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Microplastics in food packaging: Evaluating contamination in take out and dine in food containers and machine learning prediction of release

ABSTRACT

Microplastics (MPs) pose a global concern because of their potential risks to ecosystems and human health. The growing demand for fast-food delivery in today's fast-paced lifestyle increases human exposure to MPs released from food packaging containers, posing risks to food safety and well-being. This study investigates the presence of MPs in food containers used for take-out and dine-in services. Containers made from different polymers, namely polyethylene terephthalate (PET), polypropylene (PP), high-density polyethylene (HDPE) and polystyrene (PS), were analysed for microplastic abundance. Quantification was performed using three treatments: normal water (NW), hot water (HW) and cold water (CW). The influence of pH (4, 5, 7, 8 and 9), temperature (15, 30, 45, 60 and 90 °C) and exposure time (0.5, 1, 1.5 and 2 h) on MP release was examined. ATR-FTIR, SEM and AFM were employed to identify the polymer constituents and the morphology of the released particles. Average MP abundance was 474.44 ± 33.08 µg/container for NW, 659.48 ± 45.04 µg/container for HW and 556.58 ± 43.08 µg/container for CW. The highest release was obtained at pH 8, 90 °C and 2 h of exposure, with an average of 293.98 ± 13.86 particles/L. Building on the experimental data, a leakage-free machine-learning framework was developed to predict MP release from routine usage conditions. Five regression algorithms were compared, and an extreme gradient boosting model tuned with the Grey Wolf Optimizer (GWO-XGBoost) gave a coefficient of determination of 0.984 for particle count and 0.989 for released mass on unseen experimental conditions, with a negligible train-to-test gap. Shapley additive explanations (SHAP) showed that thermal exposure and polymer type were the dominant controllable drivers of release. The combined experimental and data-driven approach clarifies the fate of MPs in food packaging and offers a practical tool to support mitigation and control.

Keywords: MPs; Food containers; Quantification; Fourier-transform infrared spectroscopy (FTIR); Polymer degradation; Environmental exposure; Machine learning; XGBoost

1. INTRODUCTION

Plastic, an inseparable aspect of modern human life, is witnessing an unprecedented surge in usage and waste production owing to the expanding global population. The Central Pollution Control Board (CPCB, 2020) reported an estimated 34,69,780 tonnes per annum of plastic waste generated during 2019–2020 [1]. MPs, defined as particles smaller than 5 mm, are produced through the breakdown of larger plastic waste. Their widespread presence has become a major environmental issue, creating serious risks for ecosystems, wildlife and human well-being [2,3].

As plastic waste fragments over time, it gives rise to MPs and even smaller nanoplastics, perpetuating the hazard to life. Assessing the impact of MPs on human well-being and food safety is therefore a critical step in understanding the magnitude of this global problem [4].

India, the world's second-largest consumer of plastics, generates an estimated 9.46 million tonnes of plastic waste each year [5]. Inadequate management and disposal have led to gradual fragmentation into MPs, with severe repercussions for the country's water bodies [6], soil [7,8] and wildlife [9,10]. These MPs have also infiltrated the food chain, introducing risks to human health [11,12]. Human exposure to MPs through inhalation and food consumption has been estimated at 203 to 332 particles per person per day [13,14].

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A thriving global market for fast-food delivery has emerged from the bustling modern lifestyle, and single-use containers for take-out food carry a notable environmental burden [15]. Food-packaging plastics such as PET, PP, polylactide, low-density polyethylene, HDPE and PS are widely used [16]. The release of MPs from PET bottles and from PS, PP and PET dine-in or take-away containers has been confirmed in several studies [17-19]. Fadare et al. [4] demonstrated that common containers and disposable cups release detectable MP particles into their contents, with polyethylene identified as the dominant polymer in 76% of contaminated samples. Eti et al. [20] confirmed migration of heavy metals and chemical constituents from food-contact plastics, with rates varying by polymer and simulant acidity. Gambino et al. [21] reported higher MP concentrations in bottled than tap water, with reusable PET bottles showing greater contamination than single-use bottles. Walenna et al. [22] found PE and PP to be the predominant MPs in agricultural soils, while Seewoo et al. [23] reported that polycarbonate and PS had the highest evidence of monomer leaching into food.

The COVID-19 pandemic, which forced the closure of dine-in restaurants, further encouraged take-away delivery [24] and increased the frequency of human contact with plastic products. Plastic containers are expected to grow in use because they are light, economical and easy to handle [25]. Although previous studies have reported MP release from plastic food containers, a systematic evaluation under realistic food-contact conditions including the combined effects of pH, temperature and exposure time remains limited, particularly in the Indian context. This study provides a comprehensive quantification of MP release across multiple polymers (PP, HDPE, PET and PS) under simulated real-use scenarios, coupled with advanced morphological and chemical characterization.

A further limitation of the existing literature is that MP release is treated almost entirely as an experimental outcome, with little attempt to model it quantitatively. Because release depends on several interacting factors, the polymer, the acidity of the food, the temperature and the contact duration, a purely experimental description cannot easily predict release for conditions that were not tested, nor rank the relative influence of each factor. Data-driven models are well suited to this

kind of multivariable, non-linear problem and have recently been used to predict complex material behavior in allied fields; for example, Utkarsh and Jain [26] used a Grey-Wolf-tuned extreme gradient boosting model to predict the swelling pressure of bentonite from routine index properties. Tree-based ensembles such as XGBoost [27] are particularly effective for small to moderate tabular datasets, and explainability methods such as shapley Additive explanations [28] allow the learned relationships to be interpreted physically rather than treated as a black box. Accordingly, the present work extends the experimental study with a leakage-free machine-learning framework that (i) predicts both the number and the mass of MPs released from food containers using pH, polymer type and the thermal-exposure condition as inputs, (ii) compares several algorithms of increasing flexibility under a strict, replicate-aware validation protocol, and (iii) uses SHAP to quantify the controllable drivers of release. To our knowledge this is the first study to couple experimental MP quantification from food containers with an interpretable predictive model, providing a quantitative basis for mitigation and safer-packaging design.

2. MATERIALS AND METHODOLOGIES

2.1. Description of sample

To determine the presence of MPs in fresh consumer plastic food containers, commonly used take-away and dine-in containers were purchased from local stores in four cities of Gujarat, India (Surat, Ahmedabad, Vadodara and Vapi). The polymeric composition was identified by attenuated total reflection Fourier-transform infrared spectroscopy (ATR-FTIR). Six frequently used containers were selected: non-transparent PP containers with PP lids; transparent PP containers with PP lids; take-away HDPE bags; PET containers; PS bowls; and transparent PP disposable cups (**Figure 1**). In total, 25 batches each of the transparent and non-transparent PP containers, 30 batches of HDPE bags, 20 batches of PET containers, 20 batches of PS bowls and 25 batches of PP cups were purchased. Information on the plastics was obtained from the package labels. For convenience the six container types are denoted A (non-transparent PP), B (transparent PP), C (HDPE bag), D (PET), E (PS) and F (PP cup).

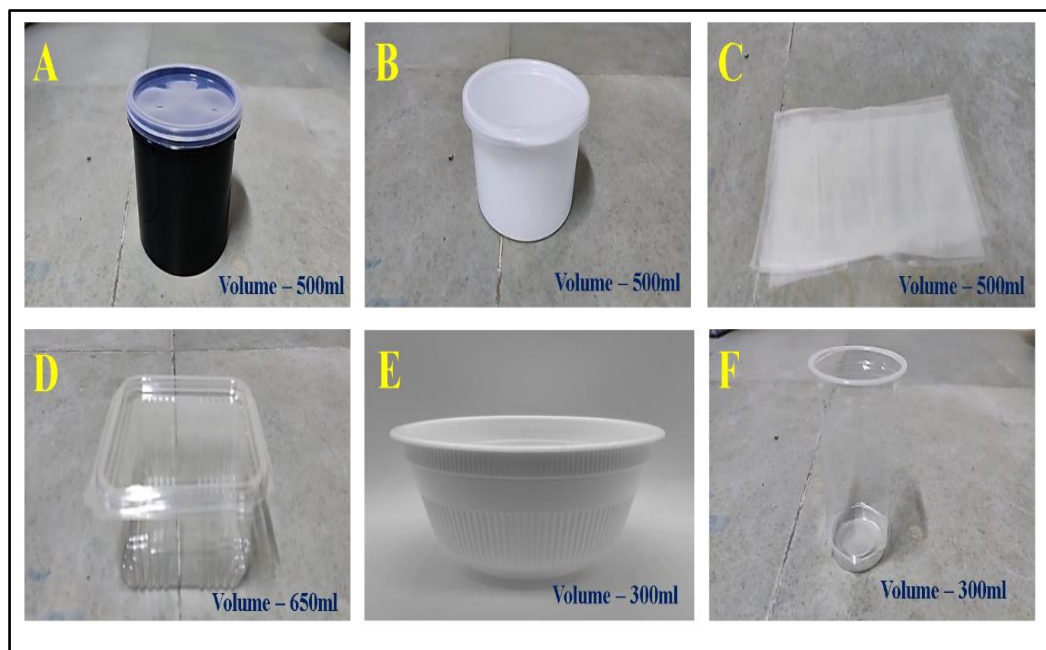


Figure 1. Food containers used for quantification of MPs. A, non-transparent PP container; B, transparent PP container; C, HDPE bag; D, PET container; E, PS bowl; F, transparent PP disposable cup.

2.2. Methodology

A laminar-flow chamber was used to prevent contamination from indoor air during the experiments, and lids covered the containers to prevent external contamination. All containers were cleaned with double-distilled water (DDW) before the experiment. The procedure was applied for the three treatments: normal water (NW), hot water (HW) and cold water (CW) representing food prepared and delivered at ambient (30–50 °C), high and low (–10 to 10 °C) temperatures, respectively. Experiments were conducted at temperatures of 15, 30, 45, 60 and 90 °C, pH values of 4, 5, 7, 8 and 9, and exposure intervals of 0.5, 1, 1.5 and 2 h. The pH conditions reflected the acidity of foods stored in such containers; solutions were prepared with a few drops of 0.1 N H₂SO₄ and 0.1 N NaOH and measured with a portable pH meter. Control tests with DDW and pH solutions confirmed the absence of MP contamination by ATR-FTIR.

For the hot condition, 300 mL of DDW at 90 °C was used at the different pH values and exposure times, simulating food consumed immediately or after delivery. For the cold treatment, 250 mL of DDW was frozen into ice cubes (–5 °C; mean cube mass 96.14 ± 3.03 g) that were transferred to each container and held for 0.5 and 1 h, as cold products are not usually stored for long. Containers were allowed to cool in the laminar-flow hood before filtration. The influence of pH was studied by pouring pre-heated pH solutions (4, 5, 7, 8 and 9) into the containers, wrapping each sample in aluminium foil and holding it at 90 °C for 1.5 h. The influence of temperature was examined at the pH giving the highest release (pH 8) for 1.5 h at 20, 30, 45, 60 and 90 °C. The influence of exposure time was studied at pH 8 and 90 °C for 0.5, 1, 1.5 and 2 h. Tests were performed in octuplicate, and mean values with standard deviations are reported. The overall experimental sequence and the subsequent computational analysis are summarised in **Figure 2**.

2.3. Microplastics extraction

Quantification of total solids. The 75 µm–1 mm size range was analysed. Each sample was passed through a stack of stainless-steel sieves (1 mm, 600, 300, 150 and 75 µm); solids retained on the 75 µm sieve were transferred to a 500 mL beaker by minimal rinsing with ultrapure water, dried at 90 °C for 24 h and weighed. The mass of total solids was taken as the difference between the beaker with dried solids and the empty beaker.

Quantification of MPs. Wet peroxide oxidation (WPO) removed organic matter [29,30]. A 0.05 M Fe(II) solution and 20 mL of 30% hydrogen peroxide were added to the solids on the 75 µm sieve; FeSO₄ catalysed the reaction while H₂O₂ oxidised the organic material. After standing for 5 min the mixture was stirred, covered and heated to 75 °C, with ultrapure water added to control vigorous boiling, and reheated for 30 min; further H₂O₂ was added until no organic matter remained. NaCl (6 g per 20 mL, ≈ 5

M) was then added to increase the density of the aqueous phase. After density separation, settled solids were discarded (MPs, if visible, were recovered with forceps), and the supernatant was vacuum filtered through WhatmanGF/C filters (1.2 μm). Filters were dried at 90 °C for 24 h and weighed; the MP mass was the difference between the loaded and the clean filter. Two control groups validated against procedural contamination. For uniform reporting throughout this study, the released microplastic mass is expressed consistently as $\mu\text{g}/\text{container}$ and the microplastic abundance as particles/L. The two metrics are retained separately because they describe different physical quantities (released mass versus particle-number concentration) and cannot be interconverted without assuming a fixed particle size and density; reporting both therefore allows direct comparison with studies that use either convention.

2.4 Characterisation and analysis of released particles

Extracted particles were observed under a Zeiss Stereo Discovery V12 microscope, and their shape and colour were recorded. Particle size was measured in Images across three classes (100–300, 301–500 and ≥ 501 μm), and plots were prepared in OriginPro 8. Polymer composition was analysed by ATR-FTIR over 500–4000 cm^{-1} (16 scans, 4 cm^{-1} resolution). Morphology was examined by scanning electron microscopy with energy-dispersive spectroscopy (SEM-EDS; 3 and 15 kV) after gold sputter-coating, and by atomic force microscopy (AFM; 10 $\mu\text{m} \times 10 \mu\text{m}$, 1 Hz/s). A quality index of 65–70% was considered acceptable [31]. No plastic particles were detected in any control.

2.5 Statistical analysis

One-way ANOVA was used to assess MP abundance across containers and treatments. Differences among cities and among treatments within a city were evaluated with the Kruskal–Wallis test. A p-value below 0.05 was considered statistically significant.

2.6 Machine-learning modelling

Dataset and variables. The experimental campaign produced 357 quantified observations, each describing the MP release measured from one container type under one combination of pH, temperature and exposure time, with three replicate trials per condition (119 distinct conditions). Three measured factors were used as model inputs: solution pH (4, 5, 7, 8, 9); polymer/container type (the six categories A–F); and the thermal-exposure condition. Temperature and exposure time were varied together in the experimental design (15 °C/0.5 h, 30 °C/1 h, 60 °C/1.5 h, 90 °C/2 h) and were perfectly rank-correlated (Spearman $\rho = 1.0$); because they cannot be separated statistically, they were represented by a single ordinal thermal-exposure level (L1–L4) so that the model is not credited with resolving an effect the data cannot distinguish. Two responses were modelled independently: the number of MPs released (particles/L) and the released mass ($\mu\text{g}/\text{container}$). Continuous inputs were standardised for the distance-based learners, and the polymer type was one-hot encoded; the descriptive statistics of the variables are summarised in

Table 3.

Data partitioning and leakage control. Because each condition was measured in triplicate, an ordinary random train/test split would scatter near-identical replicates of the same condition across both sets, leaking information and inflating the apparent accuracy. To obtain an honest estimate of generalisation, every partition was performed at the level of the experimental condition rather than the individual measurement, so that all three replicates of a given condition fell entirely within either the training or the testing set. An 80% training / 20% testing split (group-aware) was used for the final evaluation, and a five-fold grouped cross-validation (GroupK-Fold) was used for hyperparameter tuning and for cross-validated reporting. The practical importance of this choice is quantified in Section 3.5 and **Error! Reference source not found.**

Models and rationale. Five regressors of increasing flexibility were compared so that the

gain from each level of model complexity could be judged against the cost of over-fitting on a moderately sized dataset. Multiple linear regression served as a transparent baseline. Support-vector regression with a radial-basis kernel tested whether a smooth non-linear mapping was sufficient. Random forest [32] and extreme gradient boosting (XGBoost) [27] were included as tree ensembles that capture threshold effects and factor interactions, which are expected here because release rises sharply only at the harsher pH and thermal conditions. XGBoost was selected as the core algorithm because it consistently performs well on small-to-moderate tabular problems, handles mixed categorical and numerical inputs, and offers built-in regularisation; the same family of model has performed strongly in related geo-environmental prediction tasks [26]. Deep architectures such as convolutional or recurrent networks were deliberately not used: with only a

few hundred observations and four controllable factors, such models would be heavily over-parameterised, prone to over-fitting and difficult to

interpret, offering no advantage over a well-regularised gradient-boosting model on tabular data of this size..

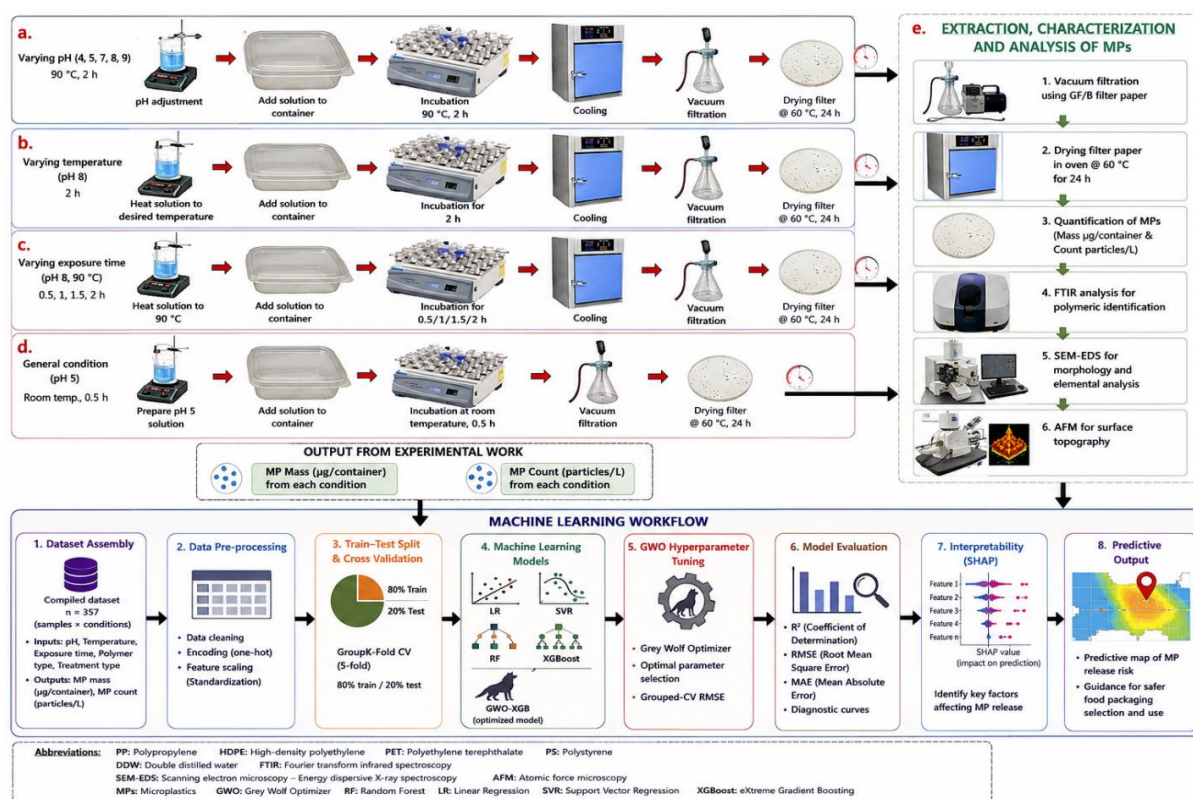


Figure 2. Schematic of the combined experimental and machine-learning workflow, from sample collection and the three water treatments through MP extraction and characterisation to data compilation, leakage-free model development, evaluation and SHAP-based interpretation.

Hyperparameteroptimisation. The XGBoost hyperparameters (learning rate, tree depth, number of trees, sub-sampling fractions, minimum child weight and the L1/L2 penalties) were tuned with the Grey Wolf Optimizer (GWO) [33], a population-based metaheuristic that mimics the social hierarchy and hunting behaviour of grey wolves. The fitness function minimised was the mean grouped five-fold cross-validation root-mean-square error, so that the search itself never used leaked information. Eight search agents evolved over twelve iterations; the resulting GWO-XGBoost configurations are listed in Table 5, and the convergence of the optimiser is shown in the supplementary material.

Evaluation and interpretation. Predictive accuracy was quantified on the held-out conditions using the coefficient of determination (R^2), the root-mean-square error (RMSE) and the mean-absolute error (MAE). Over- and under-fitting were monitored through the train-cross-validation-test gap, a learning curve and a validation curve over

tree depth (Section 3.5). The relative influence and the direction of effect of each input were assessed using shapely additive explanations (SHAP) [28] together with permutation importance. All computations were carried out in Python 3 using scikit-learn [34], XGBoost and the SHAP library.

3. RESULTS AND DISCUSSION

3.1. Quantification of MPs

Following the NOAA protocol [35], FeSO_4 and 30% H_2O_2 were used to decompose organic matter in all samples, and precautions were taken against atmospheric contamination. Because total solids were in the microgram range, a representative sample was used for quantification, and the MPs mass was expressed per container.

After NW washing, the mean MPs mass ranged from 593.58 ± 35.26 µg/container (maximum, container A) to 296.47 ± 32.65 µg/container (minimum, container C); containers B, D, E and F gave 497.82 ± 24.16 , 464.85 ± 28.39 , $548.71 \pm$

49.21 and 445.21 ± 28.82 $\mu\text{g}/\text{container}$, with a control of 25.42 ± 6.14 $\mu\text{g}/\text{container}$. After HW washing, the mean ranged from 923.75 ± 68.46 $\mu\text{g}/\text{container}$ (maximum, container E) to 413.35 ± 29.12 $\mu\text{g}/\text{container}$ (minimum, container C). After CW washing, the mean ranged from $763.42 \pm$

42.74 $\mu\text{g}/\text{container}$ (maximum, container E) to 427.84 ± 54.32 $\mu\text{g}/\text{container}$ (minimum, container B). The MPs mass per container was highest for the dark, non-transparent PP container (A) under NW and for the PS container (E) under HW and CW (Figure 3).

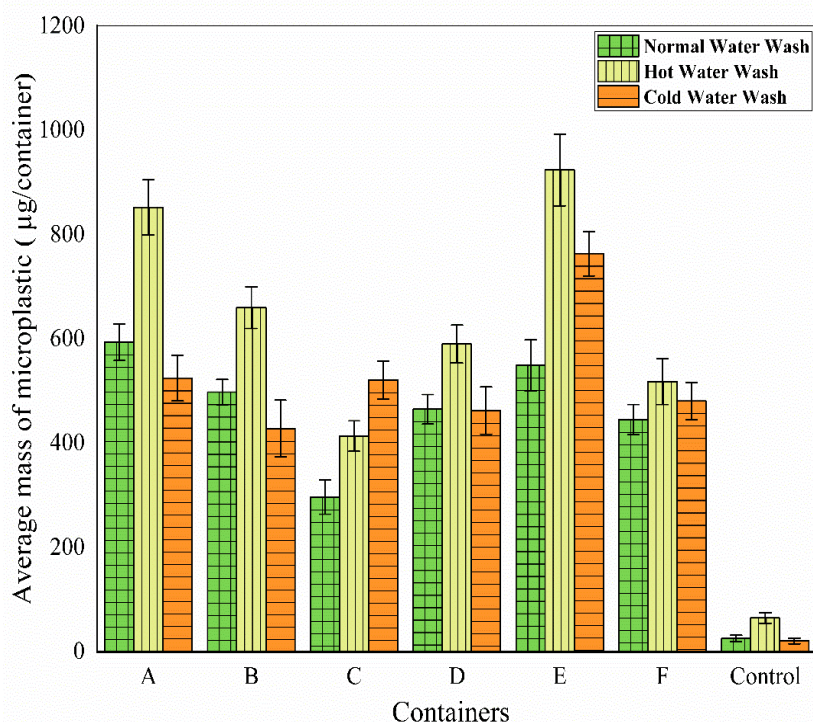


Figure 3. Average mass of MPs for all containers after the three treatments (NW, HW and CW; $n = 33$)

These values are broadly consistent with, and in several respects extend, recent reports on microplastic release from food-contact plastics, although direct numerical comparison is complicated by the different metrics used across studies (mass per container, items per container and particles per litre). On a mass basis, Fadare et al. [4] recovered roughly 3–38 mg of MPs per pack from new containers and disposable cups, about an order of magnitude higher than the 296–924 $\mu\text{g}/\text{container}$ (≈ 0.30 – 0.92 mg/container) measured here; the difference is consistent with their use of pristine packaging and a more aggressive isolation procedure. On a particle-number basis, Chen et al. [17] reported 675–5984 particles/L from disposable cups held with water at 95°C for 20 min, and Zhou et al. [18] found 723–1489 particles per cup after only 5 min of contact, both exceeding the present maximum of about 294 particles/L (up to 328 particles/L for the polystyrene bowl). The lower counts obtained here reflect the milder, more realistic contact conditions ($\leq 90^\circ\text{C}$ and controlled pH) together with the $75\text{ }\mu\text{m}$ – 1 mm size window analysed, which deliberately excludes the sub-20 μm particles that dominate those cup studies. For

polystyrene specifically, Zhu et al. [19] measured 5–173 items/container in take-out PS boxes and identified PS as the leading contributor to both particle number and human intake, in agreement with the disproportionately large mass shed by the PS bowl (container E) in the present work. The consistent ranking of PS and PP as the largest emitters across these independent datasets, despite the differing units and protocols, both strengthens confidence in the present measurements and highlights the novelty of coupling such quantification with an interpretable predictive model, which unlike the purely experimental studies above can estimate release for untested but realistic usage conditions.

3.2. Effect of pH, temperature and exposure time on MP release

Exposure to varied environmental conditions drives polymer degradation and the release of MP particles. The maximum release from containers A–F occurred under alkaline conditions (pH 8) at 90°C for 2 h (Figure 4), at 218.85 ± 16.65 , 235.71 ± 14.70 , 277.14 ± 18.06 , 240.29 ± 15.20 , 328.14 ± 15.25 and 319.71 ± 16.62 particles/L, respectively.

Release was also high at pH 4, especially for the PS container and PP cups. Under both acidic and alkaline conditions, elevated H^+ and OH^- concentrations enhance oxidation and fragment PP, PE and PS into microplastic-sized particles; similar behaviour was reported by Wang et al. [36]. Release was lowest at pH 7 and at 15 °C and rose with temperature from 45 to 90 °C (Figure 4B). The number of particles detected after 1.5 h was nearly double that at 0.5 h, and a further 10.5% increase occurred between 1.5 and 2 h (Figure 4C). The principal factors driving release were therefore alkaline pH (8), high temperature (90 °C) and longer duration (> 1 h).

Many common polymers possess carbon-based backbones (C–C–C–C) that are susceptible to thermal oxidation, including polyolefins such as polyethylene and substituted derivatives such as polystyrene, polypropylene and acrylates.

Differences in MP concentration among container types likely reflect differences in material properties arising from diverse manufacturing processes [37,38]. As reported by Guan et al. [39], the amount of MPs released increased with temperature, most probably because chain scission becomes more prevalent and the polymer structure breaks down as the temperature rises [40]. A recent study by Akbulut et al. [41] on MP release from single-use plastic beverage cups investigated the effect of different exposure times (0, 5, 10 and 20 min) and temperatures (4, 50 and 80 °C) on MP release into water from single-use cups made of four different materials: polypropylene (PP), polystyrene (PS), polyethylene (PE)-coated paper cups and expanded polystyrene (EPS). Washing the cups with ultrapure water prior to use reduced the MP release by 52–65%.

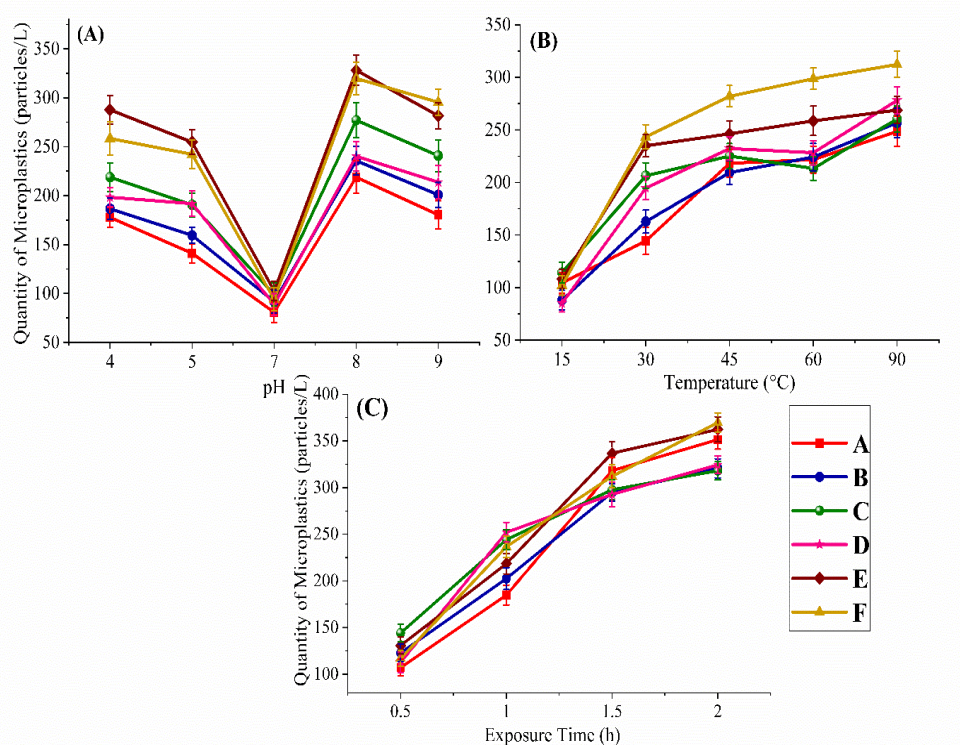


Figure 4. Quantification of microplastics (MPs) released from six types of food containers (A–F) under varying environmental conditions

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Figure 4a shows the effect of pH (4–9) on MP release at 90 °C for 1.5 h, where the minimum release was observed near neutral pH (~7), while higher release occurred under both acidic and alkaline conditions. Figure 4b illustrates the effect of temperature (15–90 °C) at pH 8 for 1.5 h, demonstrating a consistent increase in MP release with increasing temperature across all containers.

Figure 4c presents the effect of exposure time (0.5–2 h) at pH 8 and 90 °C, showing a gradual increase in MP release with prolonged exposure. The maximum MP release was recorded at pH 8, 90 °C, and 2 h, ranging from 219–328 particles/L, with the polystyrene bowl (E) exhibiting the highest release. In contrast, the minimum release was observed near pH 7 and at 15 °C, indicating that alkaline pH, elevated temperature, and longer

contact time are the major controllable factors influencing MP release.

3.3. Features of the released MPs

SEM showed irregularly shaped particles, a few to tens of micrometres in size, on the filter membranes (**Figure 5**). All containers showed increased surface roughness after treatment. After NW, PP, HDPE and PET surfaces were relatively regular with few protrusions, whereas the PS

surface was rough and broken with small folds of 45–80 μm . After HW at pH 8, 90 $^{\circ}\text{C}$ for 2 h, the HDPE bag and PS container surfaces changed drastically, while others showed pitting with deeper cavities; HW produced the highest roughness. AFM (**Figure 6**) indicated cross-sectional sizes of several microns, with HDPE and PP particles rougher than the smoother, more spherical PS particles, consistent with differences in the hardness of the plastics [42].

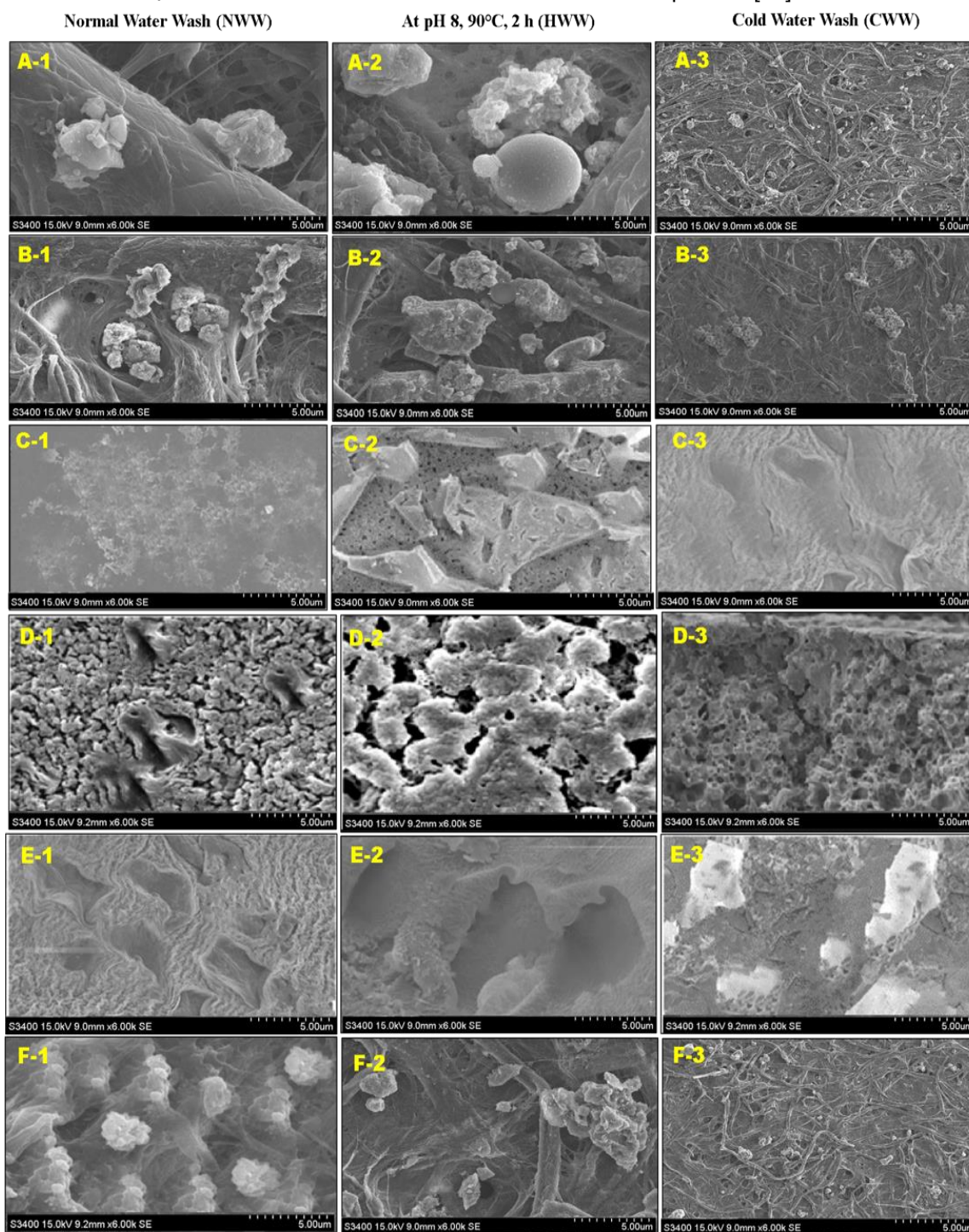


Figure 5. SEM images of containers after different treatments (1: NW; 2: HW at pH 8, 90 $^{\circ}\text{C}$, 2 h; 3: CW)

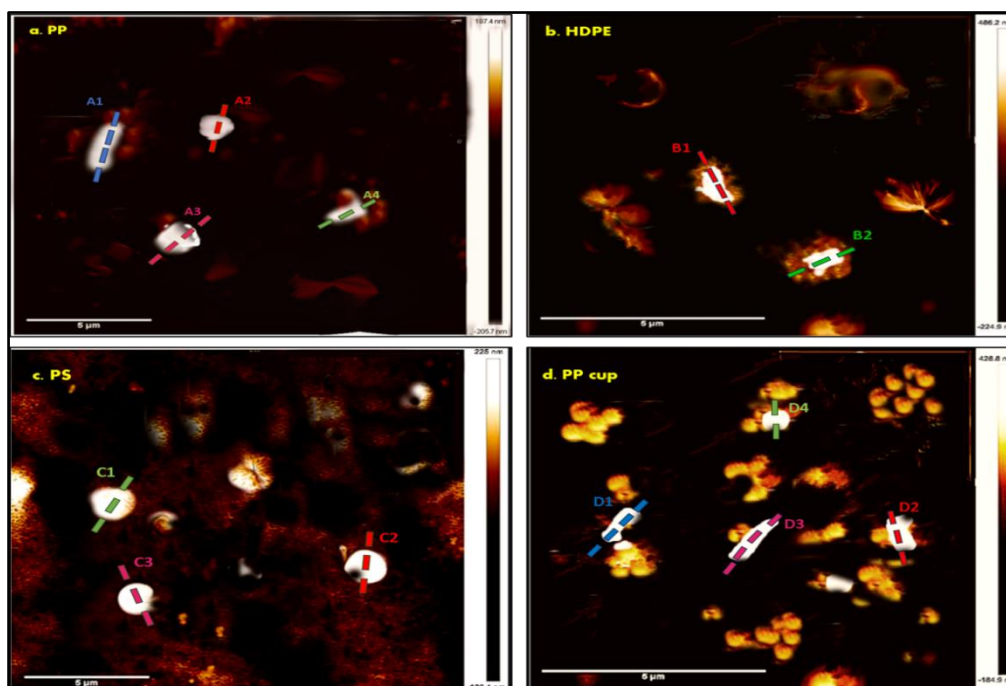


Figure 6. AFM images of the released MPs: (a) PP container, (b) HDPE bag, (c) PS container, (d) PP cups

3.4. Identification of MPs

ATR-FTIR confirmed the polymer identity of the extracted particles (**Figure 7**). The PP spectra showed CH₃ and CH₂ stretching bands (2956, 2921, 2875, 2840 cm⁻¹) and the methyl umbrella vibration at 1377 cm⁻¹; isotactic PP bands appeared near 1077, 1174 and 1071 cm⁻¹. HDPE showed CH₂ stretching at 2933–3296 cm⁻¹ and C–H modes at 1514–1681 cm⁻¹ [43]. PS showed aromatic C–H stretches (3292–3661 cm⁻¹), CH₂ stretches (2877 cm⁻¹) and aromatic ring modes near 1600, 1580, 1500 and 1450 cm⁻¹ [44]. PET was identified from C=O stretching at 1785–1765 cm⁻¹ and C–H bands at 2863–2843 cm⁻¹ and was present in all containers. Carbonyl bands (1631–1744 cm⁻¹) and hydroxyl stretches (3421–3433 cm⁻¹) indicated oxidation during manufacture and ageing [45,46].

Table 1. Size distribution of released MPs from different containers (mean ± SD)

Container	100–300 µm (%)	301–500 µm (%)	≥ 501 µm (%)
Control	46 ± 3	32 ± 3	22 ± 1
A	57 ± 3	24 ± 2	19 ± 1
B	46 ± 2	33 ± 4	21 ± 2
C	55 ± 5	32 ± 2	13 ± 1
D	61 ± 4	28 ± 1	11 ± 3
E	28 ± 2	33 ± 3	39 ± 4
F	48 ± 4	36 ± 3	16 ± 2

The released MPs were predominantly in the size range of **100–300 µm** (Table 1), although larger particles were more prevalent in the PS fraction. The smallest detected particle measured **102 µm**. Particle size plays a critical role in biological uptake and translocation. Previous studies have reported that smaller particles (0.1–1 µm) can cross mucosal lymphoid tissues, whereas particles up to approximately **130 µm** may penetrate the epithelial lining and enter systemic circulation [12, 47].

Table 2. Shape of released MPs from different containers (mean ± SD)

Container	Fibre (%)	Fragment (%)
Control	66 ± 3	34 ± 2
A	69 ± 3	31 ± 2
B	72 ± 2	28 ± 4
C	58 ± 5	42 ± 2
D	76 ± 4	24 ± 3
E	88 ± 5	12 ± 3
F	78 ± 4	22 ± 3

Fibres were the dominant shape, exceeding 60% across all containers (**Table 2**). Of 518 suspected particles identified by µ-FTIR, 52% were natural polymers (mainly cotton); rayon, acrylic, nylon, polyester, PP, PS, PE and PET were also

present (**Figure 8**). PP, PS, PE and PET were attributed to the containers themselves, whereas

rayon, acrylic, nylon and polyester were assumed to originate from external contamination.

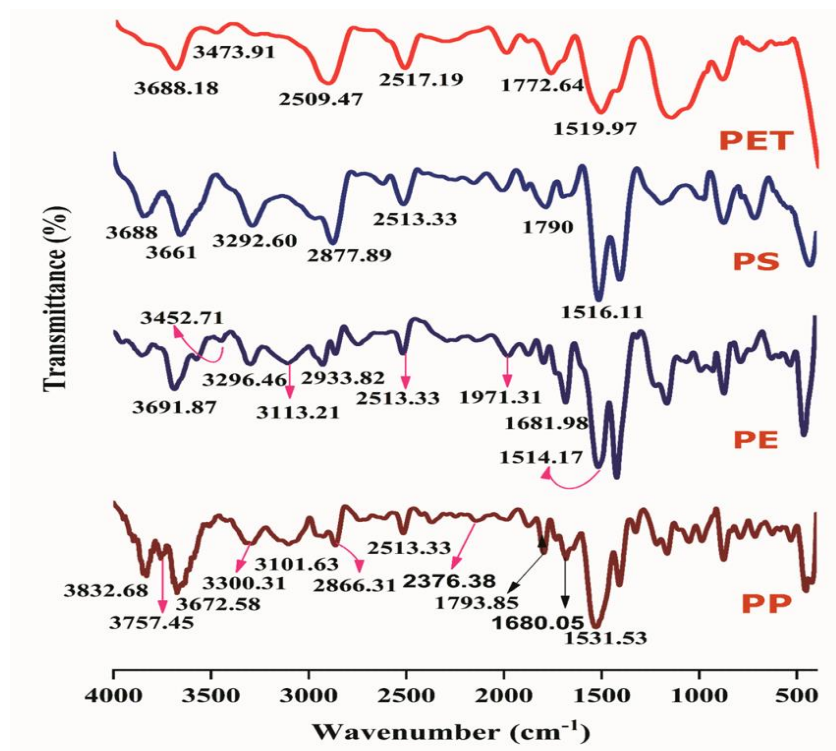


Figure 7. FTIR spectra of MPs extracted from the PP, HDPE, PS and PET containers

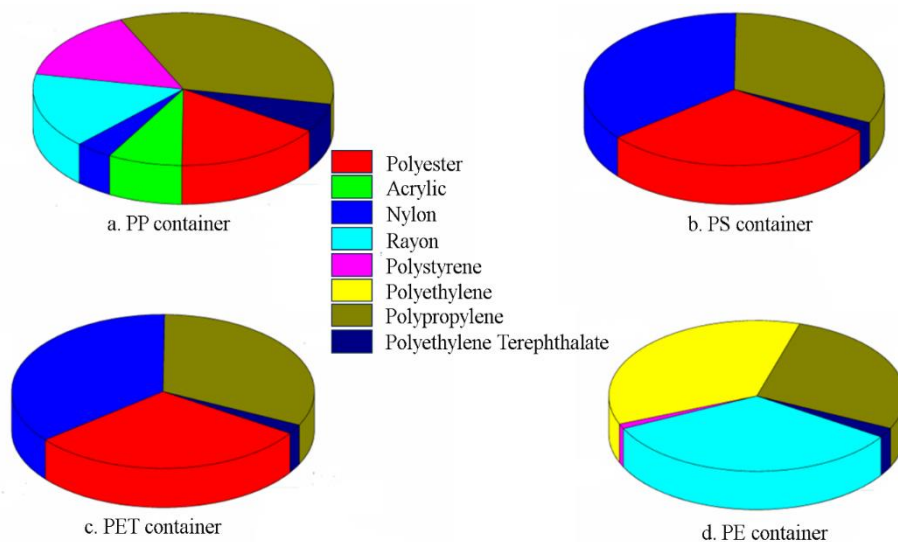


Figure 8. Chemical composition of MPs released from the different container types

3.5 Machine-learning prediction and driver analysis

Descriptive statistics and correlation. The variables span the full experimental design (Table 3) released mass is right-skewed (skewness 1.36), reflecting the much larger mass released by the PS container, whereas particle count is more symmetric. The Spearman correlation matrix (**Figure 9**) confirms that temperature and exposure time are perfectly correlated by design ($\rho = 1.0$), which is precisely why they were combined into a single thermal-exposure factor for modelling; the remaining inputs are only weakly correlated, so multicollinearity among the retained predictors is not a concern.

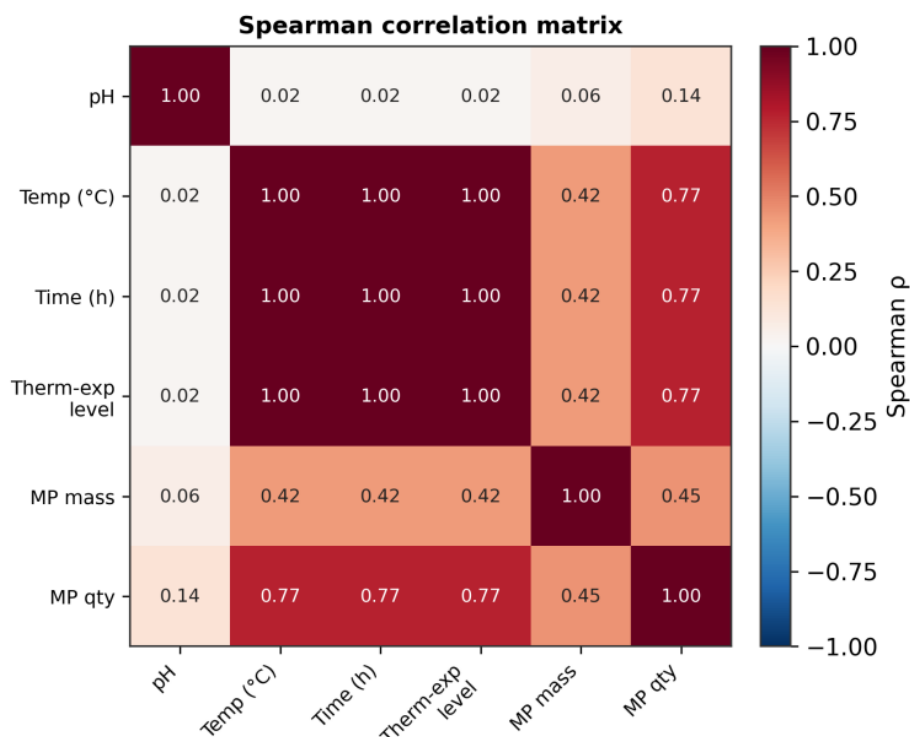


Figure 9. Spearman correlation matrix of the input factors and the two MP responses. The unit correlation between temperature and exposure time reflects the one-factor-per-block experimental design and motivates their combination into a single thermal-exposure level

Table 4; Figure 10). For particle count, the linear and support-vector models essentially failed to generalize to held-out conditions (test $R^2 = 0.03$ and 0.09), which is itself an informative result: it shows that MP release is governed by sharp, interacting thresholds rather than a smooth additive trend, so simple models cannot reproduce it. The tree ensembles performed far better, and the GWO-tuned XGBoost was the best model, reaching a test R^2 of 0.984 (RMSE 5.06 particles/L, MAE 4.21) for particle count and 0.989 (RMSE 19.77 $\mu\text{g}/\text{container}$, MAE 15.98) for released mass.

Table 3. Descriptive statistics of the variables used in the machine-learning analysis ($n = 357$)

Variable	Min	Mean	Median	Max	SD	Skew.	Kurt.
pH (–)	4.00	6.62	7.00	9.00	1.85	–0.17	–1.48
Temperature (°C)	15.0	48.4	30.0	90.0	28.71	0.30	–1.41
Exposure time (h)	0.50	1.24	1.00	2.00	0.56	0.01	–1.35
MP mass ($\mu\text{g}/\text{container}$)	325.5	632.1	567.5	1264.4	183.1	1.36	1.78
MP quantity (particles/L)	93.6	213.0	214.0	322.4	52.2	–0.26	–0.61

The very small train-to-test gap (0.009 and 0.001) and the low cross-validation scatter (standard deviation ≤ 0.004) indicate that the tuned model generalises well without memorising the training conditions. The predicted values track the

measured values closely along the 1:1 line for both training and testing points (**Figure 11**), and the residuals are small, approximately normal and centred on zero with no trend against the predicted value (**Figure 12**), confirming an unbiased fit.

Table 4. Comparison of model performance for MPs quantity (particles/L). CV R^2 is the grouped five-fold cross-validation value; the gap is $\text{Train } R^2 - \text{Test } R^2$

Model	Train R^2	CV R^2	Test R^2	Test RMSE	Test MAE	Gap
Linear regression	0.753	0.692	0.031	39.95	30.35	0.722
SVR (RBF)	0.914	0.670	0.089	38.74	30.80	0.825
Random forest	0.977	0.857	0.753	20.17	15.56	0.224
XGBoost	0.993	0.961	0.947	9.38	7.30	0.047
GWO-XGBoost	0.993	0.989	0.984	5.06	4.21	0.009

Table 5. Optimised GWO-XGBoost hyperparameters for the two responses

Hyperparameter	MPs quantity	MPs mass
learning_rate	0.296	0.300
max_depth	5	2
n_estimators	640	539
subsample	0.882	0.887
colsample_bytree	0.608	1.000
min_child_weight	10	1
reg_alpha	0.189	0.280
reg_lambda	0.737	1.071
gamma	0.461	0.190

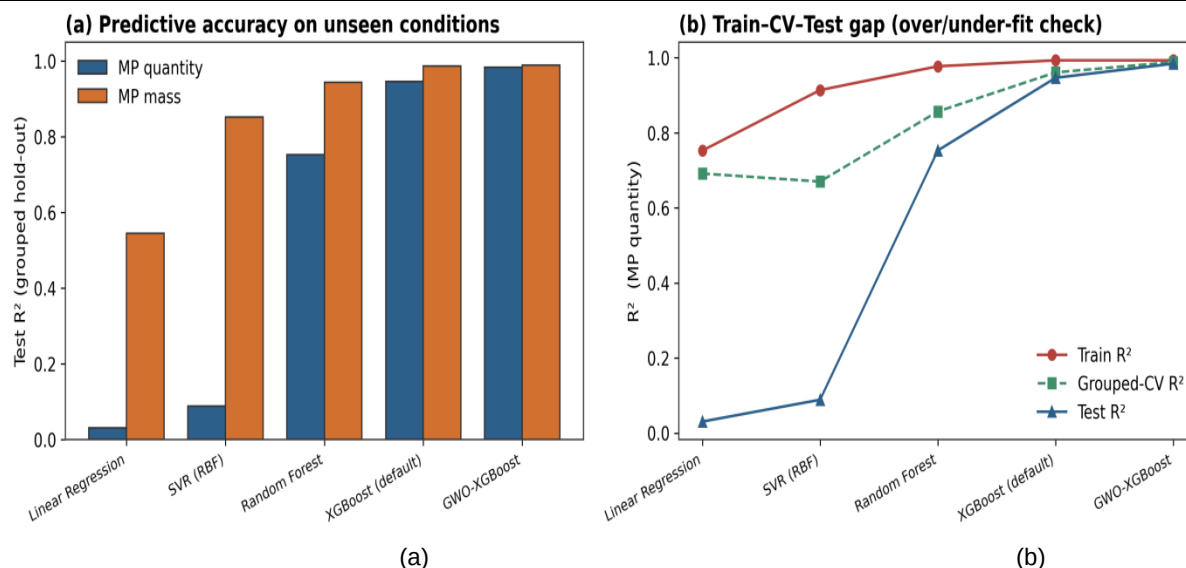


Figure 10. Comparison of model accuracy and generalisation performance for MP prediction

Figure 10a shows the comparison of test R^2 values for both response variables, highlighting the predictive accuracy of different models under unseen conditions. Among all models, GWO-XGBoost achieved the highest predictive performance, with test R^2 values of 0.984 for

particle count and 0.989 for released mass. Figure 10b illustrates the progression from training to cross-validation and test performance for MP quantity, demonstrating the generalisation capability of each model. Well-regularized models exhibited consistent and convergent performance

across datasets, whereas under-fitted models showed larger performance gaps and weaker generalisation. The GWO-XGBoost model showed the smallest train-to-test gap, indicating robust and reliable prediction performance. In contrast, linear and support-vector models performed poorly under

unseen conditions, with test R^2 values of only 0.03 and 0.09, respectively. Overall, the results indicate that GWO-XGBoost is the most effective model for predicting microplastic release, offering superior accuracy and generalisation compared to conventional machine learning models.

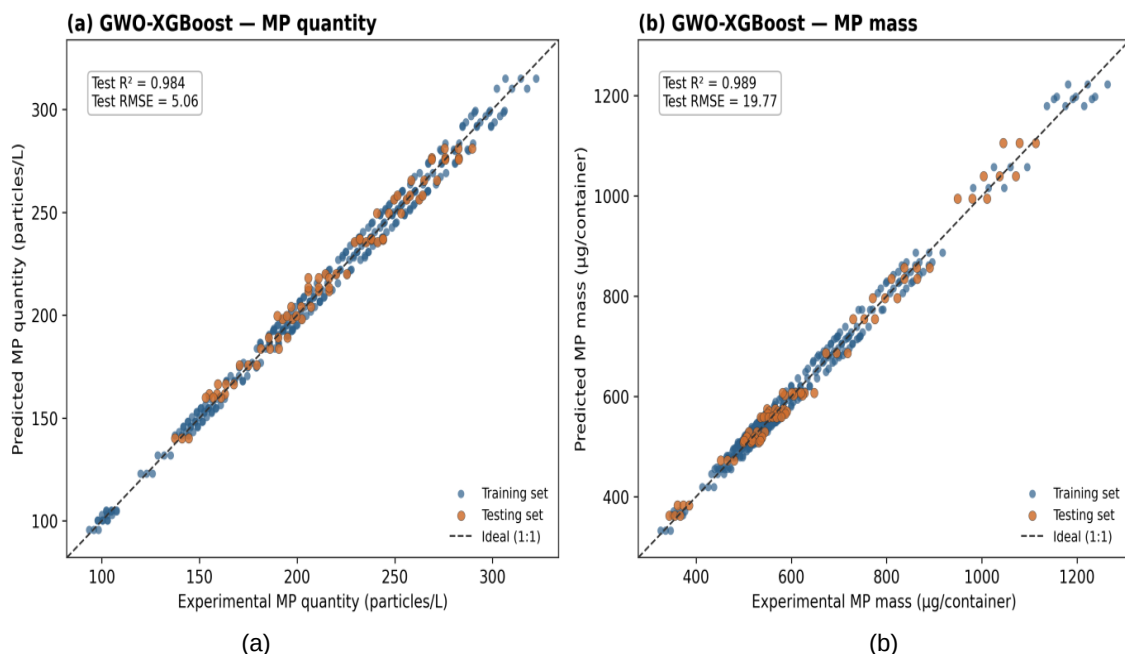


Figure 11. Predicted versus experimental values for the GWO-XGBoost model: (a) MP quantity and (b) MP mass. Training and testing points both follow the 1:1 line

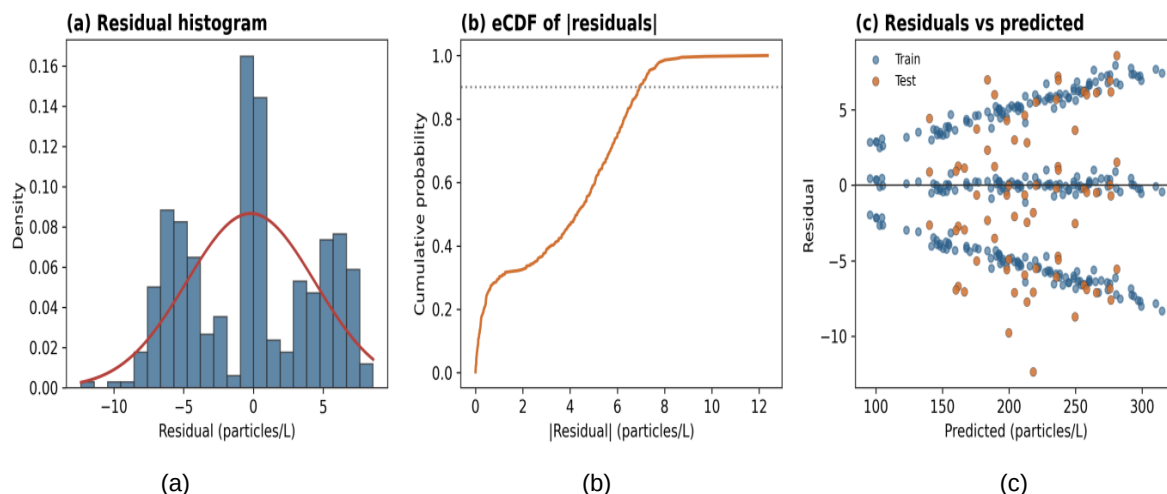


Figure 12. Residual diagnostics for the GWO-XGBoost model (MP quantity): (a) residual histogram with the fitted normal curve; (b) empirical cumulative distribution of the absolute residuals; (c) residuals versus predicted values

Drivers of release. The SHAP and permutation analyses (Figure 13, Figure 14, Table 6) revealed response-specific drivers that independently corroborate the experimental findings. For particle count, the thermal-exposure level was the

dominant control (about 45–63% of the relative importance), followed by pH and polymer type. The SHAP dependence pattern is physically sensible: high thermal exposure (L4: 90 °C, 2 h) and the acidic and alkaline extremes (pH 4 and 8) increase

release, while neutral pH (7) minimises it and the same trend measured directly in section 3.2. For released mass, polymer type became the leading driver (about 56–60%), reflecting the disproportionately large mass shed by the polystyrene container, with thermal exposure second and pH only minor. This shift in the importance ranking between the two responses is itself meaningful: the number of particles is governed mainly by how aggressively the surface is degraded (a thermal-chemical effect), whereas the mass is governed mainly by which polymer is being degraded.

Table 6. Relative importance (%) of the controllable drivers from SHAP and permutation analysis

Driver	SHAP – quantity	Perm. – quantity	SHAP – mass	Perm. – mass
pH	26.8	28.9	6.7	1.5
Thermal-exposure level	45.3	62.7	33.2	42.9
Polymer type	27.9	8.4	60.2	55.6

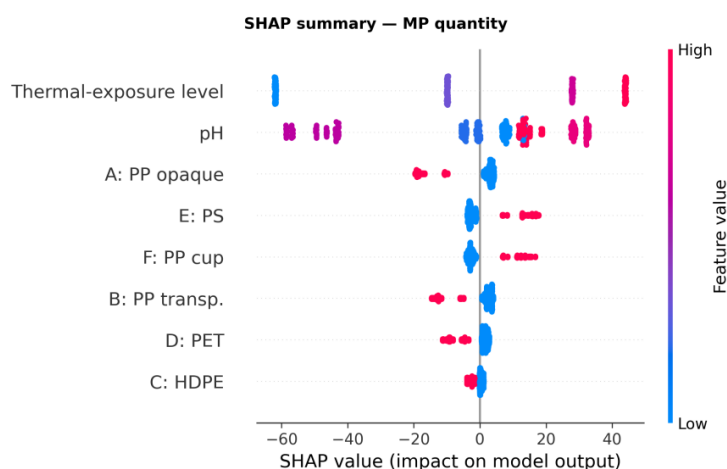


Figure 13. SHAP summary (beeswarm) plot for MP quantity, showing the magnitude and direction of each driver. Colour denotes the feature value (blue low, red high); points to the right increase the predicted release

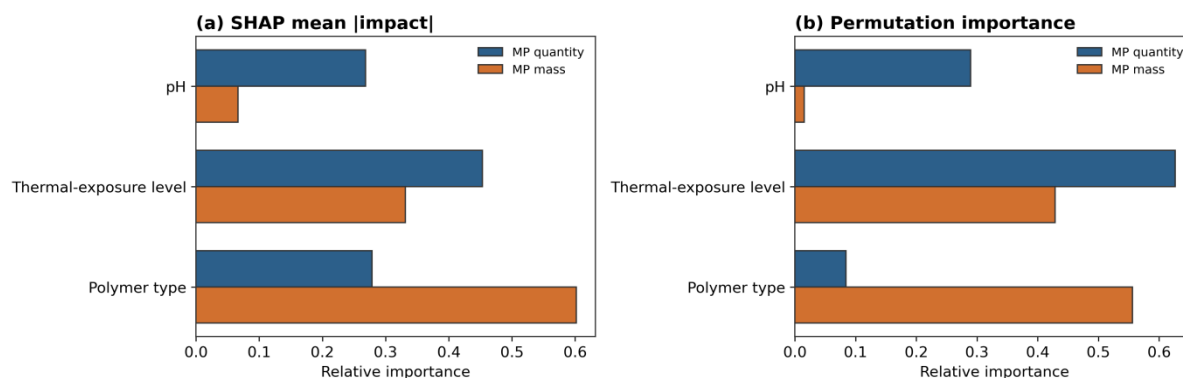


Figure 14. Relative importance of the input variables for both responses from (a) SHAP mean absolute impact and (b) permutation importance

Control of over- and under-fitting. Several safeguards were used to ensure that the reported accuracy reflects genuine generalisation rather than memorisation, which is a particular risk on a moderately sized, replicated dataset. First, the condition-level (grouped) splitting described in Section 2.6 prevents replicate leakage; its effect is quantified in **Error! Reference source not found.**

and **Figure 15c**. For particle count, a naive random five-fold cross-validation returns $R^2 = 0.986$, whereas the leakage-free grouped cross-validation returns 0.974 — an optimistic bias of about 1.2 R^2 -points that the conventional protocol would have hidden. For released mass the two estimates agree to within noise, which shows that the magnitude of the bias is response-specific and must be checked

rather than assumed. Second, the learning curve (**Figure 15a**) shows the training and cross-validation scores converging and plateauing as the sample size grows, indicating that the data are sufficient for this factor space and that the model is not simply memorising. Third, the validation curve over tree depth (**Figure 15b**) locates the under-fit

region (depth 1–2) and the over-fit region (depth ≥ 7 , where the training score stays high but the cross-validation score declines), confirming that the tuned depth lies in the stable optimum. Together with the explicit regularisation built into the boosted model (shallow trees, sub-sampling and L1/L2 penalties; **Table 5**) and the small train–test gaps in

Table 4, these diagnostics demonstrate that the final model is neither over- nor under-fit.

Table 7. Effect of replicate leakage: random versus condition-grouped five-fold cross-validation (R^2)

Response	Random K-fold R ²	Grouped K-fold R ²	Optimistic bias (ΔR ²)	
MP quantity		0.986	0.974	0.012
MP mass		0.985	0.989	−0.003

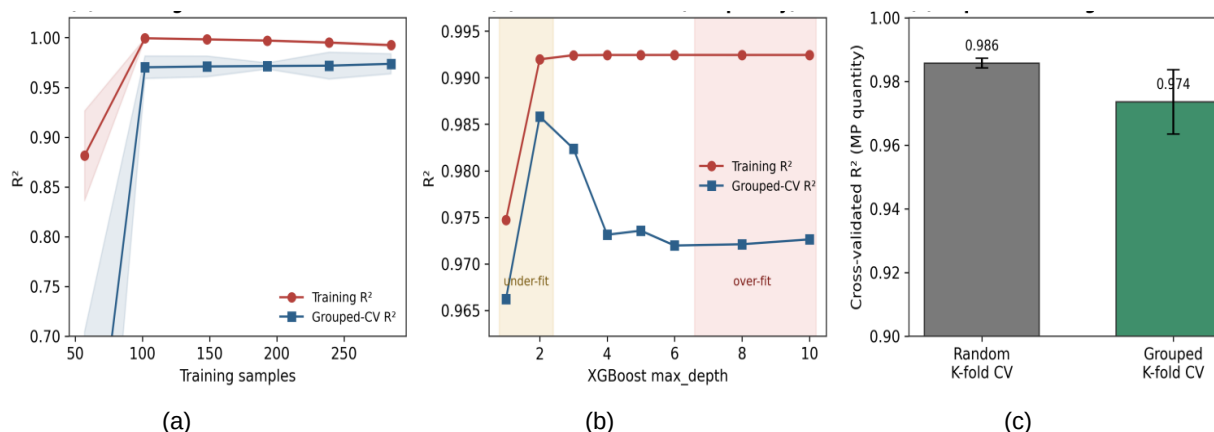


Figure 15. Diagnostics for over- and under-fitting control: (a) learning curve (training and grouped cross-validation R^2 versus training size); (b) validation curve over tree depth, with the under- and over-fit regions shaded; (c) the inflation of the cross-validated R^2 caused by replicate leakage when grouping is ignored

Figure 15 collectively confirms that the tuned GWO-XGBoost model is neither overfitted nor underfitted. The optimized tree depth lies within the stable optimal region, indicating balanced model complexity. Additionally, ignoring replicate grouping increases the cross-validated R^2 for particle count by approximately 0.012 (about 1.2%), leading to an overestimation of model performance. This highlights the importance of using leakage-free, condition-grouped validation for reliable model evaluation.

4. CONCLUSIONS AND FUTURE PERSPECTIVES

This work investigated the presence and quantification of MPs in locally available take-away and dine-in food containers. Six container types were selected after surveying several shops. The mean MP mass after NW ranged from 593.58 ± 35.26 $\mu\text{g}/\text{container}$ (container A) to 296.47 ± 32.65 $\mu\text{g}/\text{container}$ (container C); after HW from 923.75 ± 68.46 (container E) to 413.35 ± 29.12 $\mu\text{g}/\text{container}$ (container C); and after CW from 763.42 ± 42.74 (container E) to 427.84 ± 54.32 $\mu\text{g}/\text{container}$ (container B). The greatest release occurred at pH

8, 90 °C and 2 h. The polystyrene container (E) released the most MPs, because PS degrades into smaller particles through oxidation and hydrolysis under elevated temperature and prolonged exposure. FTIR confirmed that the released particles were unintentionally generated during manufacture. People may therefore unknowingly ingest considerable quantities of MPs from dine-in and take-away packaging, with possible long-term health risks.

Beyond the experimental quantification, an interpretable, leakage-free machine-learning model was developed and shown to predict MP release accurately from routine usage conditions. The GWO-tuned XGBoost model reproduced both the number and the mass of released MPs on unseen conditions with R^2 values of 0.984 and 0.989 and negligible over-fitting, and SHAP analysis identified thermal exposure as the principal control on particle count and polymer type as the principal control on released mass. This predictive map provides a quantitative basis for anticipating MP release without exhaustive testing and for prioritizing mitigation for example, avoiding prolonged hot contact and favouring polymers that

shed less mass. In addition to highlighting the extent of microplastic release from food containers, this study underscores the need for practical mitigation strategies. Consumers should reduce the use of plastic containers, particularly under high temperature, prolonged exposure, or extreme pH conditions, and instead prefer safer alternatives such as glass or stainless steel. Manufacturers are encouraged to develop more stable, low-shedding materials and adopt improved quality standards and labeling practices to inform users. Policymakers should establish stricter regulations on food-contact materials, standardize testing methods for microplastic release, and promote public awareness initiatives. Collectively, these measures can help minimize microplastic exposure from food containers and support improved environmental and public health outcomes. In practical terms, the present results translate into three concrete actions: consumers can markedly lower exposure by avoiding prolonged storage of hot or strongly acidic/alkaline foods in single-use plastic and by favouring glass or stainless steel for such uses; manufacturers can prioritise thermally stable, low-shedding polymers (avoiding polystyrene for hot-food contact) and provide clear temperature- and use-limit labelling; and policymakers can mandate standardised, condition-specific release testing of food-contact materials and set maximum-release thresholds, supported by public-awareness programmes. Because the validated model can rank these conditions without exhaustive testing, it offers a low-cost screening tool to guide such consumer choices, product design and regulation.

Future studies should assess the long-term human-health risks of chronic exposure to MPs released from food packaging under realistic use, and should examine the influence of food composition, repeated use and environmental ageing on release mechanisms.

On the modelling side, a factorial design that decouples temperature from exposure time would allow their individual effects to be resolved, and a larger, multi-source dataset spanning more polymers and brands would broaden the applicability of the model. The development of safer, biodegradable and low-emission packaging should be prioritized to minimize MP contamination and the associated ecological and public-health risks.

Competing interests

The authors declare no competing interests.

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IZVOD

MIKROPLASTIKA U AMBALAŽI HRANE: PROCENA KONTAMINACIJE U POSUDAMA ZA HRANU ZA PONETI I U RESTORANIMA I PREDVIĐANJE OSLOBAĐANJA POMOĆU MAŠINSKOG UČENJA

Mikroplastika (MP) predstavlja globalnu zabrinutost zbog potencijalnih rizika po ekosisteme i ljudsko zdravlje. Rastuća potražnja za brzom dostavom hrane u današnjem brzom načinu života povećava izloženost ljudi MP oslobođanoj iz posuda za pakovanje hrane, što predstavlja rizik za bezbednost i dobrobit hrane. Ova studija istražuje prisustvo MP u posudama za hranu koje se koriste za usluge hrane za poneti i u restoranima. Posude napravljene od različitih polimera, naime polietilen tereftalata (PET), polipropilena (PP), polietilena visoke gustine (HDPE) i polistirena (PS), analizirane su na obilje mikroplastike. Kvantifikacija je izvršena korišćenjem tri tretmana: normalna voda (NV), topla voda (VV) i hladna voda (HV). Ispitan je uticaj pH vrednosti (4, 5, 7, 8 i 9), temperature (15, 30, 45, 60 i 90 °C) i vremena izlaganja (0,5, 1, 1,5 i 2 h) na oslobađanje MP. ATR-FTIR, SEM i AFM su korišćeni za identifikaciju polimernih sastojaka i morfologije oslobođenih čestica. Prosečna obilje MP bila je $474,44 \pm 33,08 \mu\text{g/kontejneru}$ za NW, $659,48 \pm 45,04 \mu\text{g/kontejneru}$ za HW i $556,58 \pm 43,08 \mu\text{g/kontejneru}$ za CW. Najveće oslobađanje je dobijeno pri pH 8, 90 °C i 2 h izlaganja, sa prosekom od $293,98 \pm 13,86$ čestica/L. Na osnovu eksperimentalnih podataka, razvijen je okvir mašinskog učenja bez curenja za predviđanje oslobađanja MP iz uslova rutinske upotrebe. Upoređeno je pet regresionih algoritama, a ekstremni model gradijentnog pojačavanja podešen pomoću Grej Vulf optimizatora (GWO-XGBoost) dao je koeficijent determinacije od 0,984 za broj čestica i 0,989 za oslobođenu masu pod nevidljivim eksperimentalnim uslovima, sa zanemarljivim jazom između treninga i testiranja. Šepiljeva aditivna objašnjenja (SHAP) pokazala su da su termička izloženost i tip polimera dominantni kontrolisani pokretači oslobađanja. Kombinovani eksperimentalni i pristup zasnovan na podacima razjašnjava sudbinu mikroplazmatskih polimera u pakovanju za hranu i nudi praktičan alat za podršku ublažavanju i kontroli.

Ključne reči: Mikroplazmatski polimeri; posude za hranu; kvantifikacija; Furijeova transformaciona infracrvena spektroskopija (FTIR); degradacija polimera; izloženost životne sredine; mašinsko učenje; XGBoost

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