CLASSIFICATION OF POLYETHYLENE TEREPHTHALATE PLASTIC RESINS FOR PRODUCT USAGE USING NEAR-INFRARED SPECTROSCOPY

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ABSTRACT

Polyethylene terephthalate (PET) is a flexible material commonly used in beverage bottles, and the acceptability of its products is affected by various physical and chemical qualities. Conventional PET plastic resin classification techniques have proven to be expensive and unproductive. This work suggested a unique method for quickly and non-destructively classifying recycled PET (rPET) plastic bottles using near-infrared spectroscopy (NIRS) and machine learning (ML) specifically Waikato Environment for Knowledge Analysis (WEKA). Using selected NIRS wavelength ranges; absorbance values were generated, analyzed, sorted, and compiled into a dataset. This data sheet was then subjected to 43 classifiers using WEKA. The four-fold cross-validation with the J48 sub-classifier resulted in 100 percent accuracy, with 300 correct classified instances, zero (0) incorrectly classified instances, and a classifier operating time of 0.00 seconds. It also produced 0 percent relative absolute error and 0 percent root mean squared error. This process could significantly enhance production quality control and material assessment, allowing for more accurate matching of PET plastic resin qualities to specific product applications. This study highlighted the potential of NIRS as an effective, non-destructive method for classifying plastic resin in industrial settings.

Keywords: *Environmental stress cracking, machine learning, near-infrared spectroscopy, Polyethylene terephthalate, spectra, wavelength*

INTRODUCTION

Approximately 40 percent of the total plastic waste generated accounts for food and beverage packaging (Jeon et al., 2023), and around 500 million tons of plastic products are produced by humans annually (Carrera et al., 2022). Polyethylene terephthalate (PET) is one of the world's most widely used plastic packaging materials. PET plastic is popular in various industries due to its many desirable properties, including transparency, lightweight, shatter resistance, and easy processing (Hahladakis et al., 2018); several formulas and grades of PET plastic suit the requirements of different applications. Studies proved that several migrated substances in recycled PET (rPET) were detected as contaminants but in relatively small amounts hence the level of concern for public health is low and represents a low priority for risk management (Thoden Van Velzen et al., 2020).

PET plastic bottles come in various grades, and these differences can significantly impact the material's performance. It was observed in a study conducted that the characteristics of PET plastic bottles with high intrinsic viscosity (IV) values showed lower chances of environmental stress cracking (ESC) than PET bottles with low IV values (Alvarado Chacon et al., 2020), rPET bottles can be characterized by levels of extrusions, solid state polycondensation (SSP), hot wash and drying step, and series of chemical, physical, and biological analysis (Pinter et al., 2021); this can be a time-consuming, destructive, labor-intensive, and costly process (Franz & Welle, 2022). This is a problem for industrial quality control procedures that require quick plastic resin testing.

It is important to have techniques that can rapidly grade and categorize rPET plastic without destroying it according to key characteristics that are linked with product performance (Brouwer et al., 2020). This application has shown potential using techniques based on spectroscopy. Near-infrared spectroscopy (NIRS), which scans samples, can instantly detect chemical fingerprints (Zhu et al., 2019); this can be used to sort plastic resins, assess quality, and monitor processes. It can be a useful tool. The difficulty in interpreting complex NIR high-dimensional spectral information to classify PET plastic resins accurately has been an obstacle to commercial adoption.

Significance of the Study

By combining NIRS and WEKA, this study offers a disruptive solution to the inefficiencies of the standard rPET analysis method, which are costly, time-consuming, and damaging. This study addresses this issue by introducing quicker, less expensive, and non-damaging techniques for classifying rPET plastic bottles using NIRS (Wu et al., 2020). By accurately analyzing the quality of rPET plastic resins, it ensures the best material selection for optimal product applications, enabling enterprises to enhance production efficiency and reduce resource waste.

Better rPET plastic sorting and recycling procedures will substantially contribute to environmental and health-related programs contributing to the worldwide transition toward a circular economy and environmentally and health-friendly world by properly categorizing recovered materials and reusing effectively reducing landfill and ocean waste (Rajmohan et al., 2019). By integrating efficient, cost-effective tools, the manufacturing sector - particularly the plastic-producing industries - can contribute to environmental conservation by improving the quality of rPET materials. This study's findings, proving that NIRS and machine learning (ML) can successfully classify rPET plastic bottles, will expand the knowledge in the field and provide valuable insights for future research.

Scope and Limitations

The research focuses solely on classifying rPET plastic resins from three (3) specific types: water bottles, mixed-use containers, and flavored beverage bottles. NIRS and WEKA are the only tools and software used in this research. A total of 300 samples (100 samples per class) were used for machine learning, as the primary goal was to test and train the samples; validation will be performed in the next phase of the research. The study primarily concentrated on the technical aspects, leaving the larger economic or operational aspect for future exploration.

METHODOLOGY

Conceptual Design

Figure 1 illustrates the study's conceptual framework. The input consists of gathered samples of rPET plastic bottles from various brand names and industry usages. The samples will be placed in the NIRS system for data generation. Data analysis, data sorting, and data collection will be managed through human intervention. The final data generated from the NIRS process will be loaded into WEKA software for machine learning, where it will undergo analysis using various data mining classifiers for cross-validation. The output will be an analysis of the relationship between rPET plastic resins and product usage.

Research Procedures

Samples sourcing. The plan had been to sort 100 rPET plastic bottles each from water bottles, mixed-used products, and flavored drinks (Franz & Welle, 2020) of various brands and manufacturers into community waste bins, then to Materials Recovery Facilities (MRFs) in nearby General Trias City Province of Cavite Philippines, namely Rosario, Noveleta, Kawit, Imus, and Trece Martires. With weeks' worth of collection, the goal of obtaining 300 rPET plastic bottles from different brands and manufacturers seemed difficult to achieve. This was due to the fact that around 10 companies had monopolized the plastic bottling industry in the Philippines.

On the second attempt, the collection of rPET plastic samples was simplified and refined. The goal remained the same: to collect 100 rPET plastic samples each from water bottles, mixed-used bottles, and flavored drinks bottles, all from various brand names. However, this time the focus shifted away from the source and manufacturer. The samples were collected from MRFs and community bins, and additional products were purchased from local and international stores selling different brands. This strategy made it easier to accumulate the samples.

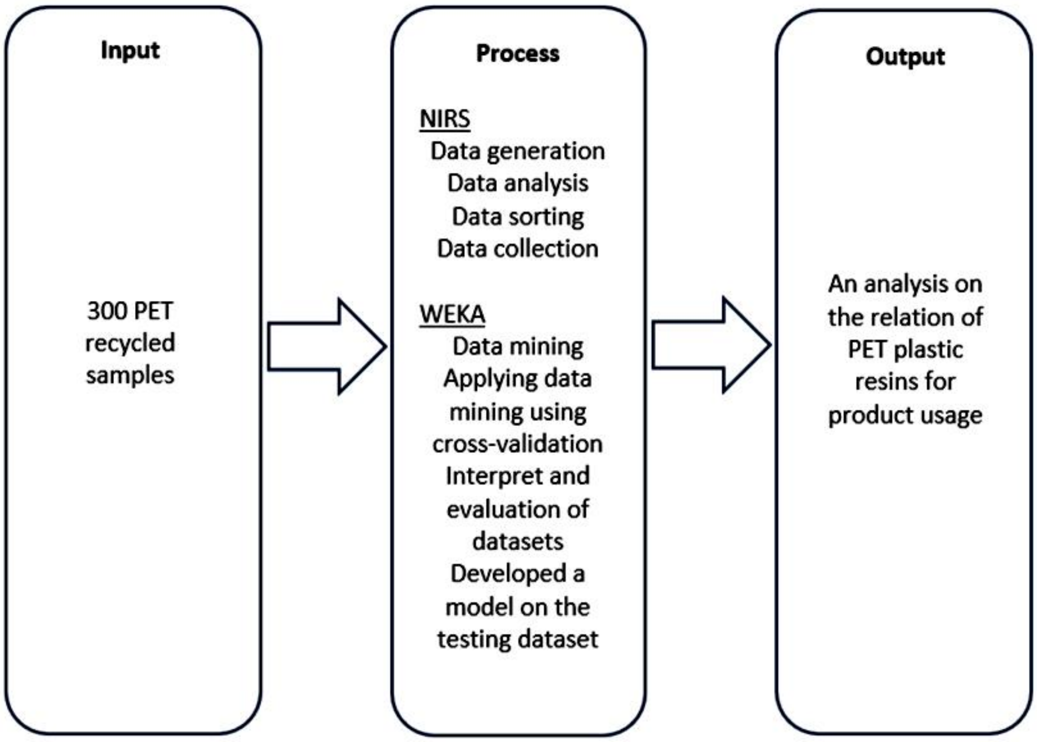

Figure 1. Conceptual framework of the study

Near-Infrared Spectroscopy. This study used the Indium Gallium and Arsenic (InGaAs)-based NIRS instrument from Cavite State University (CvSU). The apparatus, developed by scientists and engineers from CvSU, has a pending patent. It had an InGaAs NIRS sensor that could obtain absorbance data in the wavelength range from 929 nm to 1709 nm (Arboleda, 2018). In this study, the procedure involved acquiring NIR spectra from the specimens by placing each sample into the scanner of the CvSU InGaAs-based NIRS instrument one after another. It was necessary to allow the instrument to warm up for 30 minutes to ensure that both the light output of the spectrometer and the electronics were stable before collecting spectra. The spectral precision of the samples for each group was measured after the instrument had been warmed up.

Preprocessing. This was done by scanning 100 rPET plastic bottle samples from commercial water bottle samples that had been used for various types of water, including mineral, distilled, purified, infused, pH balanced, spring, and sparkling; Additionally, 100 pieces of rPET plastic bottle samples were taken from commercial mixed-used products, which had been used as containers for condiments, beauty products, sanitary items, domestic goods, and supplements. Another 100 pieces of rPET plastic bottle samples of commercial flavored drinks, including containers for juice, energy drinks, and dairy products (Eustaquio & Jr, 2020). Before scanning, the caps of all samples were removed, and the PET plastic bottles were manually crushed with feet so that the wavelength of the NIRS could properly and accurately capture the specimen compositions (Abad, 2024), and it would not just pass through the specimen as shown in Figure 2.

The total samples, consisting of rPET plastics grouped into three categories based on their product usage, were scanned using the CvSU InGaAs-based

NIRS instrument. Scanning was performed on the top, middle, and bottom parts of each specimen across the instrument's full electromagnetic range, from 929 nm to 1709 nm, at a rate of 10 minutes per specimen (Figure 3). From these scanned values, human analysis of the entire result data was conducted; the lowest wavelength range of 929 nm and highest electromagnetic range of 1709 nm were manually hand-picked for limit intention while the middle two electromagnetic ranges of 1225 nm and 1467 nm were identified through the examination of the highest data accuracy amongst others which had shown the consistent data in a linear continuity of absorbance values (Samadi et al., 2020).

Dataset. Figure 4 illustrates the NIRS data generation flow diagram of the study. It shows that SA, SB, and SC represent the names of the sample groups. The process began with NIRS, which obtained absorbance values from selected electromagnetic ranges. A total of 300 different recycled PET plastic bottle samples were used , followed by their classification. One hundred pieces of each of the following rPET bottles were used: 100 samples from commercial water bottles (SA.1-100), 100 samples from commercial mixed-used bottles (SB.101-200), and another one hundred pieces (SC.201-300) of commercial flavor drink bottles (Arboleda, 2018).

Figure 2. Crashing of PET plastic samples before performing NIRS

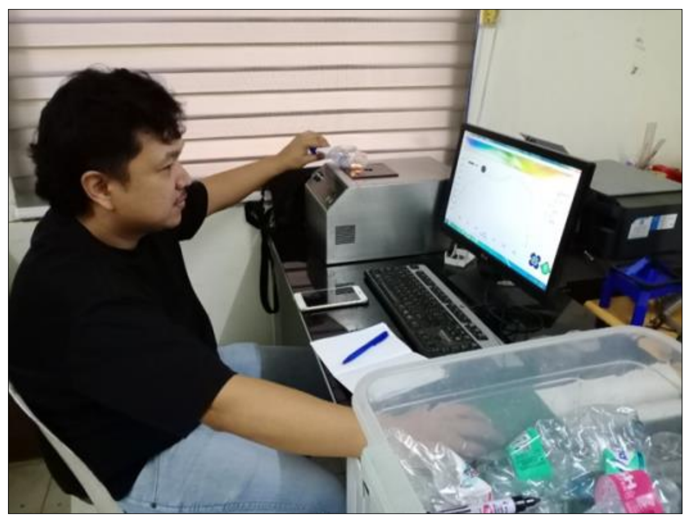

Figure 3. Conducting actual NIRS

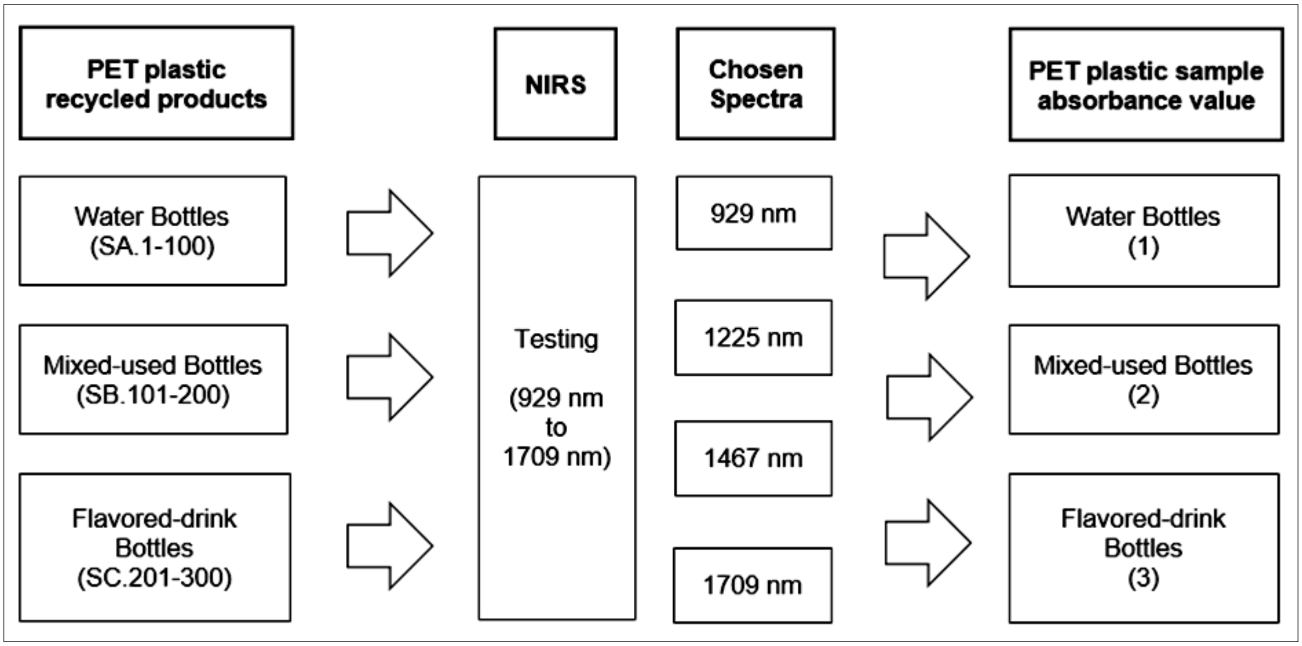

Figure 4. NIRS data generation flow diagram

The spectral results of these three groups were then tabulated in Microsoft Excel according to their respective electromagnetic ranges to identify any differences. The absorbance data for all 300 rPET plastic samples were generated, organized into tables and graphs, and subjected to human analysis, sorting, and collection.

Machine learning. The collected datasets were now loaded into WEKA (Figure 5), which will determine the most accurate classifier (Table 1), and rate the samples with the highest possibility of being classified (Saini et al., n.d.) PET plastic resin for product usage. Using the 300 samples (100 samples per class) (Hermosura et al., 2024) is sufficient for simulation; it was proven that in planning the sample size for the classification models in machine learning greater than 75 test samples per class is the reasonable precision determinant and will give a good result. However, more than 100 samples per class provided can be associated with deep learning (Neo et al., 2023) wherein models are trained using large amounts of data and algorithms (Ramos et al., 2024).

RESULTS AND DISCUSSION

NIRS Result

From the 300 specimens introduced to the electromagnetic range of 929 nm to 1709 nm, a total of 232,300 absorbance values were produced. *Table 2.* displays the absorbance values for the selected electromagnetic range; highlighting how the absorbance values from electromagnetic ranges 929 nm, 1225 nm, 1467 nm, and 1709 nm overlap.

Figure 6 created, using Microsoft Excel, shows the average absorbance values for all three groups in graph form. The graph reveals that the average absorbance of recycled PET plastic bottles containing flavored beverages was higher than that of recycled PET plastic water bottles and mixed-used plastic bottles for the electromagnetic ranges of 929 nm and 1709 nm.

No.	1: 929 um Numeric	2: 1225 um Numeric	3: 1467 um Numeric	4: 1709 um Numeric	5: **Classes** Nominal
1	0.66198	0.77345	0.77622	0.61561	Mixed us...
2	0.66198	0.77345	0.77622	0.61561	Mixed us...
3	0.66198	0.77345	0.77622	0.61561	Mixed us...
4	0.66198	0.77345	0.77622	0.61561	Mixed us...
5	0.66198	0.77345	0.77622	0.61561	Mixed us...
6	0.81061	1.00751	1.01871	0.7772	Mixed us...
7	0.81061	1.00751	1.01871	0.7772	Mixed us...
8	0.81061	1.00751	1.01871	0.7772	Mixed us...
9	0.81061	1.00751	1.01871	0.7772	Mixed us...
10	0.81061	1.00751	1.01871	0.7772	Mixed us...
11	0.78526	1.01685	1.06074	0.78974	Mixed us...
12	0.78526	1.01685	1.06074	0.78974	Mixed us...
13	0.78526	1.01685	1.06074	0.78974	Mixed us...
14	0.78526	1.01685	1.06074	0.78974	Mixed us...
15	0.78526	1.01685	1.06074	0.78974	Mixed us...
16	0.80927	1.05213	1.09434	0.79734	Mixed us...
17	0.80927	1.05213	1.09434	0.79734	Mixed us...
18	0.80927	1.05213	1.09434	0.79734	Mixed us...
19	0.80927	1.05213	1.09434	0.79734	Mixed us...
20	0.80927	1.05213	1.09434	0.79734	Mixed us...
21	0.83291	1.12324	1.16566	0.81139	Mixed us...
22	0.83291	1.12324	1.16566	0.81139	Mixed us...
23	0.83291	1.12324	1.16566	0.81139	Mixed us...
24	0.83291	1.12324	1.16566	0.81139	Mixed us...
25	0.83291	1.12324	1.16566	0.81139	Mixed us...
26	0.83291	1.12324	1.16566	0.81139	Mixed us...
27	0.84325	1.14253	1.20106	0.82972	Mixed us...
28	0.84325	1.14253	1.20106	0.82972	Mixed us...
29	0.84325	1.14253	1.20106	0.82972	Mixed us...
30	0.84325	1.14253	1.20106	0.82972	Mixed us...
31	0.84325	1.14253	1.20106	0.82972	Mixed us...
32	0.8574	1.11885	1.19319	0.85128	Mixed us...

Figure 5. The csv dataset converted to arff.

Table 1. Used Classifiers of WEKA software

Categorized Classifier	Sub-Classifier
Bayes Classifier	BayesNet NaiveBayes NaiveBayesMultinomial NaiveBayesMultinomialText NaiveBayesMultinomialUpdateable NaiveBayesUpdateable
Functions Classifier	Logistic MultilayerPerceptron SimpleLogistic SMO
Lazy Classifier	IBk Kstar LWL
Meta Classifier	AdaBoostM1 AttributeSelectedClassifier Bagging ClassificationViaRegression CVParameterSelection FilteredClassifier IterativeClassifierOptimizer LogitBoost MultiClassClassifier MultiClassClassifierUpdateable MultiScheme RandomCommittee RandomizableFilteredClassifier RandomSubSpace Stacking Vote WeightedInstancesHandlerWrapper
Misc Classifier	InputMappedClassifier
Rules Classifier	DecisionTable JRip OneR PART ZeroR
Trees Classifier	DecisionStump HoeffdingTree J48 LMT RandomForest RandomTree REPTree

The water bottles and mixed-used bottles had similar average absorbance values for the said electromagnetic ranges which fell ranging of 0.8676-1.2246 μm for 929 nm and 0.8500 and 1.3553 μm at 1709 nm respectively. Additionally, the spectra for all three groups fell within the average ranges of 1.1697-1.2927 μm for 1225 nm and 1.2227-1.3557 μm for 1467 nm.

Table 2. Range values of absorbance for the chosen NIRS electromagnetic range

ELECTROMAGNETIC RANGE	PET RECYCLED PLASTIC		
	WATER BOTTLES[A]	MIXED-USED BOTTLES[B]	FLAVORED-DRINK BOTTLES[C]
	WAVELENGTH IN MICROMETERS (MM)		
929 nm[d]	0.8959 – 0.9746	0.6119 – 0.9561	0.8774 – 1.4150
1225 nm	1.2239 – 1.3647	0.7734 – 1.3075	0.9413 – 1.3755
1467 nm	1.2822 – 1.4269	0.7762 – 1.3591	1.0053 – 1.4335
1709 nm[e]	0.8793 – 0.9494	0.6156 – 0.9279	1.0706 – 1.4775

[a] Bottles that contained water like distilled, purified, infused, alkaline, sparkling, and spring or mineral.

[b] Bottles that contained soap, detergents, oil, condiments, acids, and beauty and supplement products.

[c] Bottles that contained beverages like juices, dairy milk, soda, soft drinks, tea, energy drinks, and ready-made coffee.

[d] Minimum wavelength of Cavite State University's (Indang, Cavite) indium gallium and arsenic (InGaAs)-based near-infrared spectroscopy.

[e] Maximum wavelength of Cavite State University's (Indang, Cavite) indium gallium and arsenic (InGaAs)-based near-infrared spectroscopy.

NIRS - near-infrared spectroscopy is an absorption spectroscopy technique that determines the chemical composition of a molecule or solution by measuring how much near-infrared light it absorbs. It operates in the near-infrared electromagnetic spectrum.

PET - polyethylene terephthalate is a polyester-based thermoplastic resin that is widely employed in a variety of applications, including synthetic fibers. Depending on the manufacturing and heating history, it can exist as either a transparent or semi-crystalline polymer.

μm - a symbol of micrometers. In near-infrared spectroscopy, the wavelength is generally reported in micrometers (previously termed "microns"), which corresponds to the electromagnetic range of 780 nm to 2500 nm.

WEKA Result

Figure 7 shows the representation of the chosen NIRS spectra for absorbance value and classes, with red, blue, and cyan representing the three groups of PET plastic resins (100 samples per class). Each classification value is assigned a color by an algorithm. If the class value has two categories, the distribution is represented in two colors.

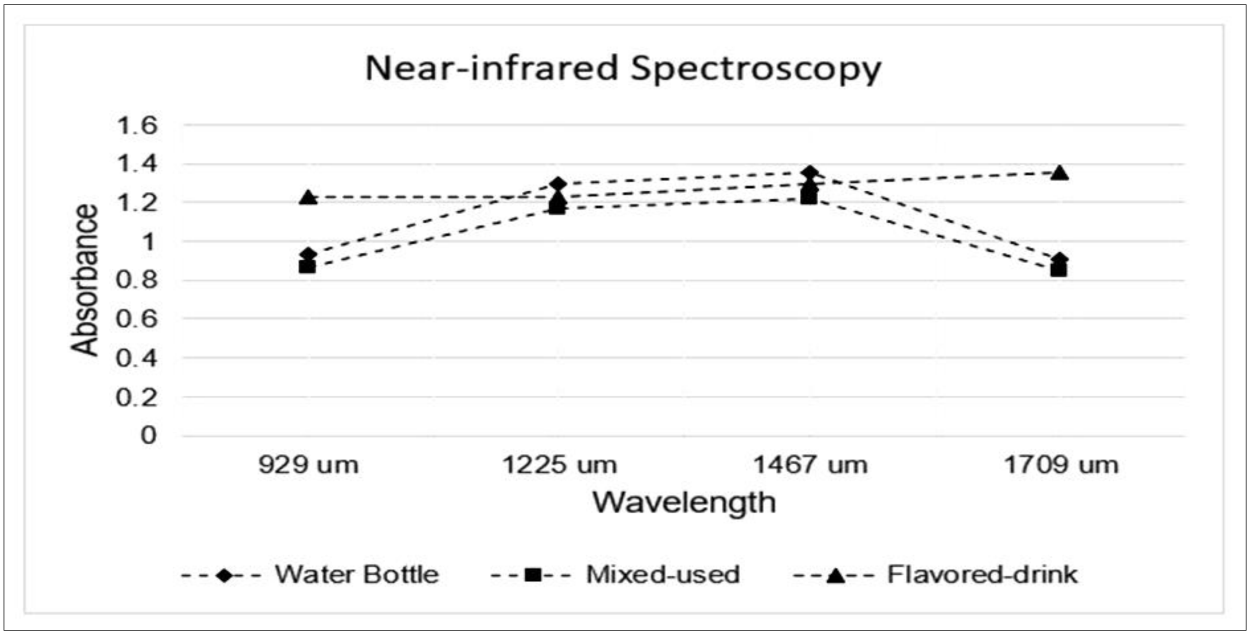

Figure 6. Average spectra of PET recycled plastic water, mixed-used, and flavored drink bottles

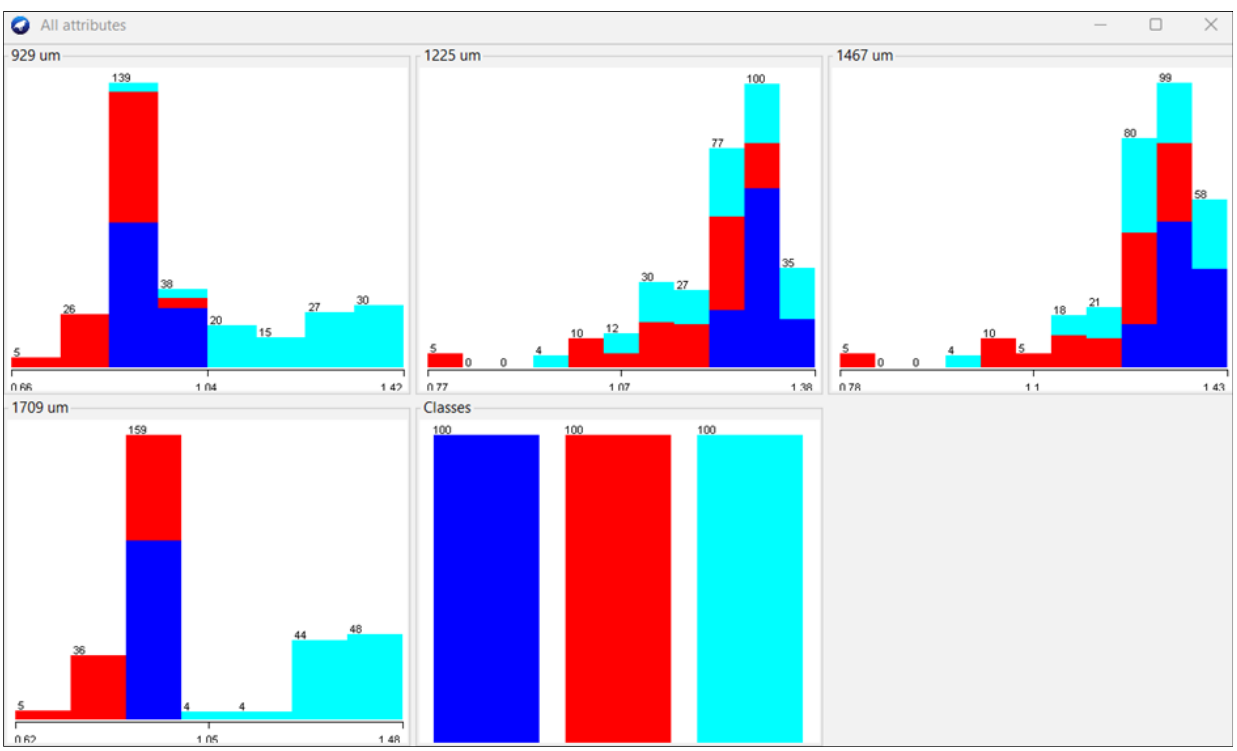

Figure 7. Visualization of PET plastic resin and product usage

Table 3 presents the complete simulation result of the four-fold cross-validation using different classifiers in WEKA. The highlighted sections of the table show that "IBk", "RandomizableFilteredClassifier", "J48", and "RandomTree" all achieved a 100% accuracy rate, with 300 correct classified instances and 0.00 seconds of classifier operating time. These four results were first evaluated by a human analyst, who filtered out other classifications based on their percent relative absolute error, and percent root mean squared error. As a result, 2 out of 4 were eliminated.

Under the Tree Classifier, "J48", and "RandomTree" both had 0% relative absolute error and 0% root mean squared error, making them stand out compared to "IBk" and "RandomizableFilteredClassifier", which had non-zero results.

Table 3. Total accuracy and estimated time of the used classifier in WEKA

Categorized Classifier	Sub-Classifier	Correctly Classifi	Accuracy Rate (%)	Estimate Time (sec)	Incorrectly Classified Instances	Accuracy Rate (%)	Relative Absolute Error (%)	Root Relative Squared	Total Number of Instances	
Bayes Classifier	BayesNet		90.33	0.01						
	NaiveBayes		84.00	0.01						
	NaiveBayesMultinomial		81.67	0.00						
	NaiveBayesMultinomialText		33.33	0.00						
	NaiveBayesMultinomialUpdateable		81.67	0.00						
	NaiveBayesUpdateable		84.00	0.00						
Functions Classifier	Logistic		86.67	0.04						
	MultilayerPerceptron		87.67	0.11						
	SimpleLogistic		87.33	0.12						
	SMO		85.00	0.05						
Lazy Classifier	IBk	300	100.00	0.00	0	0.00	0.5859	0.6616	300	
	Kstar		98.67	0.00						
	LWL		81.00	0.00						
Meta Classifier	AdaBoostM1		90.00	0.01						
	AttributeSelectedClassifier		100.00	0.02						
	Bagging		99.33	0.01						
	ClassificationViaRegression		97.00	0.08						
	CVParameterSelection		33.33	0.00						
	FilteredClassifier		92.67	0.00						
	IterativeClassifierOptimizer		98.33	0.21						
	LogitBoost		98.33	0.01						
	MultiClassClassifier		86.00	0.01						
	MultiClassClassifierUpdateable		83.00	0.03						
	MultiScheme		33.33	0.00						
	RandomCommittee		100.00	0.02						
	RandomizableFilteredClassifier	300	100.00	0.00	0	0.00	0.5848	0.6611	300	
	RandomSubSpace		98.00	0.01						
	Stacking		33.33	0.00						
	Vote		33.33	0.00						
	WeightedInstancesHandlerWrapper		33.33	100.00						
Misc Classifier	InputMappedClassifier		33.33	0.00						
Rules Classifier	DecisionTable		94.00	0.01						
	JRip		98.00	0.02						
	OneR		95.00	0.00						
	PART		100.00	0.01						
	ZeroR		33.33	0.00						
Trees Classifier	DecisionStump		66.67	0.00						
	HoeffdingTree		83.67	0.01						
	J48	300	100.00	0.00	0	0.00	0.0000	0.0000	300	(Size of the tree: 19)
	LMT		100.00	0.05						
	RandomForest		100.00	0.03						
	RandomTree	300	100.00	0.00	0	0.00	0.0000	0.0000	300	(Size of the tree: 21)
	REPTree		99.67	0.00						

To determine the most qualified classifier, a second human evaluation was conducted to compare “J48” and “RandomTree”. Technically, the main between their output was the “size of the tree.” In “Tree Classifier”, the size of the tree refers to the total number of nodes, including both leaf nodes and internal nodes. A larger tree typically indicates greater model complexity, which may fit the training data well but risks overfitting. In contrast, a smaller tree size indicates simplicity and interpretability but may underfit the data. A smaller tree size was selected to ensure model simplicity and interpretability while maintaining acceptable classification performance and reducing the risk of overfitting. This evaluation concluded that the Tree classifier – “J48” sub-classifier was the best among all the classifiers.

Detailed Accuracy by Class Using WEKA

Figures 8 and 9. provide the classifier output of the Tree classifier– “J48” sub-classifier’s four-fold cross-validation. They display the classifier model (full training set) with verified cross-validation results, showing full class accuracy of 100% in 0.00 seconds taken to build the model for a total of 300 instances. The figures also present the stratified cross-validation summary and the confusion matrix.

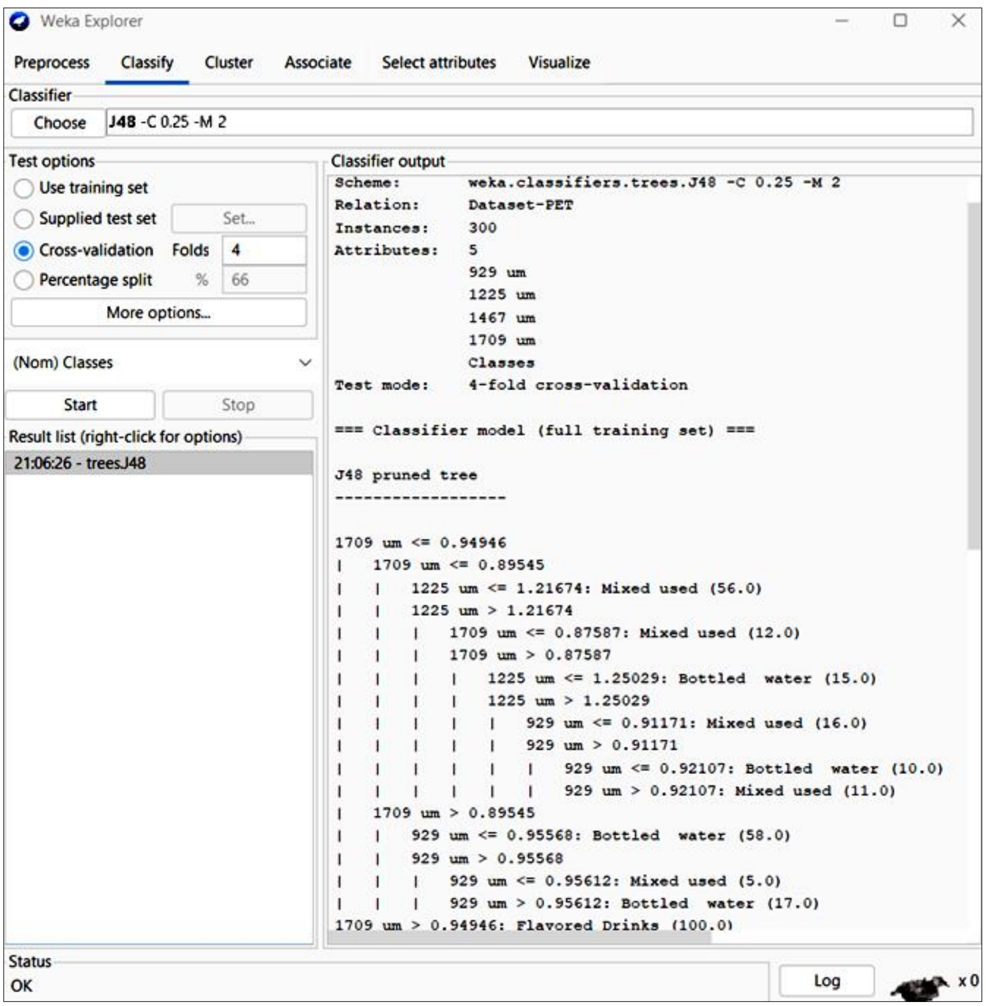

Figure 8. Cross-validation of Tree Classifier - J48 Sub-Classifier (1)

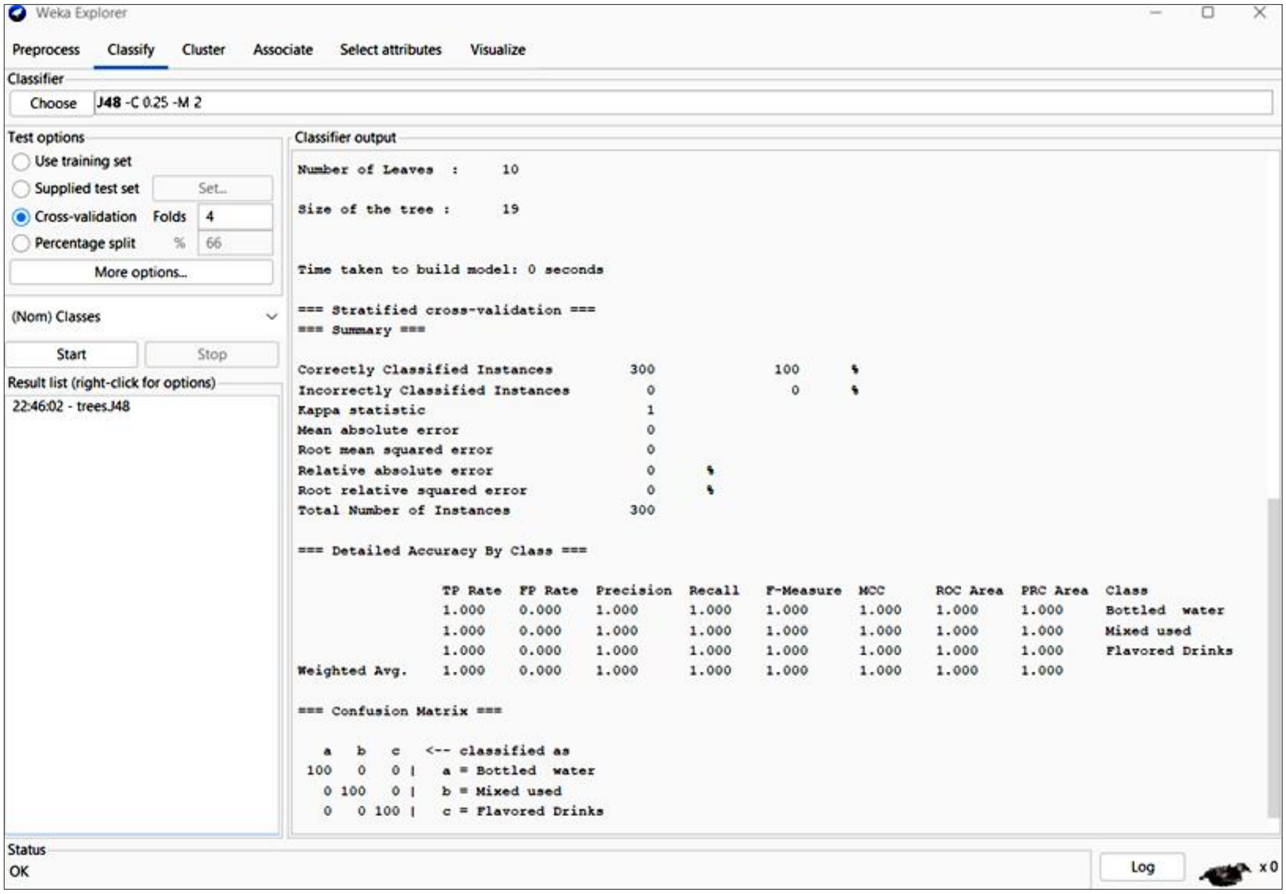

Figure 9. Cross-validation of Tree Classifier - J48 Sub-Classifier (2)

The dataset is accurate across all classes, achieving a weighted average of 1.0 in precision, true positive rate (TR Rate), Recall, F-Measure, MCC, ROC Area, and PRC area with a weighted average of zero (0) for the false positive rate (FP Rate). The stratified cross-validation summary shows 100% accuracy with 100 correctly classified instances and zero (0) incorrect classified instances, resulting in a 0% inaccurate rate. The Kappa statistic value was 1.0, and both the mean absolute error and root mean squared error are zero (0). Additionally, the relative absolute error and root relative squared errors were both 0%.

Figure 10 depicts a visual representation of the plot matrix based on the selected classifier's visualization. Blue represents plastic water bottles; red represents mixed-used plastic bottles, and cyan represents flavored drinks plastic bottles. Although there were instances where the values of 2-3 classes were overlapped, the Tree classifier–J48 sub-classifier was still able to detect the accuracy.

CONCLUSION, RECOMMENDATION, and FUTURE WORK

This paper demonstrated that NIRS, combined with machine learning (ML) cross-validation through classifiers, can be utilized to accuratealy and quickly classify rPET plastic resins based on key quality criteria. NIR fingerprints can effectively capture the inherent chemical and physical variations in rPET. Based on the results, it can be concluded that the 300 samples (100 samples per class) are sufficient to test its accuracy in ML using WEKA. Since ML focuses on training and testing samples to determine accuracy rates, a separate validation is not necessary for this study. Validation should only be applied

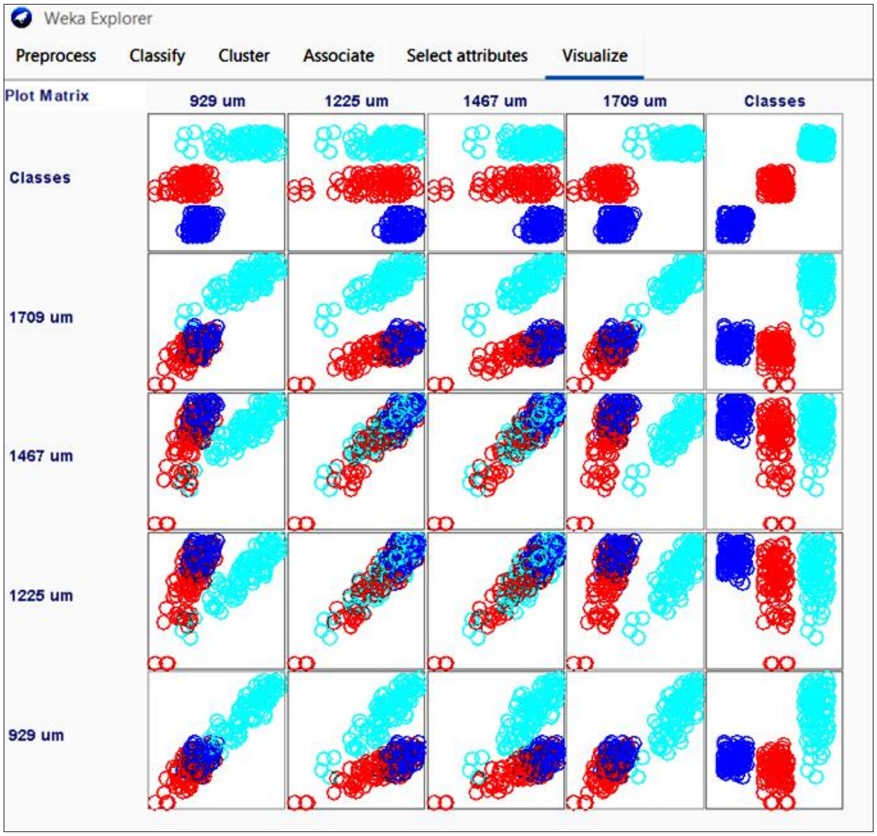

Figure 10. Plot Matrix of Tree Classifier – J48 Sub-Classifier

if the results are to be scaled up for broader application.

Using NIRS, it was possible to identify and categorize unknown spectra, with the categories of plastic resins being correlated with performance criteria and product requirements. This enables efficient mapping of plastic resin categories to application requirements, ensuring consistent product quality.

The concepts and methods developed in this paper provide a solid foundation for inline analysis of product quality and PET plastic resin across the entire value chain. This scientifically proven methodology allows producers, converters and even recycling companies to characterize rPET plastic bottles, offering a reliable way to compare material characteristics with usage guidelines, refinement processes, and industrial applications.

It is also recommended that NIRS scanners be developed, implemented, and used to identify bulk recycled plastics in real-time during sorting at accredited material recovery facilities (MRF). In the future, comparing the spectra of water bottles, mixed-used bottles, and flavored drink bottles using NIRS would allow for more accurate segregation and categorization, ensuring proper sanitation and safety. Additionally, further legislation is needed to ensure the identification of virgin PET plastic bottles (vPET), rPET plastic bottles, and mixed PET plastic bottles (mPET) which contain varying percentages of rPET and vPET. Specifications and labeling that indicate the number of times a plastic bottle has been recycled should also developed to better educate and inform end.

Although PET plastics can be recycled as many times, it is essential to establish limits on how many times rPET and/or mPET can be recycled. This would ensure that PET products have proper life span. Retired plastic PET products can be re-purposed for non-consumption-related applications, such as garments, grocery bags, school supplies, and other suitable uses.

Lastly, patenting the methodology in this study could take this research to the next level. With the proper support and network, this could become a significant advancement in the industry.

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