a ten-fold cross-validation, which means the split is 90:10 inside the training set. The best model was selected with the ten-fold training. The precision on the test set represented the final performance of the model.

For the classification model, the performance was mainly judged by its accuracy. Accuracy represents the percentage of items in the data set for which the classification results are consistent with the actual measured results. Besides, the model was also evaluated by its sensitivity, specificity, and Kappa value of the model. A more detailed explanation of the concepts can be found in Figure S3.

For the quantitative model, the performance was described by R-squared and root mean square error (RMSE). The calculation of RMSE is shown in Eq. 5:

$$RMSE = \sqrt{\frac{\sum (y_i - y_{pre})^2}{m}} \quad (5)$$

where y_i is the true value, y_{pre} is the predicted value, and m is the number of data points in the dataset.

For analyzing the importance of input descriptors, the VarImp function from the Caret package was used to evaluate the importance of descriptors in SVM, NN, and RF modeling. It should be noted that for linear SVM for binary classification, there is no parameter importance; instead, a coefficient similar to a linear correlation

was used to describe the correlation between different descriptors and the target. Here, the function ‘coef’ was used to determine the importance of the descriptor for the binary classification linear SVM. However, this is not the case for the ternary classification SVMs (nor for linear and Gaussian). Ternary classification SVMs have different parameters of importance for the three different categories. For NN, Gaussian SVM and triple classification SVM, the meaning of importance can all be interpreted as the loss of accuracy when the model removes a certain parameter. For the RF model, the package “randomForestExplainer” was further adopted (Paluszynska et al. 2020; Rigatti 2017). Accuracy decrease (RMSE increase in the quantitative model) and mean minimal depth were selected for further analysis.

2.4 Corroboration of meta-analysis and machine learning

For machine learning, to test whether the model’s understanding of the database is the same as the results of the meta-analysis, a data experiment was conducted on the five most important descriptors according to the modeling (biochar pH, soil pH, pyrolysis temperature, application rate, and soil organic matter).

For these five descriptors, data experiments were conducted one by one. For each descriptor, the minimum value in the test set was used to replace all the values in the test set. The trained model was then used to predict and record the percentage of “hazardous” in the prediction results. Subsequently, the value was replaced with the minimum value + 0.1 * the range of the parameter (here, the range means the maximum in the test set minus the minimum in the test set), and the resulting percentage was recorded, and so on, until it was replaced with the maximum value.

3 Results

3.1 Analysis of the dataset

We compiled a dataset of 61 studies reporting both positive and negative effects of biochar on soil organisms. Because this dataset contained studies using various feedstock types, different endpoint and many different test organisms, it is important to make the studies comparable. The “effect” used in the paper represents the difference between the experimental group to which biochar was applied and the control group to which no biochar was applied at a given endpoint, expressed as a percentage of the control. A value of –100% represents the maximum negative effects with no more growth, reproduction or survival of all organisms. Positive effects can go much beyond 100%. Figure 1 gives a first impression of the dataset by showing the relationship between effect and application rate. Negative effects are visible over the whole range of applications from the lowest to

the highest applied amount. Positive effects are rather concentrated at medium application rates between 10 and 100 g/kg.

The linear correlations between the observed effect and single biochar and soil descriptors are weak (see Figure S2), with no R^2 having an absolute value greater than 0.3. Also, 11 of the 22 numerical descriptors have a very low p-value in correlations with effect.

To perform a meta-analysis, subgroups were made according to Table S4, including subgroups created from different biochar pH, pyrolysis temperature, application rate, soil pH, different endpoints, test organisms, and biochar type. The meta-analysis showed that the weighted mean value of the biochar effect for the entire dataset was 0.60%, and the difference between that and 0% was insignificant (p-value < 0.05, 95% CI was between –2.15 and 3.34). The weighted mean values of different subgroups were calculated based on different subgroups. The differences between the subgroups from categorical descriptors are listed in Fig. 2.

The reproduction group exhibits no statistically significant difference from 0, and its 95% CI overlaps with 0 (p-value > 0.05). For the growth and survival groups, the effect of the former was statistically significantly positive, while the latter was statistically significantly hazardous with a mean value of –21%. The animal group showed a statistically significantly negative effect of –9.8%. In contrast, the results for plants showed that the application of biochar significantly benefited the plants by 10%. Regarding the performance of different types of biochar, the application of plant and waste feedstock biochar feedstock did not show statistically significant effects. Biochar with sludge as feedstock showed statistically significant positive effects of 65% (p-value < 0.05), and biochar made from feedstock type “mix” showed significant negative effects of –25%.

Considering the impact of biochar properties, the group with biochar pH < 6 showed a statistically significant positive effect of 10%, while the other two groups had CIs overlapping with 0. Based on the grouping of biochar production temperatures, the effect of biochar produced at less than 550 °C showed a statistically significant positive effect, while the effect of biochar produced at greater than 550 °C was statistically significantly negative. According to the grouping by biochar application rates, the group with high application rates showed a statistically significant negative effect of –32%, while the group with low application rates showed a statistically significant positive effect of 9.7%. The group with a medium application rate showed no significant effect.

For the impact of soil properties, the grouping based on soil pH appeared to have insufficient data because of the high number of missing values for soil pH. Statistically

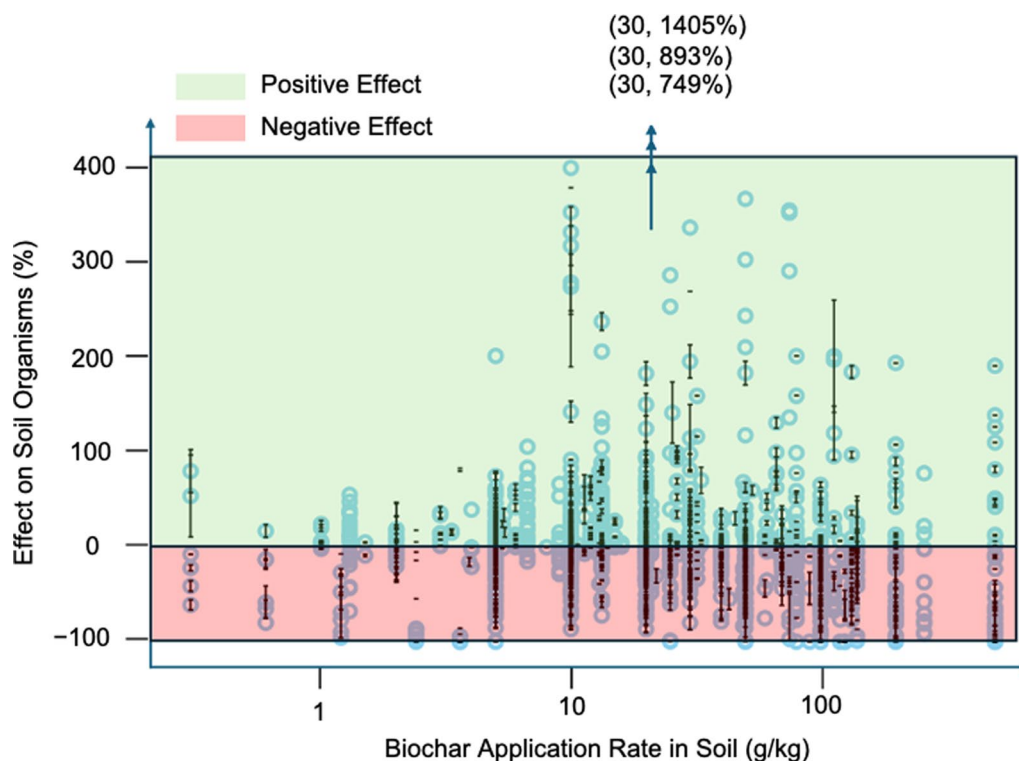


Fig. 1 The effects of biochar with application rate in g/kg soil relative to the biochar-free control sample. The green part means biochar showed a positive effect on the targeted organism, while the red part stands for negative effects. (Three data points ($Y > 500\%$) outside the range of y-axis are not shown but are listed above the plot.)

significant positive effects of biochar were observed in the soil $pH < 5$ and $5 \leq pH < 6$ groups. No significant effect was observed in the group with $pH \geq 6$. However, the $5 \leq pH < 6$ group contained only 14 data points.

3.2 Performance of binary classification models

Four models—supporting vector machine (SVM) (linear), SVM (Gaussian), neural network (NN), and random forest (RF)—were used for the binary classification of biochar effects into beneficial or hazardous. The models relate the effect (%) compared to the biochar-free control based on 14 biochar properties, 5 soil properties, 1 organism type and 3 endpoint types. The details about how the data were pre-processed can be found in Table S5. In Table 1, the results of the four models used for the binary classification are presented.

When comparing linear SVM with Gaussian SVM, the performance of the former was relatively poor. The classification accuracy of the linear SVM remained almost the same between the training and test sets. The 95% CI for the training set is even slightly smaller than that for the test sets. The prediction accuracy of the linear SVM was only 0.65. The Kappa value indicates that the prediction results are not better

compared with the random guessing. The specificity of the linear SVM is higher compared to the sensitivity, suggesting a model with a better recognition of the category “hazardous”. The Gaussian SVM has better values in all the parameters, except that its 95% CI is slightly overlapping with that of the linear SVM.

The overall performance of the NN and RF models is better than that of the two SVMs, with NN achieving an accuracy of 0.85 and a Kappa value of 0.7 for the training set, illustrating the excellence of NN for classifying the training set. While the performance of NN in the training set is better than that of RF, the performance of NN in the test set is lower than that of RF. Also, NN and RF both showed better specificity compared to sensitivity.

We also aimed to develop a ternary classifier including a neutral group with effects between -10% and $+10\%$ based on the sensitivity result shown in Table S7. An optimized RF was trained on a training set selected from the dataset without a neutral category. The optimized RF was found to have better accuracy in performing the binary classification task with the test set selected from a comprehensive dataset. The optimized RF had an accuracy of 0.79, while the binary RF had an accuracy of 0.76.

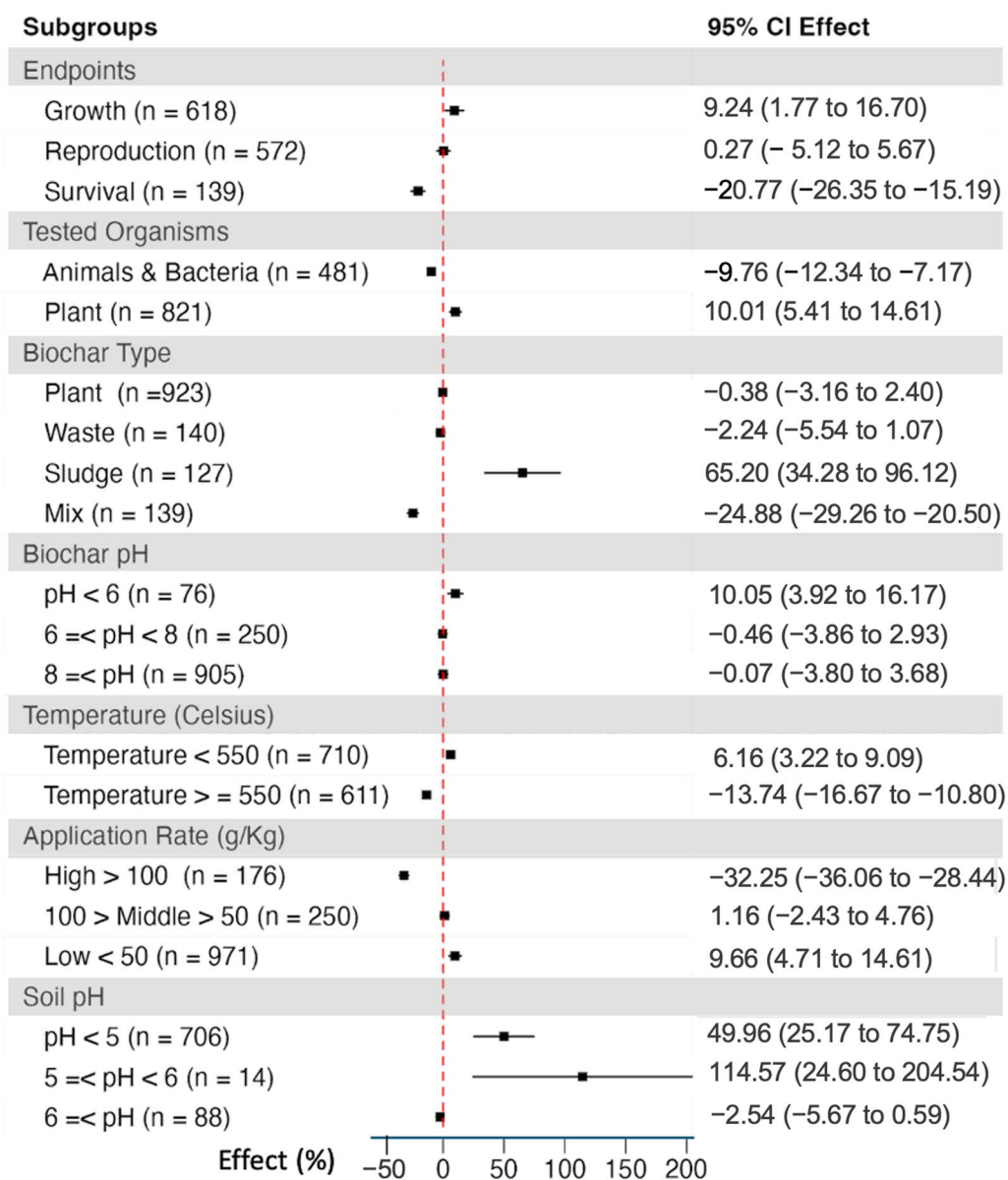


Fig. 2 Meta-analysis of the effects of biochar on soil organisms (plants, animals, bacteria) based on subgroups for selected descriptors. The red line indicates 0% effects. Data points to the right are positive effects and those to the left represent adverse effects

To further evaluate the generalizability and robustness of the random forest classifier, we trained a series of sub-models using only specific portions of the dataset, including data limited to plants or animal/bacteria, specific endpoint types (growth or reproduction), and entries with fewer missing values. As shown in Table S8, these sub-models achieved comparable accuracy (0.69–0.77) and consistent sensitivity levels.

3.3 Performance of the quantitative random forest model RF, as best-performing method, was selected for quantitatively predicting the biochar effect. The comparison between predicted and measured values for the optimum model is shown in Fig. 3.

We reached an R^2 of 0.74 for the training set and 0.48 for the test set. The RMSE for the test set was 50%, while the RMSE for the training set was 39%. The results

Table 1 Performance of four binary classification models to classify biochar effects into beneficial or hazardous

Binary classification models	SVM linear	SVM Gaussian	NN	RF
Test set				
Accuracy	0.65	0.71	0.73	0.76
95% CI	0.59–0.70	0.66–0.76	0.67–0.77	0.71–0.80
Sensitivity	0.57	0.68	0.69	0.70
Specificity	0.72	0.74	0.76	0.82
Kappa	0.29	0.42	0.44	0.51
Training Set				
Accuracy	0.65	0.73	0.85	0.8
95% CI	0.62–0.68	0.70–0.76	0.83–0.87	0.77–0.82
Sensitivity	0.56	0.71	0.85	0.77
Specificity	0.73	0.75	0.85	0.8
Kappa	0.29	0.46	0.70	0.60

The values in bold font represent the best performing models

suggested a certain difference between the accuracy in the training set and the test set. It can also be seen from the distribution of the data points in Fig. 3 that most of them are located within one RMSE.

3.4 Feature importance of binary random forest and quantitative random forest

In this section, the feature importance of the optimized RF and the quantitative RF is presented.

Figure 4 shows the four most important descriptors ranked in two different ways: the one in Fig. 4a, c is ranked by the mean accuracy decrease (for the quantitative model: RMSE increase) and gini decrease (for the quantitative model: node purity decrease) while the one in Fig. 4b, d is ranked by the distribution of minimal depth. The accuracy decrease (RMSE increase) means the decrease of model accuracy (the increase of RMSE) when a descriptor is removed. The gini decrease (node purity decrease) is a measure of how each variable contributes to the homogeneity of the nodes; the higher the value, the more important the descriptor. For the distribution of minimal depth, it indicates how early or late the decision tree makes a judgment. The smaller it is, the more important the descriptor is.

As shown in Fig. 4a, b, for the binary classification RF the same five descriptors appear in both evaluations. The five descriptors are “Biochar pH”, “Pyrolysis Temperature”, “Soil pH”, “Temperature”, and “Biochar Electrical Conductivity.” For the quantitative RF, both “Biochar pH” and “Soil pH” appeared as important parameters in both evaluations (Fig. 4c, d).

For summarizing the importance of the main descriptors in all models (binary classification models, ternary classification models and quantitative models), the top five important descriptors assessed by times of appearance are shown in Fig. 5. The descriptors ranked first to fifth in the model were also assigned values from 5 to 1, and the total scores of each descriptor were added up. The descriptors with five highest score are also shown in Fig. 5.

Figure 5 shows the descriptors with the highest score and the highest times of appearance. Biochar pH, application rate, soil pH and pyrolysis temperature were already among the top five most important parameters for the optimized binary RF or quantitative RF. Soil organic matter is another descriptor which is relevant as shown by the high overall score.

Finally, we conducted a data experiment to confirm the model’s understanding of the correlation between parameters and effects. The descriptors targeted by the experiment are the five parameters that appear in Fig. 5. These five parameters were varied over the full range each parameter covered within the used test set. The results are shown in Fig. 6. As the five parameters increased from their minimum to maximum values, the percentage predicted to be hazardous increased overall. Except for soil pH, the increase of the parameters caused the percentage predicted as hazardous to be higher than the original result. For soil pH, decreasing its value caused the percentage predicted as hazardous to decrease much below the original test set.

4 Discussion

4.1 Biochar effect on soil organisms

The available data show that the effect of biochar on soil organisms is distributed widely between negative and positive values. Negative and positive effects appeared at both low and high application rates. Averaging all the effects in our database, the result of a positive effect of 0.60% is almost indistinguishable from 0, and the calculated 95% CI also includes 0, indicating that analyzing the whole dataset together, biochar has statistically no effect on soil organisms. However, considering the average effect based on subgroups is crucial for a more detailed analysis. When distinguishing between the two categories “Plants” and “Animals/bacteria,” the calculated average effect is positive for plants and negative for animals/bacteria. The occurrence of a positive effect for plants is consistent with the conclusion of other meta-analyses (see Table S1). However, this positive effect is only one part of the whole picture as our meta-analysis including animal data clearly shows that biochar application can potentially be harmful to animals. Biochar has a mainly positive effect on growth, almost no effect on reproduction, and a significantly negative effect on survival.

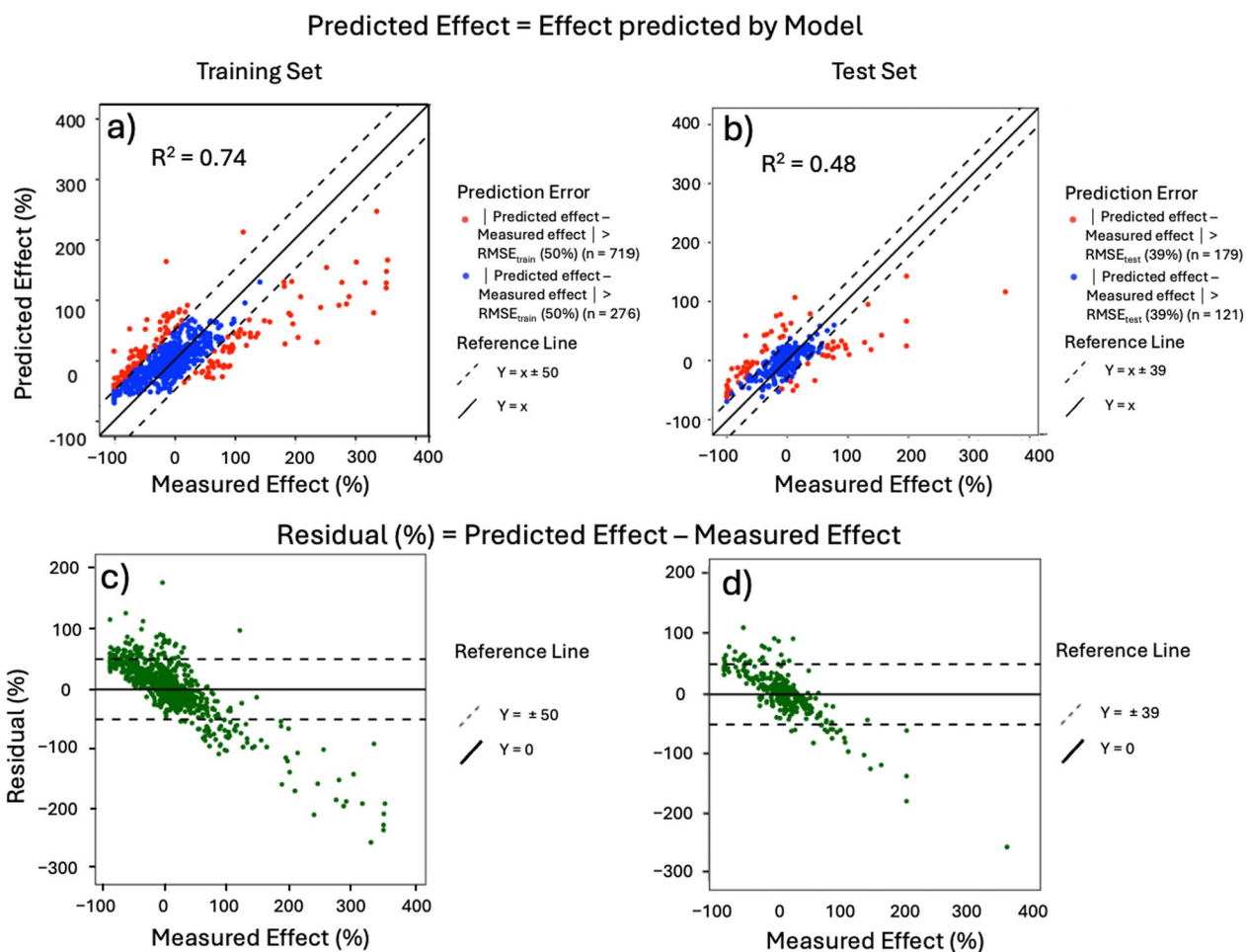


Fig. 3 Quantitative RF model to predicting the effect in % relative to the control based on biochar and soil properties and organisms and endpoint type. The two dashed lines in the figure represent $y = x + \text{root mean square error (RMSE)}$ and $y = x - \text{RMSE}$ ($\text{RMSE}_{\text{train}} = 50\%$ and $\text{RMSE}_{\text{test}} = 39\%$). The points falling in between two lines indicate that the deviation of quantitative prediction is within the range of RMSE. **a** The correlation between the predicted and measured values for the training set. Three data points with large measured effects —(1404%, 772%), (893%, 446%), and (749%, 552%)—are omitted to improve readability. **b** The correlation between the predicted and measured values for the test set. **c** The residual plot for the training set. **d** The residual plot for the test set

We will discuss the specific mechanism of the effects later, but it is worth mentioning that the average impact on different toxicity endpoints may also come from the different proportions of plants and animals in different toxicity tests. For example, in the growth dataset, 548 data points are from plants, and 67 are from animals; in the reproduction dataset, 297 are from plants, and 275 are from animals; and in the survival dataset, there are only animal data.

4.2 Mechanisms of biochar effects on soil organisms and their corroboration with the result of meta-analysis and machine learning

Meta-analysis and machine learning are considered here together to understand and validate the underlying mechanisms for the beneficial or adverse effects of

biochar. From the machine learning model, three of the five most important descriptors are biochar properties, and two are soil properties. This conclusion supports the information from the prior knowledge on which the meta-analysis grouping relied. Considering possible bias due to the same literature source, it is worth mentioning here that the significant descriptors derived from our model are also consistent with the groupings of some meta-analyses using data sources older than 2010 (Liu et al. 2013). Application rate, biochar pH, pyrolysis temperature, and soil pH are also the basis of the subgroups in the meta-analysis.

The effects of biochar, as a complex mixture, mainly depend on the difference between the biochar and the soil properties, such as higher specific surface area (Li

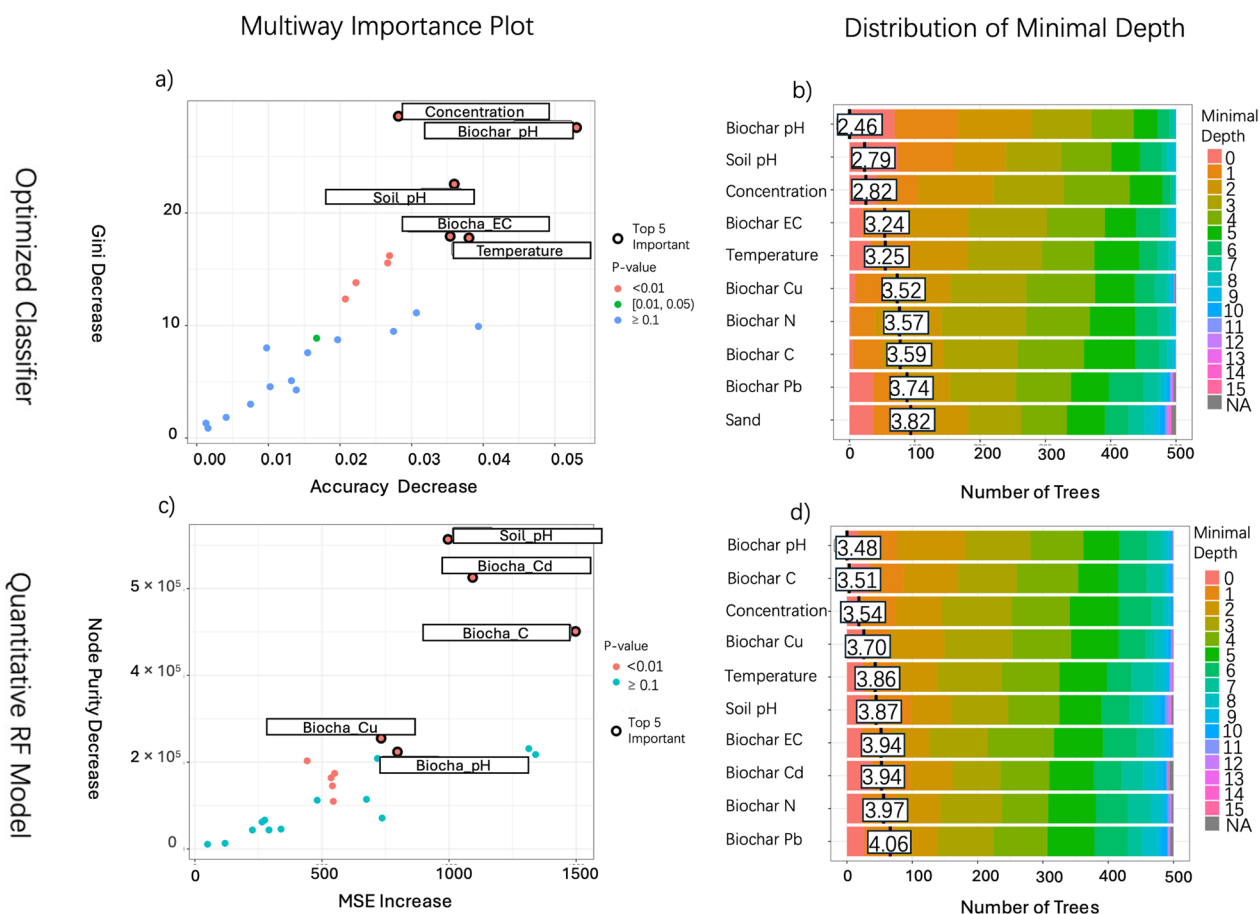


Fig. 4 **a** Feature importance of descriptors in the optimized classifier RF model, described by accuracy decrease and gini decrease and **b** by minimal depth of descriptors. **c** Feature importance of descriptors in the quantitative RF by mean square error decrease and node purity decrease **d** by minimal depth of descriptors in quantitative RF by the distribution of minimal depth

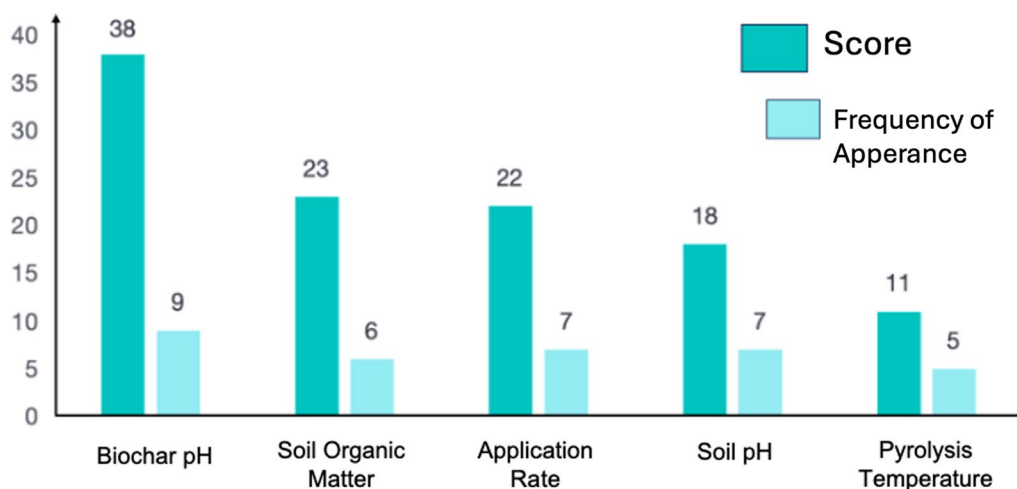


Fig. 5 The descriptors that get the top five scores and the frequency of appearance. Scores were assigned based on the ranking of descriptors' importance in the model, with the first to fifth ranked descriptors being assigned from five to one, respectively

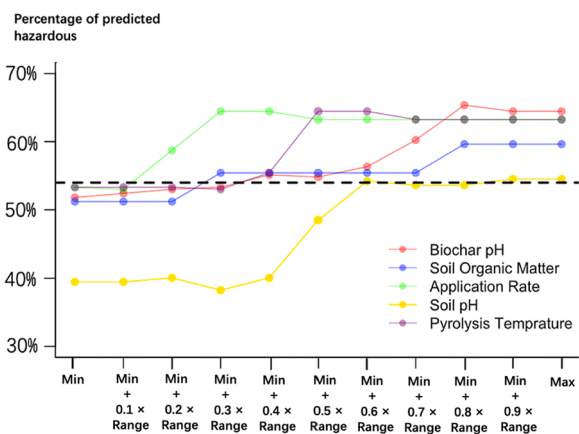


Fig. 6 Influence of changing the five most important parameters shown in Fig. 5 on the percentage of the full dataset predicted to be hazardous. The dashed dark line stands for the percentage predicted in the original test set

& Sun 2019), higher element content (Jones et al. 2012), and higher heavy metal content (Yang et al. 2021). On the positive side, adding biochar helps the soil to accumulate water (Mao et al. 2019), increase porosity (Toková et al. 2020), reduce bulk density (Toková et al. 2020), and provide a habitat for soil microorganisms and some small animals (Li et al. 2020). On the negative side, biochar pollutants and excessively high pH will reduce the abundance of soil microorganisms and inhibit algae growth and seed germination (Mierzwa-Hersztek et al. 2018).

The biochar application rate has always been considered an important indicator of the biochar effect. For example, the International Biochar Initiative states that the optimal application rate of biochar should be determined experimentally based on the specific properties of the land to which it is applied (Initiative, n.d.). Gao et al. concluded from a meta-analysis that the optimal application rate of biochar should be between 20 and 40 g/kg (Gao et al. 2021). In our study, the conclusion of the meta-analysis was consistent with the above analysis, and the average effect of biochar in three different groups of application rates decreased with the increase in application rate. Compared to other biochar-related meta-analyses, Farhangi-Arbiz et al., Liu et al., and Bai et al. also concluded that application rate is negatively related to the effect of biochar (Bai et al. 2022; Farhangi-Arbiz et al. 2021; Liu et al. 2013). The negative relationship between application rate and effect was corroborated by our model. When the application rate was increased, the number of negative predictions made by the model also increased. From a mechanistic perspective, this may be because excessive biochar adsorbs and fixes soil nutrients, resulting in a decrease in the effective nutrient content of the soil. For example, Case et al. reported

that the use of biochar reduces the availability of nitrates and ammonium salts in the soil (Case et al. 2012). Brtnicky et al. believe that for other lands that already have salinization, water-soluble salts released by excessive biochar will enter the soil solution, which may also lead to increased salinization (Brtnicky et al. 2021).

The pH change caused by biochar is also an important source of influence for the above-mentioned effects. The discussion on biochar pH involves multiple aspects. On the one hand, the high pH of biochar is believed to buffer the pH of acidic soil well and increase crop yields (Molnár et al. 2016). On the other hand, high pH reduces the rate of soil nitrification and thus affects the utilization rate of N in the soil (Uzoma et al. 2011). At the same time, high-pH biochar is sometimes fatal to soil organisms, especially earthworms (Noguera et al. 2010). The different possible mechanisms by which biochar pH affects toxicity depend not only on the biochar pH but also on the pH of the soil. The meta-analysis showed that low-pH biochar had, overall, a statistically positive effect, while the medium and high pH biochar did not. The application of biochar in acidic soils shows a significant positive effect, while the positive effect begins to become insignificant when the soil pH is > 6. This can be validated by the data shown in Fig. 6. The increase in the percentage of hazardous effects for soil pH suggests that after exhaustion of the buffering effect of the soil, the positive effects of biochar become smaller.

The positive effect of biochar on phosphorus availability tends to exist in acidic soils because of reduced leaching due to decreased soil bulk density and increased adsorption, while for alkaline soils, the previously mentioned salinization significantly reduces the availability of phosphorus, which decreases the positive impact (Brtnicky et al. 2021). For the impact on soil fauna, especially on earthworms, at high pH ammonium can become toxic (Liesch et al. 2010). Once the increase in pH is too high, earthworm mortality may lead to an overall negative effect. It was suggested that the mortality rate of earthworms can reach 100% when applying biochar with pH > 10 (Cui et al. 2023). This shows that it is of particular importance to include soil animals in the effect analysis—previous meta-analyses have stated that biochar tends to be more beneficial with higher pH, but these studies missed the high mortality of soil animals caused by high biochar pH (Farhangi-Arbiz et al. 2021).

The temperature at which the biochar was synthesized is another very important parameter affecting toxicity. It is generally believed that biochar synthesized at a temperature below 550 °C performs better because it contains less PAHs and heavy metals and higher amounts of bioavailable C, N, and P (Tomczyk et al. 2020). The results of the meta-analysis also show that biochar

produced by low-temperature pyrolysis generally exerts a positive effect, while the opposite is true for high-temperature biochar. Another noteworthy difference is that among the biochars pyrolyzed from four different raw materials, only the average effect of biochar from sludge shows a significantly positive value. This may be due to the high phosphorus content in sludge. The phosphorus content of biochar is positively correlated with its effect (Figure S2).

Beyond individual effects, interactions between biochar properties also appear critical in determining its overall impact on soil organisms. As shown in Figure S2, the pyrolysis temperature is positively correlated with biochar pH ($R^2=0.48$) and heavy metal content (e.g., Cd and Pb), while also increasing the levels of PAHs ($R^2=0.75$). Considering the positive relations between biochar pH and pyrolysis temperature, it is reasonable that the increase of biochar pH and pyrolysis temperature in Fig. 6 together leads to an increase in negative predictions. Pollutant content is considered relevant to biochar toxicity: elevated PAH and heavy metal content may directly inhibit microbial and animal activity (Lu et al. 2016). Thus, high-temperature-pyrolyzed biochars, although potentially improving carbon stability, may simultaneously pose greater ecological risks, especially when high pH biochar is applied to soils that are already neutral or alkaline. Conversely, low-temperature biochar with lower pH and contaminant levels may exert more beneficial or neutral effects. The co-variation among these descriptors suggests that future models and guidelines should integrate descriptor interactions rather than consider each in isolation.

4.3 Model performance and data gaps

The machine learning model we developed can effectively categorize biochar based on its properties in a specific soil. We achieved an accuracy of the binary classification of 0.79, which means that we can accurately determine whether biochar has a positive or negative effect under a given set of conditions. The model results can be well corroborated with the meta-analysis and previous knowledge about the biological effects of biochar. For categorizing biochar, RF showed better performance compared to SVM. RF is recommended to be adopted when dealing with high-dimensional datasets such as ours, which contains 23 descriptors (Liaw & Wiener 2002; Rigatti 2017). In other machine-learning studies to predict the effect of materials, similar results were found: Zhou et al. (2023), who modeled the effect of metallic nanoparticles using RF, NN, and SVM, showed that RF performed best with a dataset containing 14 descriptors (Zhou et al. 2023). Chen et al. compared the performance of RF, linear regression, and XGboost for predicting the effect

of nanomaterials on the soil microbiome based on five descriptors (Chen et al. 2024). Again, RF performed best among the three models. These authors all state that RF performed well when dealing with complex and high-dimensional data.

For the quantitative model, the R-squared of the model in the training set reached 0.74, but it dropped in the test set to 0.48. Although our dataset consists of 1329 data points, this might not be enough for the model to establish a good quantitative relationship between the 23 descriptors and the adverse effects. Other researchers got a higher R-squared for modeling with less descriptors; for example, the models for predicting the effect of nanoparticles by Zhou et al. were trained based on a dataset consisting of 701 data points using 14 descriptors and reached an R-squared of 0.82 (Zhou et al. 2017). This finding suggests that compared to the toxicity of nanoparticles, the higher heterogeneity of our dataset and the complex, often nonlinear, interactions between biochar, soil, and organisms resulted in a lower predictability. The model is suitable for trend estimation but may be limited in precise effect prediction, especially for underrepresented test conditions. Furthermore, its extrapolation to novel biochar types or soil systems beyond the training data range should be done cautiously. Future work should focus on expanding the dataset, especially with more detailed and standardized measurements for soil fauna and microbial responses. Considering the complexity of biochar as a mixture and the unclear understanding of the mechanisms of negative effects, more data are needed for a further improvement of the model accuracy.

The results in Table S8 show that when faced with relatively limited data, the binary classification accuracy of the trained model decreases, but remains high (greater than 0.7). This illustrates the availability and robustness of our method for databases with limited data. Similarly, this also tells us that the accuracy of the model can be further improved with more data. While most of the studies performed high-quality experiments on biochar application, we found several aspects that could be improved in the study design and reporting. First, there are uneven records of experimental parameters given in the various studies. Some studies record the various characteristics of biochar and the soil properties relatively well whereas in others both biochar and the used soils have an incomplete set of characterization data. The records of biochar properties are generally more complete compared to the physical and chemical properties of the soils. For example, there are almost no missing values for biochar pH in the database, while one-third of the studies do not even report the soil pH. This is quite a surprising fact since a basic characterization of the soil used in a study is usually considered in soil science to

be a prerequisite for publishing any results. The lack of data and the relatively poor data quality clearly impacted the accuracy of the model and became the barrier for the further improvement of the quantitative prediction. There are several ways in which one can deal with missing data: one approach is to discard parameters for which "missing values reach more than one-third" (Zhou et al. 2023). However, this would result in our dataset having only very few parameters remaining in the dataset. For instance, the two important descriptors soil pH and biochar carbon content would be discarded because of the number of missing values. We therefore adopted the approach to only discard parameters when the missing values reach more than 50%. In the final dataset there are therefore many missing values which necessitates the use of "data imputation". Here, the method we adopted was to use the median of a specific descriptors to fill in the missing value. This is a common way to fill the data gap for data series containing extreme values (Bidyuk et al. 2022). Using the median to fill in missing values can reduce the impact of extreme values compared to using the mean. For biochar, the pH range is wide (ranging from 4.10 to 12.76 in our database) and the pyrolysis temperature range is also wide (ranging from 180 to 1200 °C in our database). For such complex materials with diverse processing conditions, the median method is more appropriate.

Another issue with the dataset is that there are fewer experiments focusing on effects on soil animals whereas a lot of attention is paid to the biochar impacts on plants from an agricultural perspective. Considering the possible negative effects on soil fauna, more toxicological research on animals may be critical. Finally, we also recognize the lack of long-term data as an important gap in the current dataset. Most existing studies focus on short-term responses, whereas the long-term effects of biochar application on soil ecosystems remain poorly understood. These may include potential benefits such as sustained improvements in soil structure and nutrient retention, or adverse outcomes like gradual accumulation of contaminants or delayed toxicity to soil fauna. Addressing these unknowns through long-term field studies will be essential to evaluate the ecological sustainability of biochar use and improve future predictive models.

5 Conclusions

The demand for biochar is growing because of its good carbon sequestration potential and its beneficial effects on plant growth. However, our study clearly shows that we also need to turn our attention on the potential negative effects of biochar.

Based on the meta-analysis, application guidance for biochar could be provided. For general agricultural soils,

an application rate of less than 50 g/kg is recommended, where pyrolysis temperature below 550 °C are preferable for ecological safety. Biochar with high pH is encouraged to be applied in acidic soil for better performance.

Using a machine learning model, we provide a first classifier that can predict with an accuracy of 0.79 whether, under given biochar characteristics, the application in a soil with given properties will result in positive or negative effects. The model's understanding of biochar properties is similar to the results of the meta-analysis, which also suggests that a high pH of biochar will increase the likelihood of biochar exhibiting harmful effects. At the same time, the benefits of biochar buffering in low-pH soils are also significant. The strength of the model is that the recommended application rate of biochar for a particular type of biochar and a specific soil can be obtained. What needs to be noticed is that the model was trained based on experiments from agricultural soils, which means that the model might not be accurate when dealing with situations in polluted or industrial soils.

Future research on biochar should focus on providing more data on negative effects, in particular on soil fauna, and ensuring a good characterization of the biochar and the soil to allow any future model to better relate material and soil properties to effects. This is an urgent need prior to large-scale uses of biochar for climate change mitigation.

Abbreviations

IBI	International Biochar Initiative
EC50	Median effective concentration
LC50	Median lethal concentration
ML	Machine learning
PAHs	Polycyclic aromatic hydrocarbons
SVM	Supporting vector machine
NN	Neural network
RF	Random forest
RMSE	Root mean square error
WOS	Web of Science

Supplementary Information

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Additional file 1.

Additional file 2.

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Author contributions

Yucan Dong: methodology, software, formal analysis, investigation, Writing—Original Draft. Merve Tunali: Conceptualization, Writing—Review & Editing, Supervision. Bernd Nowack: Conceptualization, Writing—Review & Editing, Supervision, Project administration, Funding acquisition.

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Availability of data and material

The code, the dataset and the raw results are available at: https://github.com/LifelsStrange-Part/Biochar-Effect_ML

Declarations**Competing interests**

The authors declare no competing interests.

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