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Machine learning prediction and interpretation of the impact of microplastics on soil properties☆

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ABSTRACT

The annual microplastic (MP) release into soils is 4–23 times higher than that into oceans, significantly impacting soil quality. However, the mechanisms underlying how MPs impact soil properties remain largely unknown. Soil-MP interactions are complex because of soil heterogeneity and varying MP properties. This lack of understanding was exacerbated by the diverse experimental conditions and soil types used in this study. Predicting changes in soil properties in the presence of MPs is challenging, laborious, and time-consuming. To address these issues, machine learning was applied to fit datasets from peer-reviewed publications to predict and interpret how MPs influence soil properties, including pH, dissolved organic carbon (DOC), total P, NO_3^--N, NH_4^+-N, and acid phosphatase enzyme activity (acid P). Among the developed models, the gradient boost regression (GBR) model showed the highest R^2 (0.86–0.99) compared to the decision tree and random forest models. The GBR model interpretation showed that MP properties contributed more than 50% to altering the acid P and NO_3^--N concentrations in soils, whereas they had a negligible impact on total P and 10–20% impact on soil pH, DOC, and NH_4^+-N. Specifically, the size of MPs was the dominant factor influencing acid P (89.3%), pH (71.6%), and DOC (44.5%) in soils. NO_3^--N was mainly affected by the MP type (52.0%). The NH_4^+-N was mainly affected by the MP dose (46.8%). The quantitative insights into the impact of MPs on soil properties of this study could aid in understanding the roles of MPs in soil systems.

1. Introduction

Plastic waste generation and its accumulation in the environment are important environmental issues. Soil is among the largest acceptors and long-term sinks of waste plastics in the environment (Horton et al., 2017). Although research in this area is limited, plastic pollution in soil causes severe environmental and health issues (Rist et al., 2018). Once plastic waste enters the soil, large pieces of plastic disintegrate into micro-sized particles (<5 mm) known as microplastics (MPs) through their exposure to physical abrasion, UV light, and mechanical forces, such as tillage practices (Gao et al., 2020). Electronic-waste dismantling areas (Chai et al., 2020), plastic-waste dumping sites, and plastic-waste littering on land are the primary sources of MPs in the soil. Moreover, a wide array of plastics is used in the agricultural sector, leading to MP accumulation in soils. Mulch films, weed-barrier sheets, and greenhouse covers are commonly used for crop production (Piehl et al., 2018; Rochman, 2018). The application of municipal waste, compost, biosolids, treated irrigation water, and plastic-coated fertilizers to soils are also important sources of MP (Corradini et al., 2019).

Additionally, widespread atmospheric deposition of MPs occurs even

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in remote areas that are far from the point sources (Evangeliou et al., 2020). The distribution and abundance of MPs vary substantially across land use types. MP levels in soils can reach more than 40,000 particles/kg (Zhang & Liu, 2018). MP contamination levels of approximately 300–67,500 mg/kg and 62.5–78.0 items/kg in industrial and farmland soils, respectively, were recently reported (Fuller & Gautam, 2016; Liu et al., 2018). MP can alter the inherent physical, chemical, and biological properties of soils. In a five-week garden experiment, de Souza Machado et al. (de Souza MacHado et al., 2018a) observed that the presence of up to 2% (w/w) of four common MP types (polyacrylic fibers, polyamide beads, polyester fibers, and polyethylene fragments) had notable effects on soil properties. Specifically, these MPs influence soil properties, including bulk density, water-holding capacity, hydraulic conductivity, and soil aggregation. For example, Feng et al. (Feng et al., 2022a) found that the occurrence of various MP types (such as polyethylene, polystyrene, polyamide, polylactic acid, polybutylene succinate, and polyhydroxybutyrate), particularly at a concentration of 2% (w/w), reduced the richness and diversity of bacterial communities in soils. Moreover, MPs were shown to alter the composition of soil microbial communities. Interestingly, when MPs derived from biodegradable plastics were introduced into the soil, higher relative abundances of bacterial genera such as *Bacillus* and *Variovorax* were observed (Qi et al., 2020). Additionally, plants can absorb MPs *via* their root systems, leading to MP accumulation in different plant tissues (Zhang et al., 2022). Consequently, MPs enter the human body through food chain contamination and cause various health issues. Owing to their small size, MPs can be inhaled and may cause abrasions in the respiratory system, depending on an individual's vulnerability and the MP particle properties (Prata, 2018).

Unlike modeling or simulation studies, soil-related research aimed at analyzing and quantifying contaminants and their impacts on soils is time- and resource-consuming and complex (Cornelis et al., 2001; Nanni & Demattê, 2006). Furthermore, the effects of experimental conditions, such as time, spiked MP concentrations in soils, soil moisture content, and soil temperature, on soil properties in the presence of MPs remain unclear. Additionally, soils have spatially heterogeneous properties (such as soil texture and nutrient availability) within a specific area because of the high variability in environmental and climatic factors, such as rainfall, activity of microorganisms in the soil, and topography (Li et al., 2021). Given the complex nature of soils and the experimental limitations, the research results cannot be generalized for all soil types. Thus, the development of mitigation measures and investigation of how the presence of MPs alters soil properties are difficult.

Using an empirical approach prior to conducting experiments can lead to a reduction in time, cost, and resource requirements for identifying optimal environmental conditions. However, in specific research areas that focus on the presence of MP in soils and their impact on soil properties, the application of such empirical methods has not been widely explored (Palansooriya et al., 2022a). Machine-learning (ML) is a progressive arm of computational algorithms designed to imitate human intelligence by learning from the surrounding environment (Zhong et al., 2021). This method has been validated in various environmental science studies. A notable exemplar lies in the domain of identifying heavy metal immobilization through biochar application within soils (Palansooriya et al., 2022a; Sun et al., 2022), to provide an accurate and reliable classification of soil texture classes (Kaya et al., 2022), to develop models for predicting of heavy metal adsorption in soils and identifying the effect of key factors on metal adsorption in soils (Guo et al., 2023; Jia & Hou, 2023; Yang et al., 2021), and to model the soil moisture distribution (de Oliveira et al., 2021; Guio Blanco et al., 2018). Compared with statistical analysis, ML-based models can predict nonlinear and complex relationships between the dependent and independent variables in systems related to environmental engineering and environmental sciences (Yuan et al., 2021; Zhu et al., 2019). To date, ML has not been used to investigate the changes in soil properties following the addition of MP into soils.

To address this research gap, data on MP properties, experimental conditions, soil type, presence of other additives, and soil properties were extracted from the literature using tree-based algorithms, such as decision tree (DT), random forest (RF), and gradient boost regression (GBR), which were used to develop models for predicting changes in soil properties, including pH, dissolved organic carbon (DOC), total P, NO_3^--N, NH_4^+-N, and acid phosphatase enzyme activity (acid P), following the presence of MP in soils. An optimal ML model was used to interpret the importance and impact of the input features on the predicted soil properties. We also investigated the effects of MP properties (type, size, shape, and dosage) on soil properties. Such data-driven model-based predictions and interpretations can provide quantitative insights into the role of MP in soils. Although certain MP properties, such as polymer structure, shape, size, and dosage in soils, have garnered attention, the resultant soil property changes remain understudied. Studies have suggested that the presence of MP in soils can modify soil properties; however, in certain cases, the impacts appear insignificant. These findings lead to the formulation of various hypotheses to support these observations. Notably, a considerable proportion of scientific research has focused on examining alterations in soil chemical properties, microbial diversity, and microbial abundance, often overshadowing investigations of changes in soil physical properties. Considering these research gaps, we sought to address the knowledge deficit by collecting rich data from various experimental publications. By pioneering the application of ML techniques to analyze these data, we aimed to discern how MP properties and experimental conditions collectively influence soil property alterations. Our study is a pioneering endeavor in this field and provides crucial insights into an unexplored dimension. This is the novelty of the present study.

2. Materials and methods

2.1. Data collection and formatting

After a thorough literature survey, research articles related to soil property changes owing to the presence of MP in soils published between 2017 and 2022 were selected using the Web of Science and Google Scholar. Through a preliminary search, 48 research papers describing the changes in the physical, chemical, and biological properties of soil following MP addition were selected. The selected articles were included if they contained data on the physical, chemical, and biological properties of the soil. From the 48 research articles selected, (Blöcker et al., 2020; Boots et al., 2019; Brown et al., 2022; Chen et al., 2020; Chen et al., 2022; de Souza MacHado et al., 2018; de Souza Machado et al., 2019; Dong et al., 2021; Fan et al., 2022; Fei et al., 2020; Feng et al., 2022a; Feng et al., 2022b; Gao et al., 2021; Gao et al., 2020; Guo et al., 2021a,b; Hou et al., 2021; Jiao et al., 2022; Li et al., 2022; Li et al., 2021; Lian et al., 2021; Liu et al., 2017; Liu et al., 2019; Liu et al., 2022a,b,c,d; Lozano et al., 2021; Meng et al., 2022; Meng et al., 2019; Ng et al., 2021; Palansooriya et al., 2022b; Qi et al., 2020; Ren et al., 2020; Rillig et al., 2021; Sun et al., 2022a; Wang et al., 2020; Ren et al., 2022; Wang et al., 2022b; Yan et al., 2021; Yang et al., 2021b; Yu et al., 2021; Yu et al., 2022; Zhang et al., 2019; Zhang et al., 2022; Zhao et al., 2021; Zhou et al., 2021; Zhu et al., 2022; Ren et al., 2021; Li et al., 2022; Chen et al., 2022; Li et al., 2021; Jiao et al., 2022; Hou et al., 2021; Wang et al., 2020), data were obtained from tables or extracted from figures using Web Plot Digitizer Software (https://apps.automeris.io/wpd/). All data were screened to avoid repetition. All input features were broadly classified into four categories, i.e., MP information (MP properties), experimental conditions, soil type, and other additives, which are shown in detail in Table S1.

2.2. Data imputation

Drawing on the compiled data concerning alterations in the physical, chemical, and biological attributes of soils after MP incorporation, a notable trend emerged. Specifically, a significant proportion of soil chemical property variations exhibited promising characteristics suitable for the construction of ML models. Due to insufficient data volume, the number of data points available for the other two soil properties was limited: less than 100 data points for physical attributes and less than 150 for biological traits. In contrast, the chemical attributes of the soil, encompassing parameters like pH, dissolved organic carbon (DOC) concentration (mg/kg), ammonium nitrogen (NH_4^+-N) content (mg/kg), nitrate nitrogen (NO_3^--N) content (mg/kg), total phosphorus (total P) content (mg/kg), along with the biological property acid phosphatase (acid P) activity in soils (μg (pNP)·g/h), were robustly evaluated and earmarked as prime candidates for training the ML model (**Table 1**). Given these considerations, our meticulous assessment directed our focus towards specific soil parameters exhibiting ample data availability, forming a rationale for concentrated attention in the ML modeling process. Thus, a comprehensive evaluation of the array of soil properties led to the selection of these six pivotal attributes. These attributes were chosen based on their suitability for modeling and the extensive data available, thus serving as the cornerstone of our analytical investigation. However, not all data included all six soil properties simultaneously. To use the manually collected data, we compiled six sub-datasets to develop individual predictive models for the same types of input variables to predict the six selected properties of the MP-added soils. Except for pH, the values showed wide ranges and unbalanced distributions. Therefore, log transformation was conducted for the other five properties to reduce the gaps between the data. This transformation step is useful for converting the original data to a normal distribution to improve model convergence and performance (Shi et al., 2023; Sigmund et al., 2020). A box plot illustrates the data distribution for each soil property (Fig. S1).

The input variables for ML training, both categorical and continuous, are listed in Table 1. The richness of the MP types caused us to further categorize them based on their elementary composition. For example, high-density polyethylene, low-density polyethylene, phenanthrene, polypropylene, and polyethylene contained only C and H and were marked as "CH." The category "CH–B" was added to distinguish plastics containing benzene rings, such as polystyrene. Additional details on the MP type, MP shape, experiment type, soil type, presence of other additives, and continuous variables are listed in Table 1. After labeling the categorical variables, the one-hot encoding method (Cerda et al., 2018; Dahouda & Joe, 2021) was employed to encode the categorical data for ML model development. We also filled in missing values for the continuous variables before ML modeling, using the k-nearest neighbor method (Pan et al., 2015).

Table 1
Detailed information on categorical and continuous input variables in the collected dataset.

Categorical input variables	MP types	CH (high-density polyethylene, low-density polyethylene, polyethylene, phenanthrene, polypropylene), CH–B (polystyrene), CHCl (polyvinyl chloride), CHF (polytetrafluoroethylene), CHO (biodegradable plastics, polyhydroxybutyrate, polylactic acid, polyacrylic, bisphenol, oly(3-hydroxybutyrate-co-3-hydroxyvalerate0)), CHO–B (polyethylene terephthalate, (poly) butylene adipate terephthalate, polycarbonate), CHN (polyacrylonitrile), CHON (polyamide, polyurethane), CHOS (polyester)
	MP shapes	Fiber, Cylinder, Film, Foam, Fragment, Particle, Powder, Round
	Experiment types	Field, Laboratory, Pot, Greenhouse
	Soil types	Clay, Clay loam, Loam, Loamy sand, Sand, Sandy clay loam, Sandy loam, Silt, Silt loam, Silt clay loam
	Other additives	Biochar, Biomass, Fertilizer, Heavy metal, Organic compounds, Nanoparticles, Water
Continuous input variables		MP size, MP dosage, Incubation time
Output variables		Dissolved organic carbon (mg·kg^{-1}), NH_4^+-N and -NO_3^--N (mg·kg), Total P (mg kg), Acid phosphatase enzyme activity (μg (pNP)·g/hr)

2.3. Model development and evaluation

Based on previous studies, tree-based ML algorithms can be adapted to soil-related data (Palansooriya et al., 2022a; Shi et al., 2023). Therefore, three tree-based algorithms–DT, RF, and GBR–were employed to train the predictive models using the collected data. The DT algorithm splits the input variable data into small groups by identifying specific ranges based on the minimum sum of squared errors (variance between the predicted and actual values) to build a tree with a set depth. The RF algorithm is an ensemble-learning method that uses many trees. The RF model was developed using bagging or bootstrap aggregation to use the data to build trees based on set hyperparameters (Prasad et al., 2006). The performance of RF is the average performance of all trees. The GBR algorithm is another ensemble-learning method that develops a model based on a boosting strategy (Zhang & Ma, 2012). The boosting strategy involves developing a series of weak models to predict errors according to the chain rules to obtain a final robust model (Cai et al., 2020). Details regarding these tree-based algorithms have been reported in our previous study (Li et al., 2021).

To train the tree-based ML models, all data in the dataset were randomly divided into training and testing sets at a ratio of 80:20 (Li et al., 2022a; Li et al., 2022b). The training set accounted for 80% of the data and was used for hyperparameter tuning and training of the predictive model. A testing set with 20% of the data was used to evaluate the ultimate prediction performance of the trained model. During hyperparameter tuning, the maximum depth of the tree and the minimum number of samples required to split an internal node were tuned for the DT model; the maximum depth and number of trees were optimized for the RF model; and the maximum depth of trees, number of trees, learning rate, and subsampling rate were adjusted for the GBR model to adapt the compiled dataset. To reduce overfitting caused by improper hyperparameters, a five-fold cross-validation method was applied during hyperparameter tuning. The final optimized hyperparameter was the mean performance of the validation, which was performed five times. The coefficient of determination (R^2) and root mean square error were used to evaluate the prediction accuracy of the trained ML models (Li et al., 2020; Severson et al., 2019).

Using the developed ML models, the importance of the input variables and their correlations with the predicted targets were determined. ML model is similar to a function that builds a bridge between inputs and outputs from the ML architecture with a large number of fitting parameters. Thus, for tree-based ML, the importance of the input variables to the output targets can be simultaneously determined from the Gini Index during model training. The tree-based model provides a score for each feature, and the feature importance is calculated according to the increase in model performance based on Gini splitting during tree development (Cai et al., 2020). Moreover, the Shapley additive explanations method was used to validate the feature importance results of the tree-based model (Jeong et al., 2021). For feature correlation, the partial dependence plot method was integrated with the ML models to visualize the relationships between the continuous variables and output targets (Lopez et al., 2021).

3. Results and discussion

3.1. ML model development and evaluation

First, the tree-based ML algorithms DT, RF, and GBR were used to predict one soil property (i.e., pH) in the presence of MPs. The optimal hyperparameters for each model were tuned during the training phase using five-fold cross-validation to minimize the prediction errors

(Figs. S2 and S3). The five-fold cross-validation R^2 was the highest, showing a value of 0.83 (Fig. 1). The R^2 value of GBR based on the test set was 0.92 (Fig. 2a), which was much higher than those of DT (0.87) and RF (0.81) (Fig. S4). These results indicate that the GBR model with optimal hyperparameters most accurately predicted pH changes in soils with MP. Therefore, the GBR method was applied to develop predictive models for DOC, total P, acid P, NO_3^--N, and NH_4^+-N in the soil.

After hyperparameter tuning based on five-fold cross-validation (Figs. S5–S9), the final optimal hyperparameters for each GBR model are determined as shown in Table 2. Using the optimal hyperparameters, the five-fold cross-validation R^2 was 0.80–0.97 in predicting soil properties (Fig. 1). Additionally, the testing set from the collected data was used to evaluate the performance of the GBR models for unseen data (Fig. 2). The test R^2 for predicting soil properties was 0.86–0.99, which was close to the range obtained in five-fold cross-validation. Therefore, the developed GBR models exhibited a generic prediction ability without overfitting.

3.2. ML-based interpretation for determining the roles of important factors in MP-added soil

Fig. 3 shows how the MP properties, experimental type and conditions, soil type, and the presence of other additives simultaneously alter soil properties. Among the analyzed input features, four categories of inputs had a relatively close impact ratio on soil pH, with feature importance ranging from 19.5% to 34.5%, among which the MP information had a feature importance of 20.9% (Fig. 3a). Analysis of the role of the different MP properties showed that the MP size contributed 71.6% in altering the soil pH. The soil pH was maintained at 6.45–6.55 when the MP size was less than 3.8 mm. However, the soil pH increased and then decreased significantly as the MP size increased from 3.8 to 8 mm, with a peak at approximately 4 mm (Fig. S10a). The MP shape is the second most important factor influencing the pH of the soils. Zhao et al. (2021) reported that MP shape, particularly foams and fragments, can increase soil pH, possibly because of their association with a higher soil aeration and porosity. Although we did not determine the precise mechanisms by which the MP size affected soil pH, we developed hypotheses to explain these results. The presence of MP in soils alters their bulk density, percentage of water-stable aggregates, and water-holding capacity (de Souza MacHado et al., 2018b). De Souza MacHado et al. (de Souza MacHado et al., 2018b) observed that polyethylene fragments, polyamide beads, and polyester fibers can interact with soil particles and form large soil clumps. Small MPs have a high surface area, and thus can interact with soil particles and may promote the alteration of the soil structure. The formation of soil clumps can negatively affect soil erosion as it leads to the leaching of basic cations, such as Ca^{2+}, Mg^{2+}, K^+, and Na^+, from the soil resulting in pH changes. According to Fei et al. (2020), the growth of Burkholderiaceae and Pseudomonadaceae families were stimulated by the addition of polyvinyl chloride and polyethylene (1%, w/w) to soils. Both these families can fix N (the process that converts atmospheric N into NH_4^+-N in soils); therefore, biological N fixation may be increased in soils, which can affect N cycling. This can alter the H^+ equilibrium in soils because the conversion of organic N into NH_4^+-N consumes H^+, which may explain how MPs alter soil pH (Zhao et al., 2021). Importantly, pH alteration does not depend solely on the MP size. The nonlinear observations of the pH of soil containing MPs of different sizes (Fig. S10a) may be due to the simultaneous effects of other MP properties and experimental conditions.

As a primary form of labile C in soils, DOC plays a vital role in C cycling and is a sensitive indicator of soil quality changes following a disturbance (Guo et al., 2020), since short-term changes cannot be determined by evaluating the total organic C in soils (Li et al., 2016; Liu et al., 2017). We found that the DOC in soils was less affected by MP properties (15.8% importance) than by the soil type and co-existence with other additives (such as biochar, compost, and fertilizers) (Fig. 3b). Almost all nonrenewable petrochemical-based plastics are recalcitrant and persist long after entering the soil (Chamas et al., 2020; Rillig, 2018). Physical degradation of plastics in soil, which occurs through flaking, cracking, or embrittlement, can alter the overall chemical structure of the plastic, whereas chemical degradation of plastics occurs through the oxidation of long polymer chains (Chamas et al., 2020). However, the degradation of plastic and plastic-based products requires 10–1000 years; thus, DOC from MPs may not be available in soils within a short period of time. The MP size and shape are the two most important factors that exert influence on soil DOC. Furthermore, the soil DOC decreased with increasing MP size (Fig. S10b). Lehmann et al. (2021) showed that MP shape is an important determinant of soil aggregate formation and organic matter decomposition, which are closely related to the DOC of soils. The DOC acts as a binding agent and promotes the aggregation of soil particles into larger structures known as aggregates. These aggregates improve the soil structure, porosity, and water-holding capacity. The interaction between DOC and soil particles, particularly clay and silt particles, helps

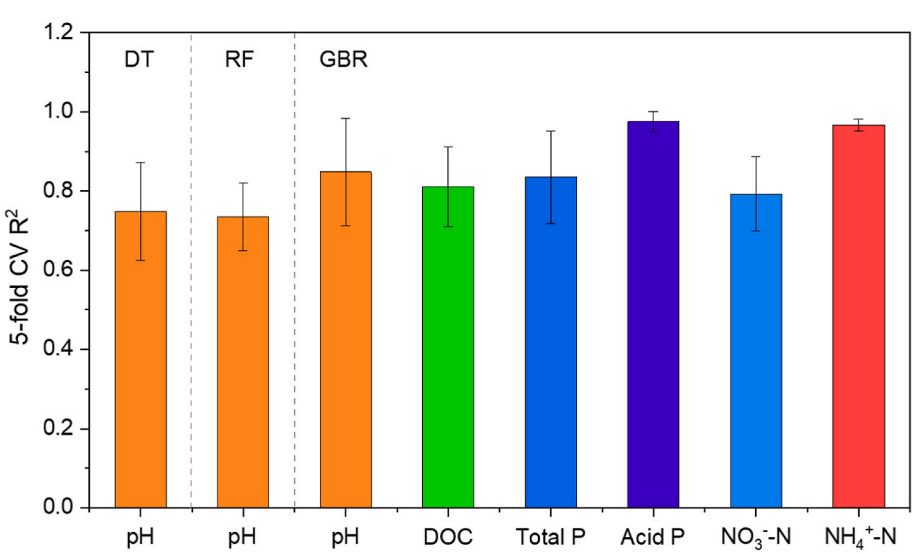

Fig. 1. Average R^2 with standard deviation obtained for the developed machine learning models with optimal hyperparameters, based on five-fold cross-validation for predicting chemical properties of soils with microplastics. Acid P, acid phosphatase enzyme activity; DOC, dissolved organic carbon.

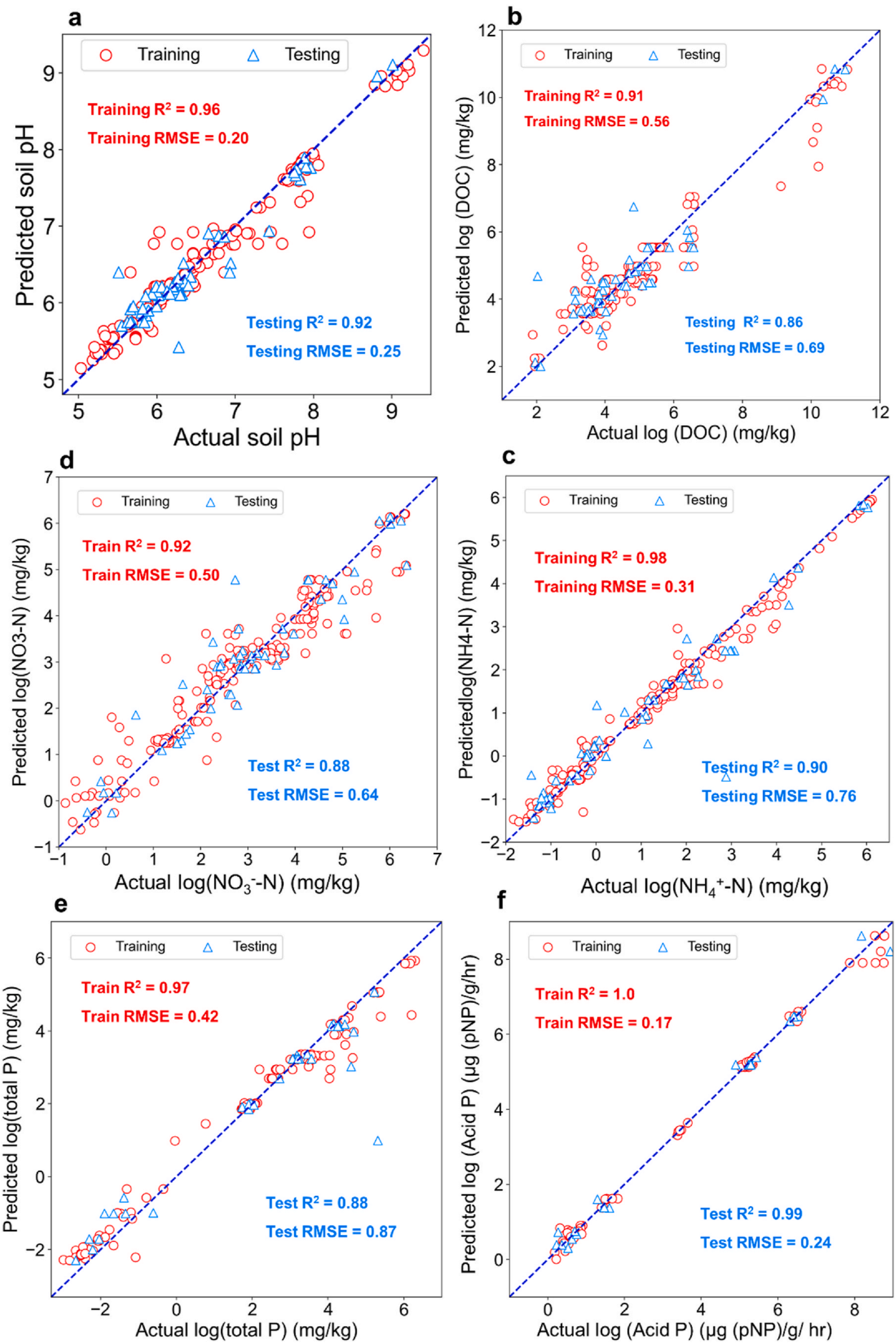

Fig. 2. Predicted vs. actual values during training and testing of gradient boosting regressing (GBR) models for predicting pH (a), DOC concentration (b), NO_3^--N concentration (c), NH_4^+-N concentration (d), total P concentration (e), and acid P (f) of soils with MPs. Acid P, acid phosphatase enzyme activity; DOC, dissolved organic carbon.

Table 2
Optimal values of hyper-parameters of gradient boost regression (GBR) models for predicting chemical properties of MP-containing soils and the number of data points for GBR model development.

Hyper-parameters	n-estimators	max_depth	learning_rate	subsample	No. data points
pH GBR model	9	6	0.4	1	254
DOC GBR model	5	5	0.5	0.5	253
Total P GBR model	5	5	0.4	0.7	164
Acid P GBR model	3	7	0.9	0.7	115
NO_3^--N GBR model	11	4	0.5	1	275
NH_4^+-N GBR model	5	8	0.5	1	284

form stable aggregates. The presence of DOC acts as a "glue" that binds particles together, enhancing aggregate stability. Moreover, DOC serves as a vital energy source for soil microorganisms. Microorganisms, including bacteria and fungi, feed on DOC, breaking it down into simpler compounds *via* microbial respiration. This microbial activity contributes to the breakdown of organic matter and release of carbon dioxide and other byproducts. The activities of these microorganisms affect the structure and aggregation of surrounding soil. Lehmann et al. (2021) found that polypropylene, polyethylene films, and polypropylene particles decreased the decomposition of organic matter in soils. Additionally, MPs can affect soil aggregates within a short period of 42–63 d (Lehmann et al., 2019). This is supported by our findings showing increased DOC in the soils after 40 and 60 d of soil incubation (Fig. S10b). Furthermore, a relatively small-sized MP can easily disrupt soil aggregation by becoming entrapped in soil pores and decreasing the soil bulk density (de Souza MacHado et al., 2018a). As supported by the present study, decreasing the MP size to <1000 μm increased the DOC levels in the soil (Fig. S10b). Lehmann et al. (2021) observed that MP foams tended to decrease the number of newly formed aggregates (>2 mm in size) and overall aggregate stability. Additionally, MP films negatively affected aggregate formation and positively affected aggregate stability. MP films accelerate water evaporation, decrease moisture content and bulk density, and increase soil porosity (Jiang et al., 2017). The artificial pore structure introduced by the MP films breaks the planes that form aggregates, thereby preventing the formation of new aggregates. The dosage and type of MP also caused changes in soil DOC; the DOC increased with increasing MP dosage (Fig. S10b). Chen et al. (2022) also observed that the addition of (poly)butylene adipate terephthalate MP (10%, w/w) to soils resulted in a higher DOC of 66.3 mg/kg compared to that in control soils with 38.4 mg/kg of DOC. This result indicates that the accumulation of MP (both petrochemical-based and biodegradable) stimulates soil enzymatic activity, leading to the degradation of MP and the accumulation of labile C in soils. Under different MP types at different application rates, this could possibly change the soil microbial biomass and activity to varying degrees and then affect soil CO_2 emissions, leading to an increase (with increasing application rates of MP) in the soil DOC content (Gao et al., 2021).

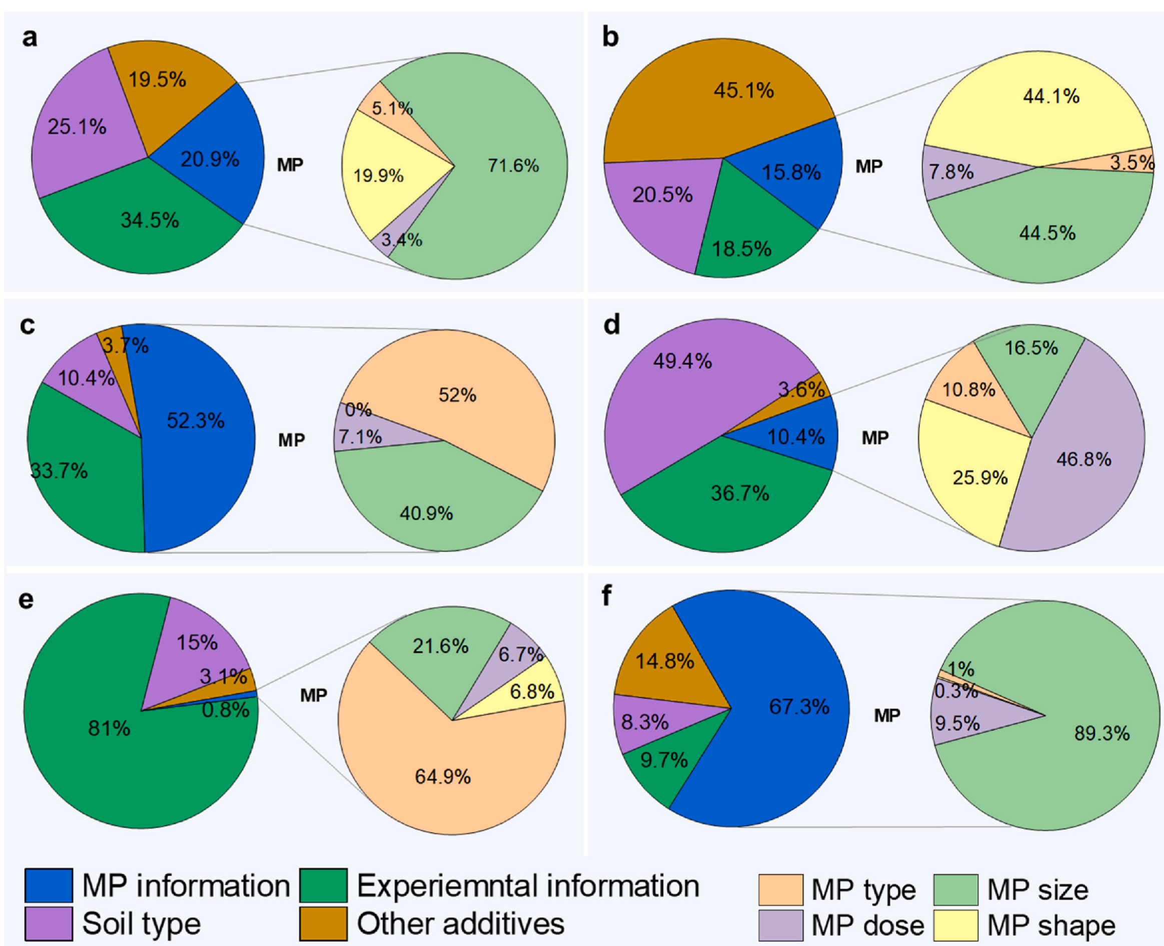

Fig. 3. Importance of various types of input features to pH (a), DOC concentration (b), NO_3^--N concentration (c), NH_4^+-N concentration (d), total P concentration (e), and acid phosphatase enzyme activity (f) of MP-added soils. MP, microplastic; DOC, dissolved organic carbon.

N is an essential nutrient that ensures the growth of plants and biota in the soil. Among the different forms of organic and inorganic N, NO_3^--N, and NH_4^+-N are present in soils. Shen et al. (2022) stated that although some studies on the impact of MPs on N transformation and N cycling have been conducted, data on how MP size, shape, dose, and types affect N in soils are limited. MPs can profoundly alter N cycling by altering the N dynamics in soils. Although MP structures contain negligible amounts of N, they can significantly modify N cycling. As shown in Fig. 3c, changes in NO_3^--N in soils are the most strongly affected by MP properties (up to 52.3%), followed by the experimental conditions (*i.e.,* soil incubation period and type of experiment, either indoors or outdoors). MP type and size were two critical features, and larger MPs decreased the NO_3^--N concentration (Fig. S11a). NH_4^+-N was predominantly affected by the soil type, followed by experimental and MP data, with 49.4%, 36.7%, and 10.4% importance, respectively (Fig. 3d). Among the MP properties, MP dosage was the most important and had a positive impact on the concentration of NH_4^+-N in the soil (Fig. 3d and S11b). Furthermore, the concentration of NH_4^+-N decreased significantly with increasing MP size, whereas the MP dosage had a positive impact on the NH_4^+-N concentration in the soils. Liu et al. (Liu et al., 2022b) observed that the addition of polypropylene MP significantly increased NH_4^+-N levels from 0.94 mg to 1.53 mg N/L. The addition of 1% (w/w) polyethylene MP to soils significantly increased NH_4^+-N and decreased NO_3^--N in soils compared to those in the control soils (Shi et al., 2022). These results agree with our findings (Fig. S11). Small MP can adsorb and trap NO_3^- and NH_4^+ in soils (Li & Liu, 2022). MPs have charged surfaces that can adsorb mineral ions such as Cd^{2+}, Ni^{2+} (Li et al., 2019), Pb^{2+}, and Cu^{2+} (Zou et al., 2020). However, the surface charge of the MP depends on the environmental pH. The isoelectric points (the pH at which a specific molecule carries no net electrical charge) of polyethylene, polypropylene, and polystyrene MPs are 3.2, 6.5, and 5.9, respectively. If the environmental pH is higher than the isoelectric point, the net surface charge of MPs is negative.

As shown in Fig. S10a, almost all pH values are above 6.2, and MPs were mainly negatively charged in the soil (Zhang et al., 2020). The negative MP surface electrostatically repels anions such as NO_3^- and attracts cations such as NH_4^+ into the soil. We found that the type and dose of MPs strongly affected the NO_3^--N and NH_4^+-N concentrations in soils. Particularly for NH_4^+-N, the major fixation mechanism is the sorption of cations on clay mineral surfaces and their penetration into the interlayers of illite- and vermiculite-like clay minerals in soils (Nieder et al., 2011). Negatively charged MPs can adsorb NH_4^+, and at high MP doses, more binding sites are available for NH_4^+; therefore, less NH_4^+ is available in the soil. With the decreasing size of MPs, they have high surface areas available for NH_4^+ binding. Unlike NH_4^+, NO_3^- ions are negatively charged. The electrostatic repulsion between the negatively charged MPs and NO_3^- results in their lower adsorption by the MPs compared to NH_4^+. Therefore, more NO_3^- ions are available in the soil (Fig. S11). Further, MPs influenced soil microbial community composition and activity. Microbes play a significant role in nutrient cycling, including N transformation. Changes in microbial communities due to the presence of MPs could affect the rates of nitrification (conversion of NH_4^+ to NO_3^-) and other nitrogen-related processes. Shi et al. (2022) observed MP-induced soil N immobilization and reduced soil N bioavailability.

P is another important nutrient that limits global agricultural production (Holford, 1997). According to the present study, the total P in soils was significantly affected by the experimental conditions (81% importance), such as the soil incubation period, whether the experiment was conducted indoors (in a laboratory or greenhouse) or outdoors as a field experiment (Fig. 3e). The MP properties did not have an obvious impact on the total P in the soil, which agrees with the experimental results. Feng et al. (2022) observed that, compared to the control soils (160.0 mg/kg), the available P (part of total P) only slightly decreased to 152.34, 147.88, 152.46, and 151.09 mg/kg after adding polyamide, polylactic acid, polybutylene succinate, and polyhydroxybutyrate (2% w/w), respectively. The incubation duration also plays a key role in changing P dynamics in soils. The total P concentration increased with increasing incubation time (Fig. S12a). After 60 d of incubation, the total P in the soil increased significantly. Soil type also influenced alterations in the total P in the soil, with 15% significance (Fig. 3e). P typically shows a strong affinity for oxygen; therefore, rather than elemental P, orthophosphate forms, including $H_2PO_4^-$, HPO_4^{2-}, and PO_4^{3-}, are abundant in soils that are available to plants (Eidt, 1979). Other soil constituents, such as organic amendments and clay minerals, may have positively charged surfaces, and thus, they can adsorb orthophosphate ions in soils. Generally, P has a strong affinity for aluminum oxides in soils with a pH between 4 and 7 (Penn & Camberato, 2019).

Acid P is an index of phosphatase enzyme activity in soils. According to our ML interpretation, acid P was significantly influenced by MP, with a shareholder ratio of 67.3% (Fig. 3f). Many researchers have demonstrated the importance of MP. For example, Liu et al. (Liu et al., 2022b) suggested that MP only increased acid P in soils by 8.3%, and the addition of polypropylene, polyvinyl chloride, and polytetrafluoroethylene MP to soils significantly increased acid P in soils by 14.6%, 12.4%, and 11.7%, respectively. More specifically, MP size was the most important property, accounting for nearly 90% of all MP properties; an increase in MP size decreased acid P (Fig. 3f and S12b). This result indicates that other MP properties have a slight impact on acid P, which was proved by other researchers. For example, Xu et al. (2020) observed that different types of MPs at different doses had non-significant effects on acid P in soils. In addition, Daughtridge et al. (2021) reported that active soil enzymes are essential to ecosystem processes as they catalyze reactions that are important in biogeochemical cycles (Daughtridge et al., 2021). These enzymes are extremely sensitive to ecological and anthropogenic alterations in soil environments; therefore, they are often used as indicators of soil quality (Aponte et al., 2020). The Acid P enzyme catalyzes the cleavage of phosphate bonds and releases phosphate through hydrolysis (Margalef et al., 2017). Therefore, it can be deduced that MPs in soils influence the microbial community and P release by changing the acid P activity in soils.

4. Conclusions, limitations and future prospects

Amidst the myriad soil properties and intricate compositions of soils and MPs, notable variability in research outcomes has emerged in the existing literature. Although examinations of the occurrence of soil MPs are relatively common, investigations into the impact of MPs on soil ecosystems remain scarce. Notably, most of these studies focused on exploring soil chemical properties, as they are more amenable to laboratory-based assessments. It is pertinent to emphasize that a significant number of studies have prioritized the evaluation of singular chemical, physical, or biological property alterations in response to the presence of MPs, with limited exploration of the holistic modification of overall soil properties. Scientific investigations have incorporated a diverse array of experimental variables, including soils with varying textures, concentrations, and MP types. Consequently, the observed shifts in soil properties exhibit considerable variance, thus impeding direct comparisons across distinct research endeavors. This complexity renders the prediction of soil property alterations triggered by MPs particularly challenging. Consequently, the confluence of the diversity and scarcity of comprehensive data have culminated in limited insights into the mechanisms underlying the transformative impact of MPs on soil properties. Consequently, an evident void looms within the realm of soil science, where the predictive capacity for the alteration of soil properties owing to MP attributes remains underdeveloped. Notably, the interactions among MP properties, experimental conditions, soil types, and supplementary additives influencing alterations in soil properties are subject to considerable variation among studies. Comprehensively addressing all these contributing factors in a single study presents a formidable challenge.

To overcome this challenge, we used ML methodologies to holistically examine the combined effects of MP properties, experimental conditions, soil types, and additional additives on soil properties. Our findings underscore the significance of MP attributes, including shape, size, dose, and type as pivotal modulators of soil properties. The infusion of MPs into soils engenders a spectrum of chemical reactions and decomposition processes, augmenting our understanding of the intricate roles played by MPs in soil ecosystems. However, this study has some limitations; only the effects of MPs on the chemical properties of soil were mainly investigated, though MPs also affect soil physical properties such as bulk density, water-holding capacity, porosity, and hydraulic conductivity. Following MP exposure, soil macroaggregates were formed. Wang et al., 2022) observed that 72% of MPs were trapped within soil aggregates. MP shapes, such as films, fragments, and spheres have different surface areas that can alter the physical properties of the soil in different ways. In addition, the surface area of MPs offers a habitat for the proliferation of soil microorganisms. In addition, microorganisms can form biofilms on weathered MP surfaces and further alter them (McCormick et al., 2014). Thus, the surfaces of MPs provide a specific niche for microorganisms. The activity of microorganisms in soils plays a key role in changing soil properties; therefore, the effects of the MP shape should be further evaluated. Although the manner in which the MP shape affects these physical and biological property changes in soils can be predicted, data from existing research were inadequate for our analysis. We plan to further study the effects of MPs on the physical properties and abundances of microorganisms. In addition, our data were obtained mainly through laboratory experiments, which may not reflect real-world conditions. Since MPs are not constantly mixed under real-world conditions and many environmental factors, such as rainfall, leaching, erosion, and soil aggregation, can influence the effects of MPs on soil properties (Lehmann et al., 2021), these situations should be further examined.

This study lays the foundation for future research endeavors to direct greater attention towards comprehending the influence of MP properties on the transformation of soil properties. This exploration extended beyond the categorization and dosage of MPs, emphasizing how the morphological attributes, specifically the shape and size of MPs, interacted with soil properties. Furthermore, our findings highlight a critical point: changes in any soil property (chemical or biological) resulting from the introduction of MPs into soils stem from a complex interplay. This interplay encompasses not only MP properties but also factors such as soil type, duration of MP presence, and concurrent presence of other additives in soils.

In light of these findings, it is prudent to consider the aforementioned insights when developing regulations and policies pertaining to MP in the soil context. Moreover, this study advocates the adoption of comprehensive methodologies for the analysis and quantification of MP in soils. Additionally, this study underscores the value of further research aimed at elucidating the intricate mechanisms by which MP properties, whether isolated or intertwined with experimental conditions, orchestrate shifts in soil properties. Such inquiries hold promise for enriching our understanding of the underlying dynamics and enabling informed decision-making in soil management and environmental policies.

Author contributions

P. A. W. and J. L. contributed equally to this study. P.A.W.: data collection, writing, Writing – review & editing, and Visualization. J. L.: Methodology, data mining, modeling, writing (Writing – review & editing), and Visualization. S.S.: writing (Writing – review & editing). C. F.: writing (Writing – review & editing). Y.W.: Supervision, Funding acquisition, writing (Writing – review & editing). Y.S.O. conceptualized the Supervision, Funding acquisition, and writing (Writing – review & editing).

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.

Data availability

Data will be made available on request.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.envpol.2023.122833.

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