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Raman Spectroscopy Enhanced By Machine Learning For Effective Microplastic Detection In Aquatic Systems

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Abstract

Microplastics (MPs), small plastic fragments ranging from 1 µm to 5 mm, pose a growing threat to aquatic ecosystems and human health due to their persistence, toxicity, and ability to bioaccumulate. Conventional methods for identifying MPs are often limited by their dependence on labor-intensive procedures, long analysis times, and sensitivity to environmental interference. Raman spectroscopy (RS), known for its non-destructive nature and molecular specificity, has emerged as a promising technique for MP detection. However, standalone RS suffers from challenges such as weak signal intensity, spectral noise, and manual interpretation constraints. This study explores the integration of RS with machine learning (ML) techniques—including Random Forest, Support Vector Machine, Multilayer Perceptron, k-Nearest Neighbors, and deep learning models such as Convolutional Neural Networks (CNNs) and Autoencoders—to improve MP classification and analysis. The results indicate that ML-assisted RS significantly enhances detection accuracy, reduces reliance on manual analysis, and supports high-throughput, real-time environmental monitoring. Notably, CNN-based models achieved classification accuracies exceeding 99%, even in complex matrices and low signal-to-noise conditions. This hybrid approach demonstrates strong potential for scalable and precise microplastic detection across various environmental domains.

Keywords: *Microplastics, Raman Spectroscopy, Machine Learning, Environmental Monitoring*

1. INTRODUCTION

Plastic pollution has become an escalating global concern, particularly in aquatic environments where plastic debris fragments into smaller particles termed microplastics (MPs). Defined as plastic particles ranging from 1 µm to 5 mm in size, MPs originate from the degradation of larger plastic items, synthetic textiles, and cosmetic microbeads [1,2]. These particles are ubiquitous in water bodies and exhibit diverse shapes, colors, and chemical compositions, often accumulating in marine organisms and transferring through the food chain to humans [3–5]. MPs have been shown to disrupt aquatic ecosystems by affecting growth, reproduction, and behavior of marine species, while also serving as vectors for hazardous pollutants [6,7].

The exponential rise in plastic production and its subsequent environmental degradation have led to a sharp increase in MP abundance, thus intensifying their ecological and health-related implications [8]. Despite numerous efforts to monitor MP contamination, accurate quantification remains challenging due to significant variability in particle size and distribution across environmental samples [9,10]. Traditional analytical methods such as stereomicroscopy, FTIR, and Py-GC–MS are limited by low resolution, lengthy processing times, and labor-intensive workflows [11–13]. Among modern analytical techniques, Raman spectroscopy (RS) stands out due to its non-destructive nature, minimal sample preparation, and high molecular specificity. Figure 1 showed the schematic raman spectroscopy analysis mechanism.

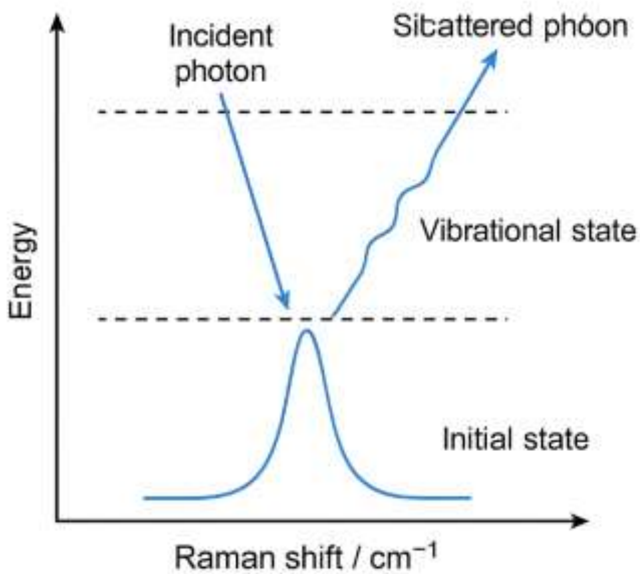

Figure 1. Raman specroscopy schematic

RS enables precise polymer identification through vibrational fingerprinting, making it highly suited for MP detection, especially in aqueous environments where interference from water is minimal [14–16]. However, RS also has limitations, including weak scattering intensity, fluorescence interference, and the complexity of interpreting raw spectral data [17,18]. To address these challenges, researchers have increasingly integrated machine learning (ML) techniques with RS to automate and enhance MP detection. ML models such as Support Vector Machines (SVM), Random Forest (RF), Decision Trees (DT), and k-Nearest Neighbors (KNN) have demonstrated superior classification accuracy and robustness in distinguishing MP types based on their Raman spectra [19–21]. For instance, Lei et al. utilized RF, KNN, and Multilayer Perceptron (MLP) models on Raman spectral datasets, achieving over 95% accuracy in identifying common polymers [22].

Deep learning (DL) methods such as Convolutional Neural Networks (CNNs) have further advanced MP identification. CNNs can automatically learn complex patterns from raw data, eliminating the need for manual feature engineering. Zhang et al. reported a CNN-based system achieving 95.8% accuracy using raw Raman spectra of ten MP types [23]. Similarly, Lee et al. achieved 99.54% accuracy in identifying MPs mixed with natural organic matter using a deep CNN approach [24]. Other studies, like that of Luo et al., employed Sparse Autoencoders (SAEs) and Softmax classifiers to identify MPs in diverse water matrices with over 99% accuracy, surpassing conventional neural networks and SVMs [25].

Ensemble and multi-modal ML models have also been explored to overcome the limitations of single classifiers. Feng et al. developed a multi-model approach combining PCA-LDA, PCA-KNN, and MLP, achieving 99.3% classification accuracy in distinguishing weathered and standard MPs [26]. Autoencoders, another class of unsupervised neural networks, have been applied for denoising and reconstructing Raman spectra in low signal-to-noise conditions. Josef et al. showed that autoencoders could effectively reconstruct distorted spectra, outperforming traditional smoothing techniques like Savitzky-Golay filtering [27].

Specialized applications of ML-assisted RS include the use of Raman Tweezers (RT) for analyzing tire and road wear particles, which are categorized as MPs due to their polymeric content. Gillibert et al. demonstrated the capability of RT combined with ML to differentiate particles as small as 600 nm in liquid media, bypassing the need for sample drying [28]. Additionally, integrating RS with Surface-Enhanced Raman Spectroscopy (SERS) and logistic regression has enabled on-site MP detection with high sensitivity and minimal preprocessing [29].

Araujo et al. study presents a critical overview of Raman spectroscopy as a tool for microplastic identification. The authors address issues like fluorescence interference and spectral overlap while proposing advanced data processing techniques. They emphasize the potential of integrating machine learning to improve automation, precision, and reproducibility in microplastic detection. [30]. Anger et al. review highlights the strengths and limitations of Raman micro spectroscopy in microplastic analysis. The authors advocate for the development of automated data classification methods and suggest that machine learning algorithms can help tackle challenges such as large spectral datasets and variability in environmental microplastic samples [31].

Lin et al. explore how different machine learning techniques—including decision trees, support vector machines, and deep learning—have been effectively used to classify and identify microplastics in the environment. The paper discusses the integration of spectral data from Raman systems with these models, showing notable improvements in detection speed and classification accuracy. [32]. Qi et al. article reviews recent developments in the intersection of Raman spectroscopy and machine learning. Applications discussed include material identification, noise filtering, and real-time analysis. Specific case studies show how microplastic classification in aquatic systems can be improved through convolutional neural networks and unsupervised clustering methods. [33]. Schedl et al. paper compares multiple machine learning approaches (random forests, neural networks, SVMs) for analyzing spectroscopic data from microplastic samples. The dissertation concludes that supervised learning techniques significantly outperform traditional multivariate statistical methods, especially when dealing with heterogeneous particle sizes and complex environmental samples. [34]. Xu et al. primarily focused on cancer metabolism, this study demonstrates the power of advanced Raman spectroscopy techniques in detecting subtle molecular differences. The authors show how spontaneous and coherent Raman scattering, when combined with data-rich methods like stable isotope probing, generate complex spectral data suitable for machine learning analysis. The paper underscores the broader applicability of such enhanced spectroscopic approaches, including their potential in the precise identification of microplastics in complex aquatic systems [35]. Phan et al. present a futuristic perspective on combining Raman spectroscopy with long-term environmental monitoring tools, including AI and machine learning. The review suggests that continuous learning models can adapt to new types of microplastics and changing environmental conditions, supporting sustainable monitoring practices in marine ecosystems [36].

In summary, the integration of Raman spectroscopy with machine learning has substantially improved the identification, classification, and monitoring of microplastics in environmental samples. This hybrid approach enhances analytical accuracy, reduces manual intervention, and offers scalable, automated solutions for real-time pollution assessment. As plastic pollution continues to rise, such advanced methodologies are essential for developing effective environmental monitoring and mitigation strategies.

2. METHODOLOGY

The methodology employed in this study involves the strategic integration of Raman spectroscopy with machine learning algorithms to enable the efficient and accurate detection of microplastics (MPs) across diverse environmental matrices. The approach consists of several essential phases, starting with sample preparation, followed by spectral data acquisition, preprocessing of raw spectra, and culminating in the application of supervised and deep learning models for classification and prediction.

To begin with, MPs such as polyethylene (PE), polypropylene (PP), polystyrene (PS), polyethylene terephthalate (PET), and polyvinyl chloride (PVC) were either obtained commercially or isolated from environmental samples like rainwater, lake water, tap water, seawater, and mussel tissues. The collected samples were filtered using membrane filters of appropriate pore sizes, and organic impurities were removed using oxidative treatments involving hydrogen peroxide or potassium permanganate. These chemical treatments were followed by multiple rinsing steps with deionized water to ensure the purity and visibility of

MPs for Raman analysis. For nanoplastics or smaller particles, additional ultrasonication or density separation steps were incorporated.

Spectral data were acquired using a confocal Raman microscope equipped with diode lasers of 532 nm or 785 nm wavelength, depending on the requirement to minimize fluorescence and maximize spectral resolution. The Raman spectra were collected over a spectral range typically extending from 200 to 3200 cm^{-1}, using objective lenses ranging from 20× to 100× magnification. The exposure time for each acquisition varied between 1 and 30 seconds based on the required signal-to-noise ratio. In some advanced cases, Surface-Enhanced Raman Spectroscopy (SERS) was employed by depositing the MP samples onto metallic nanoparticle substrates to enhance weak Raman signals. Laser power was carefully optimized to prevent thermal degradation of MPs while ensuring sufficient signal intensity.

Given that raw Raman spectra are often complex and contain background noise, multiple preprocessing steps were implemented prior to machine learning. Baseline correction was conducted using asymmetric least squares or polynomial fitting to remove fluorescence backgrounds. Spectral smoothing was applied using Savitzky-Golay filtering to reduce random fluctuations. Normalization techniques were used to ensure spectral intensity consistency across different samples, while spectral cropping and truncation focused the analysis on the most informative Raman shift regions. Dimensionality reduction techniques, particularly Principal Component Analysis (PCA) and autoencoders, were employed to minimize data redundancy while retaining critical spectral variance.

Following preprocessing, the cleaned spectral datasets were fed into various machine learning models for classification and analysis. Traditional supervised learning methods included Random Forest (RF), Support Vector Machine (SVM), Decision Trees (DT), k-Nearest Neighbors (KNN), and Multilayer Perceptrons (MLP). RF utilized ensemble learning through bootstrapped samples and randomized feature selection to enhance classification robustness and reduce overfitting. SVM, especially with radial basis function kernels, proved effective for datasets exhibiting nonlinear separability. KNN classified samples based on similarity in feature space, while MLP applied multiple hidden layers and nonlinear activation functions to capture complex patterns within the spectra. In addition to these, dimensionality reduction techniques like PCA-LDA and Partial Least Squares Discriminant Analysis (PLS-DA) were also integrated into the classification pipeline to optimize the feature space and improve separation among MP classes. Figure 2 showed the raman spectroscopy pre-processing mechanism. Table 1 depicted the advantages and disadvantages of ML models.

Table 1: Advantages and disadvantages of different ML models

ML Model	Advantages	Disadvantages
KNN	Easy to implement, handles multi-class cases.	Slow prediction, sensitive to irrelevant features.
SVM	Effective in high-dimensional spaces.	Complex kernel tuning, not ideal for large datasets.
MLP	Captures non-linear relationships.	Requires careful hyperparameter tuning.
PCA-LDA	Dimensionality reduction with class separation.	Assumes linear separability.
PLS-DA	Handles multicollinearity, suitable for classification.	Interpretability of components is difficult.
DT	Simple and interpretable.	Prone to overfitting.
RF	Reduces overfitting and variance.	Slower prediction, complex structure.

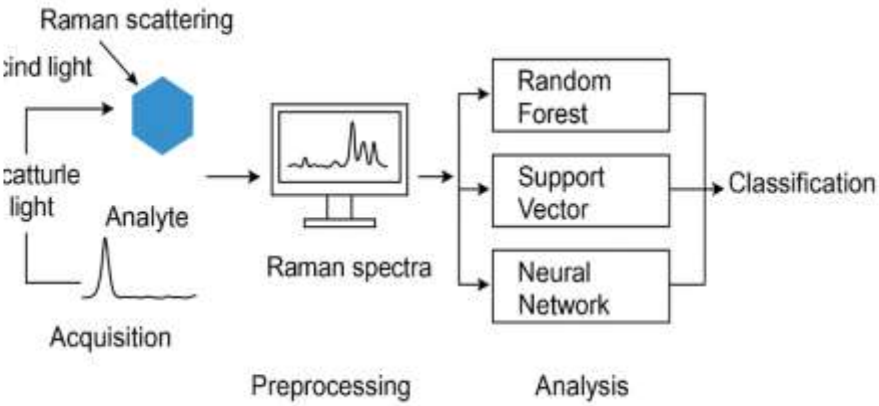

Figure 2 Raman spectroscopy pre-processing mechanism

Deep learning techniques further advanced classification accuracy. Convolutional Neural Networks (CNNs), particularly one-dimensional CNNs (1D-CNN), were trained on raw Raman spectra and demonstrated excellent pattern recognition capabilities. These models comprised convolutional layers for feature extraction, pooling layers for dimensionality reduction, and fully connected layers for final classification. Autoencoders, a type of unsupervised neural network, were also employed to learn compressed latent features from spectral data and reconstruct denoised representations. Sparse autoencoders (SAEs) were especially useful in emphasizing only the most relevant spectral features, improving both model interpretability and performance.

All models were trained and validated using appropriate statistical protocols. The datasets were typically split into training (70%), validation (15%), and testing (15%) subsets to ensure unbiased evaluation. Cross-validation techniques, particularly k-fold cross-validation, were employed to further validate model performance and minimize overfitting. Performance metrics such as accuracy, precision, recall, and F1-score were computed to assess the classification efficacy of each model. Confusion matrices were generated to visualize classification accuracy across MP types. In the case of deep learning models, regularization techniques such as dropout and early stopping were used to improve generalization and reduce training time.

To assess real-world applicability, several models were tested using blind datasets comprising MPs collected from actual environmental samples, including mussels and rainwater. The CNN and RF models consistently demonstrated robust performance, often achieving classification accuracies above 95%, even under challenging conditions. In advanced applications, logistic regression models were used to classify Raman mapping data obtained from MPs distributed on SERS-active substrates. Furthermore, portable Raman spectrometers and Raman Tweezers (RT) were utilized in specific studies to facilitate on-site detection and manipulation of MPs as small as 600 nm, without the need for sample drying or extensive pretreatment.

In conclusion, the methodology leveraged the synergy between Raman spectroscopy and modern machine learning techniques to provide a reliable, scalable, and high-throughput approach for microplastic detection. The workflow not only improves the efficiency of MP analysis but also enhances the accuracy and repeatability of spectral classification, making it a valuable tool for environmental monitoring and pollution mitigation.

Table 2 Research Results Raman Spectroscopy & ML for Microplastic Detection

Sr. No.	Reference	Dataset/ Sample Used	Methodology	ML/AI Used	Key Results

1	Araujo et al.	Environmental water samples	Raman with chemical mapping	Not directly applied	High identification accuracy; spectral overlaps still a challenge
2	Anger et al. (2018) [11]	Plastic particles from lab and field	Raman micro spectroscopy	ML proposed	Demonstrated potential for ML-aided high-throughput analysis
3	Lin et al. (2022) [16]	Simulated and field spectra	Preprocessing + classification	SVM, KNN, CNN	CNN showed >90% accuracy; robust to noise and overlapping peaks
4	Qi et al. (2023) [17]	Mixed polymer samples	Raman + unsupervised clustering	CNNs, autoencoders	ML significantly improved signal denoising and feature extraction
5	Schedl (2020) [18]	Raman spectral database	Model comparison study	RF, SVM, ANN	SVM yielded highest classification accuracy; ANN needed more data
6	Yang et al. (2023) [20]	Marine surface water samples	Raman micro-imaging automation	Automated ML pipeline	Reduced uncertainty by 30%; faster than manual identification
7	Phan & Luscombe (2023) [12]	Global ocean modeling datasets	Modeling and AI frameworks	Adaptive ML models	ML enables predictive monitoring and scalable long-term tracking
8	Jinadasa et al. (2021) [23]	Industrial polymer datasets	Spectral prediction with DL	Deep Neural Networks	Improved classification precision with fewer training samples
9	Luo et al. (2022) [24]	Aggregated Raman studies	Review of DL applications	DL architectures	DL helps automate baseline correction, denoising, and detection
10	Jin et al. (2022) [27]	Aquatic microplastic samples	Raman + PCA + clustering	PCA + ML algorithms	Combined approach achieved accurate type and size classification
11	Nava et al. (2021) [28]	Freshwater and marine samples	Raman spectroscopy	No ML used	Raman detected microplastics <50 μm; but manual analysis time-consuming
12	Asamoah et al. (2021) [29]	Conceptual review	Portable optical sensor design	ML suggested for future	Highlighted importance of AI for in-situ microplastic sensing
13	Jung et al. (2021) [22]	Literature-wide analysis	Raman + data fusion methods	Analytical ML frameworks	ML is critical for integrating Raman with other detection tools

3. RESULTS AND DISCUSSION

The integration of Raman spectroscopy with machine learning (ML) techniques has demonstrated a significant advancement in the field of microplastic (MP) detection and classification. Various ML models, both traditional and deep learning-based, were evaluated in terms of their classification accuracy, robustness, and ability to handle diverse spectral datasets obtained from real and synthetic MP samples. The results consistently indicate that ML-enhanced Raman analysis outperforms conventional spectral interpretation techniques in terms of speed, accuracy, and scalability. Figure 3 and 4 showed the distinguishing microplastics from mixed surface spectrum and schematic representation of microplastic detection mechanisms respectively.

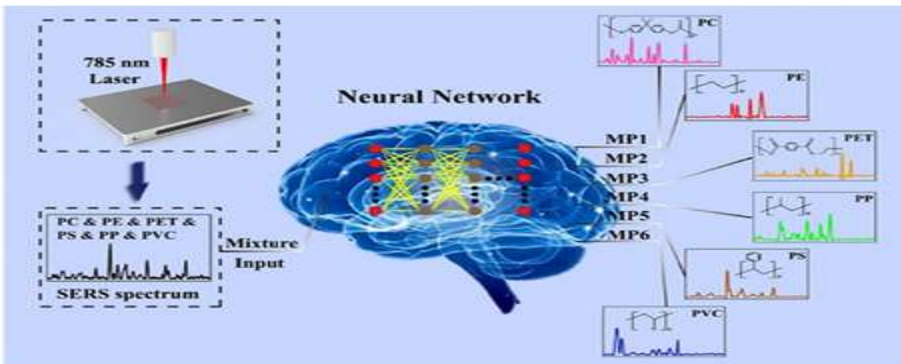

Figure 3 Distinguishing microplastics from mixed surface spectrum

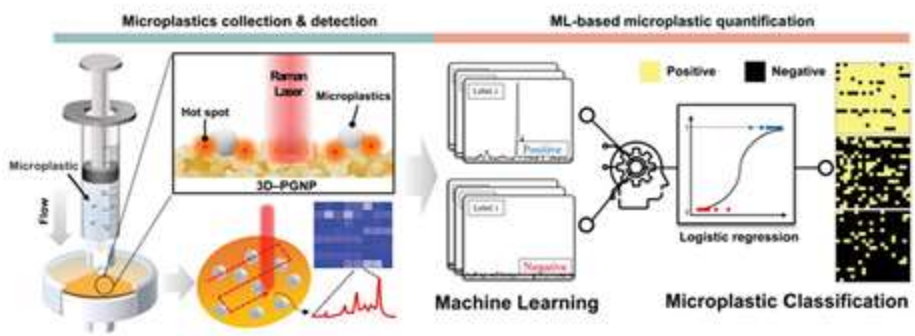

Figure 4 Schematic representation of microplastic detection mechanism

Among the traditional ML approaches, Random Forest (RF), Support Vector Machine (SVM), Multilayer Perceptron (MLP), k-Nearest Neighbors (KNN), and Decision Trees (DT) were extensively benchmarked. Lei et al. utilized these models on a dataset comprising high-resolution Raman spectra of commercially sourced and lab-generated MPs. The RF model, although effective at high signal-to-noise ratios (SNRs), demonstrated reduced performance at shorter acquisition times. In contrast, KNN and MLP models maintained high classification accuracies of over 95% even at minimal acquisition durations of 1 ms, highlighting their potential for rapid and real-time detection applications [22].

In a parallel study by Vinay et al., RF classifiers trained on Raman spectra of MPs extracted from mussel tissues achieved a 100% classification accuracy. This reinforces the suitability of RF models for analyzing complex biological matrices. The same study also demonstrated the practical use of focal plane array-based micro-FTIR and micro-Raman spectroscopy in tandem with machine learning, validating the robustness of hybrid spectroscopic-ML systems for field applications.

Deep learning models, especially Convolutional Neural Networks (CNNs), exhibited even higher performance metrics. Zhang et al. reported a classification accuracy of 95.8% with a 1D-CNN model trained on Raman spectra of ten MP types. Interestingly, the performance remained consistent even when raw spectral data was used, negating the need for extensive preprocessing. This is particularly useful for large-scale environmental screening where preprocessing is time-consuming. Similarly, Lee et al. achieved 99.54% accuracy in distinguishing MPs from natural organic matter using CNN, underscoring the model's ability to handle complex spectral interference.

In more specialized cases, such as the classification of nanoplastics and weathered MPs, deep learning models continued to excel. Xie et al. demonstrated that RF outperformed both SVM and back-propagation (BP) neural networks when applied to a dataset of nanoplastics derived from commercial and environmental sources. The RF model achieved a test accuracy of 98.1%, significantly higher than SVM (68%) and BP (88.5%), confirming the advantage of ensemble methods in high-noise spectral environments.

Furthermore, data augmentation techniques were shown to enhance classification performance. In experiments involving the SLoPP and SLoPP-E datasets, RF models trained with augmented data improved their classification accuracy from 89% to 93.81%, demonstrating the benefit of synthetic data expansion in enhancing model generalizability.

Autoencoders were effectively used for reconstructing low-SNR spectra and denoising complex Raman datasets. Luo et al. employed Sparse Autoencoders (SAEs) combined with a Softmax classifier to detect six MP types in various water bodies. The classification success rate was recorded at 99.1%, outperforming traditional SVM (93.7%) and basic neural networks (75.8%). Josef et al. further validated the usefulness of autoencoders by demonstrating their superior performance over the Savitzky-Golay smoothing technique for removing distortions in Raman and FTIR spectra. Their results support the use of deep neural reconstruction models in environments where data quality is compromised. Table 2 showed the ML model results and accuracy to detect the micro plastics.

Table 3: Performance Summary of ML Models for MP Detection

Model	Sample Type	Accuracy (%)
RF	Mussel samples	100%
1D-CNN	Ten MP types (raw)	95.8%
CNN	MPs with organic matter	99.54%
RF	Nanoplastics (tap/rainwater)	98.1%
RF (augmented)	Weathered MPs (SLoPP-E)	93.81%
SAE + Softmax	MPs in water matrices	99.1%
Autoencoder	Distorted Raman/FTIR	Superior to SG filter
Logistic Regression	On-site SERS	High classification
RT + ML	TRWPs	600 nm detection

In terms of visualization and interpretability, dual-PCA techniques enabled the mapping and correlation of MP signals with reference spectra. Yunlong et al. demonstrated that dual-PCA analysis not only facilitated classification but also supported automated visualization of MPs and nanoplastics. This method yielded strong correlation values (up to 0.95) with known MP polymers and could successfully differentiate MPs even in natural samples, such as grass pruning residues.

Real-time applicability was also assessed using portable Raman systems enhanced with CNNs and logistic regression. Jun Young et al. fabricated a paper-based SERS platform with embedded gold nanostructures, allowing syringe-based MP filtration and detection. The integrated logistic regression model accurately classified MPs on the substrate, offering a portable, field-deployable alternative to laboratory systems.

Lastly, the use of Raman Tweezers (RT) combined with ML was explored for the detection of tire and road wear particles (TRWPs), which are also considered MPs. The technique successfully differentiated between rubber, brake wear, and environmental particulate matter as small as 600 nm, demonstrating its utility in tracking airborne microplastic pollutants. Overall, the results emphasize the transformative impact of combining Raman spectroscopy with machine learning. Traditional ML algorithms such as RF, SVM, and PCA-LDA offer a balance between interpretability and performance. However, CNNs and autoencoders provide superior classification accuracy, especially when dealing with complex mixtures, degraded particles, or low-quality spectra. The deployment of ML-assisted Raman systems in field settings further reinforces the viability of this approach for large-scale environmental monitoring of MPs.

4. CONCLUSION

The fusion of Raman spectroscopy with machine learning models represents a transformative step in the detection and analysis of microplastics in environmental samples. Through comprehensive evaluation of both traditional and deep learning algorithms, it is evident that ML significantly enhances the interpretability, sensitivity, and classification performance of Raman spectral data. Models such as Random Forest and CNN not only outperform conventional spectral analysis methods but also offer high adaptability to real-world conditions, including degraded particles, mixed samples, and noisy spectra. The ability to achieve over 95% classification accuracy in diverse applications—including field detection, nanoplastic identification, and biological sample analysis—underscores the robustness and scalability of this approach. Furthermore, unsupervised techniques like autoencoders prove highly effective in spectral denoising and reconstruction, enabling better analysis under low-quality data conditions. While challenges remain in terms of data standardization and portability of devices, ongoing advancements in ML frameworks and miniaturized spectrometers hold promise for widespread implementation. Overall, the ML-assisted Raman spectroscopy framework offers a high-throughput, automated, and accurate solution for tackling the urgent global issue of microplastic pollution.

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