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Research Article

Discrimination and source correspondence of cling film using ATR-FTIR spectroscopy and chemometrics techniques

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Abstract
In forensic investigations, cling film is often used by drug dealers to wrap drugs on illegal activities. Subsequently, the identification and source correspondence of cling film has become increasingly important for investigators to establish a potential link between a suspect to the crime. In this work, a non-destructive technique of ATR-FTIR spectroscopy was used with two chemometric methods of Principal Component Analysis (PCA) and Hierarchical Clustering Analysis (HCA) to discriminate and identify the source correspondence of 81 samples of two types of cling film (PVC and LDPE). The PCA chemometric model after non-destructive ATR-FTIR spectroscopy effectively segregated and classified the two cling film classes according to types. Furthermore, HCA was performed to investigate the structure-spectral property relationship between both types of cling film. It successfully distinguished the samples into two classes (Group 1 = LDPE samples and Group 2 = PVC samples), aligning with the PCA analysis results. This study further explored whether the trained PCA model can be extended to simulated forensic case scenario and found that all seven unknowns were correctly predicted to their original source. The findings suggest that non-destructive ATR-FTIR spectroscopy and the two chemometric methods (PCA and HCA) can be essential tools for the discrimination of cling film and source correspondence in real forensic scenario.

Keywords: analytical chemistry, chemometrics, cling film, attenuated total reflectance infrared spectroscopy, principal component analysis

Introduction

Cling film, or cling wrap, is commonly used to wrap foodstuff. Within the forensic perspective, cling film is utilised to wrap illicit drugs, electric wires, and explosive devices. Subsequently, it can be used to establish a link between crime and suspects in forensic investigations. The composition of polymer-based cling film commonly consists of polyvinyl chloride (PVC) spiked with plasticisers (i.e. adipates, citrates, phthalates). However, the usage of low-density polyethylene (LDPE) has raised global health concerns, particularly regarding its impact on humans' daily life [1-2]. In forensic examinations, both destructive and non-destructive techniques can be employed to detect the composition of cling film [1-2].

Recognising the evidential value of cling film, various forensic studies have been conducted on cling film using destructive techniques such as UV–Vis Spectroscopy [3], gas chromatography mass spectrometry (GC–MS) [4], and Differential Scanning Calorimetry (DSC) [5]. However, all these are destructive techniques which can affect the integrity of samples. Therefore, the ATR-FTIR spectroscopy technique should be implemented in forensic analysis, including the examination of cling film. Such technique is rapid, non-destructive, sensitive, free from sample preparation, and requires a sample in minute portion, thereby prompting its utilisation in numerous analyses of trace evidence such as eyeliner [6], foundation cream [7], and fingernail clippings [8].

The promising accessibility of statistical software today has raised research interest in the application of chemometrics across disciplines [9-11]. PCA is an unsupervised chemometrics technique that naturally clusters and links groups of similar attributes (or variables) without the need for prior training of the mathematical algorithms [6-11]. It segregated the samples by clustering similar cling film together based on the common traits identified. The parameters were examined using a scree plot to determine the number of significant PCs in the dataset based on significant data variance. A score plot was used to display the clustering outcome, where samples with similar scores were placed close to each other, while those with dissimilar scores were located apart [6-11].

Whilst HCA is an unsupervised chemometric approach that requires no human definition of sample categories [6,7]. It improves the accuracy of analytical techniques by converting high-dimensional data into spectral data, where chemometrics can extract similarities and differences from the latter into more concise data for better interpretation [6,7]. Therefore, the purpose of this study is to extend the application of non-destructive ATR-FTIR spectroscopy combined with two approaches of multivariate statistical analyses for the discrimination of PVC and LDPE cling films. The first approach employed both PCA and HCA to assess the pattern between two types of cling films, while the second approach explores whether PCA will remain effective in source correspondence of unknown for application in forensic practice.

Materials and Methods

Sample collection

81 cling films representing nine brands (9 samples per brand) of similar batch number and production date were purchased from different outlets of the same store in Selangor, Malaysia (**Table 1**). Precautionary steps were taken by wearing personal protective equipment and gloves to avoid any contamination during sample analysis. Furthermore, careful checking was done prior to sample analysis to avoid any twisting or wrinkling on the cling film.

ATR-FTIR analysis

Visual inspection of the ATR-FTIR spectra ranging from 4000 to 400 cm^{-1} was performed to detect any similarities and differences in the cling film. The presence of peaks in the functional group was observed and recorded in the ATR-FTIR analysis. The analysis was performed using an IR Affinity-1 Spectrometer (Shimadzu, Japan) with DLATGS detector, temperature control (22 °C), and built-in Spectrum software version 5.0.1.0021 (Shimadzu, Japan). The condition parameter was used at a resolution of 4 cm^{-1} resolution with 16 scans in the range of 400-4000cm^{-1}. Prior to analysis, the sample was cleaned using methanol (Sigma-Aldrich (Germany) to eliminate the surface contamination on ATR- FTIR crystal. Background scanning was performed without placing any sample before the sample analysis. All data pre-processing was performed using baseline-corrected via the Spectrum software. To ensure the repeatability and reproducibility of the ATR-FTIR spectrometer, ten measurements were recorded at the same location in one cling film. Relative standard deviation (%) was measured during the assessment of repeatability and reproducibility of ATR-FTIR.

Data pre-processing

The chemometrics analysis was preceded by further data pre-processing using normalisation techniques on ATR-FTIR spectra to reduce potential noise in the sample and human error during sample collection [7-8]. The method reduced any interference that could affect the separation result of the chemometric method (PCA and HCA).

Principal component analysis (PCA)

In this study, spectral data were classified and discriminated using PCA by utilising the Minitab 19 statistical analysis software (USA). In PCA analysis, the dataset consists of 857 columns and 81 rows. The independent variables (IV) were the 857 columns representing wave numbers between 400 and 4000 cm^{-1}, whereas the dependent variable (DV) was the type of the cling film (PVC and LDPE).

Table 1. Brands and types of cling film samples used in the study

No.	Brand	Type	Roll Length (m)	Manufacturer	Width (cm)	No. of Samples
1.	Ezy	PVC	30 m	China	30 cm	9
2.	Wrapit	PVC	30 m	China	30 cm	9
3.	Kardli	PVC	30 m	China	30 cm	9
4.	Crystal	LDPE	30 m	Malaysia	30 cm	9
5.	Hagen	LDPE	30 m	Malaysia	30 cm	9
6.	Sun Fresh	LDPE	30 m	Malaysia	30 cm	9
7.	Kobens	LDPE	30 m	China	30 cm	9
8.	Best	LDPE	30 m	China	30 cm	9
9.	Kitchen PE	LDPE	30 m	Malaysia	30 cm	9

Hierarchical clustering analysis (HCA)

In this study, HCA was performed across all 81 cling film samples to investigate the relationship between the two types of cling film (i.e., PVC and LDPE). The clustering strategies in HCA involving single, complete, and average linkages were assessed to obtain the best separation of data. Once the clustering strategies were evaluated, the dimensions of large original variables could be transformed into new dimensions called dendrogram [10]. Similarly, HCA was performed using the Minitab 19 statistical analysis software (USA).

Results and Discussion

Visual inspection of ATR-FTIR

Figure 1 shows the IR spectrum of the LDPE cling film. Examination of the IR spectrum revealed unique structural variation peaks at 3323 cm^{-1}, indicating intermolecular hydrogen bonding due to the hydroxyl functional group. C=O stretching carbonyl functional group indicated significant absorption peaks at 1610 cm^{-1} and 1720 cm^{-1}. The values observed on the IR spectrum were C-H bending bands at 1499 cm^{-1} and 1320 cm^{-1} [12, 13]. The peaks occurring at 660 cm^{-1} and 720 cm^{-1} are associated with C=C bending and C-Cl (aliphatic) group, respectively [12,13]. **Figure 2** shows the IR spectrum of the PVC cling film. The samples revealed that the peak at 3324 cm^{-1} reflects hydroxyl functional group, while the absorption bands at 2480 cm^{-1} reflect the C=C or alkene group [12, 13]. Dioctyl adipate (DOA) and dioctyl phthalate (DOP), which were added as plasticisers [12, 13], exhibited absorption peaks at 1720 cm^{-1} and 1520 cm^{-1}, respectively. However, the next section will provide proof of concept study on using chemometrics technique to differentiate cling film samples that might be beneficial if we have some limitations on using visual inspection alone. The RSD (%) value on ATR- FTIR peaks obtained from cling film were less than 2% (RSD < 2%), indicating that the ATR-FTIR analyses exhibited good repeatability and reproducibility studies.

PCA

Figure 3 displays the scree plot derived from the ATR-FTIR dataset of the two types of cling film. A scree plot identifies the number of significant PCs in the dataset to capture significant data variance. Most variations in the dataset can be explained by the first ten PCs, with PC1 and PC2 capturing the first and second most maximum variability. The scree plot indicates that PC1 and PC2 are sufficient to describe the majority of data structure, allowing for dimension reduction in PCA analysis. Furthermore, there is a sharp decline in variance proportion after PC2, indicating minimal contribution from further PCs (**Figure 3**).

Apart from the scree plot, the data visualisation in PCA (PC1 vs. PC2) was plotted through score plots in two dimensions (2D). The 2D score plot visualised the relationship between samples defined by the first two PCs (i.e., PC1 and PC2) (Figure 4). Both PCs explained the total variance of 90.2% (PC1 = 83.1% and PC2 = 7.1%). The LDPE (Group 1) and PVC samples (Group 2) formed a cluster in one region on the left and right sides, indicating significant differences in their chemical compositions as observed in the ATR-FTIR spectra (Figures 1 and 2). It is interesting to note that the groupings evident in the 2D PCA score plot reflect the direct visual inspection under consideration, enabling the discrimination of the PVC and LDPE samples according to their types. The analysis was further verified using a paired t-test analysis to assess differences between the PVC and LDPE samples. The results indicate statistically significant differences between both cling film types with $p > 0.05$. The reasons use of a paired *t*-test because PVC and LDPE spectra were obtained under identical measurement conditions, allowing direct pairwise comparison and minimisation of instrumental variability in ATR- FTIR analysis. This approach enhances statistical sensitivity when validating PCA-based discrimination.

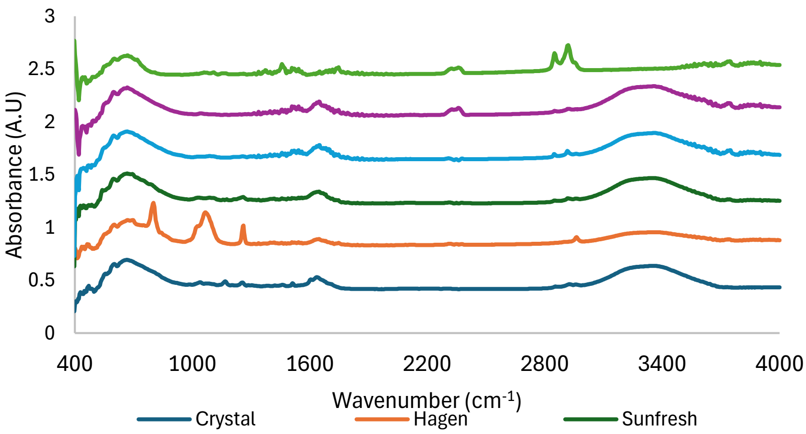

Figure 1. ATR-FTIR spectra of LDPE cling films

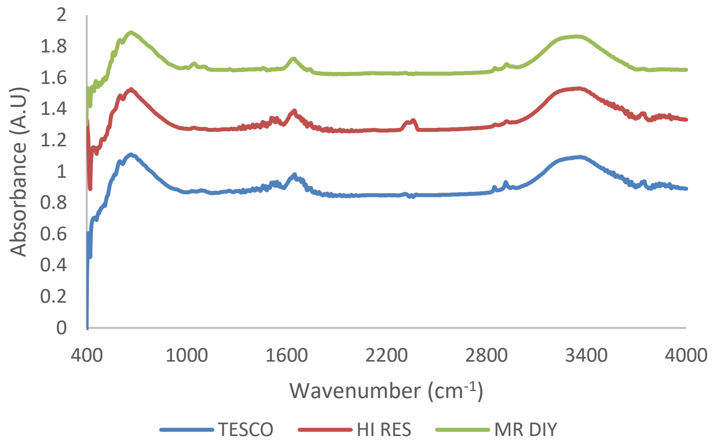

Figure 2. ATR-FTIR spectra of PVC cling films

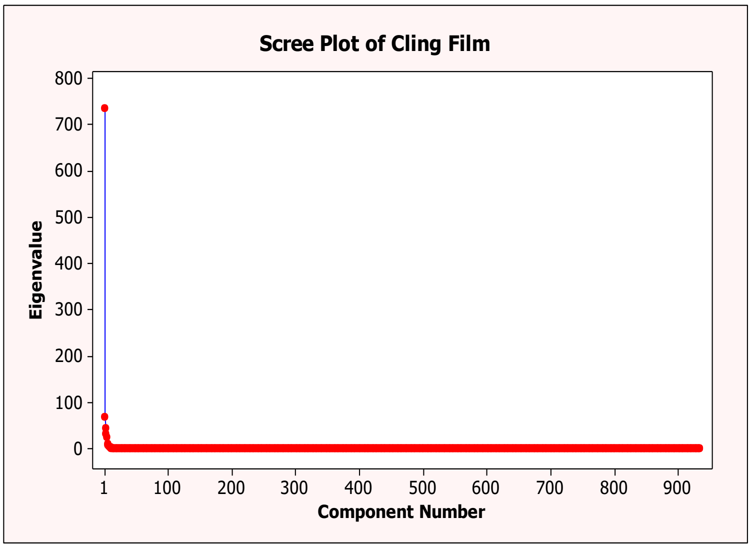

Figure 3. Scree plot to choose the number of PCs used in PCA analysis

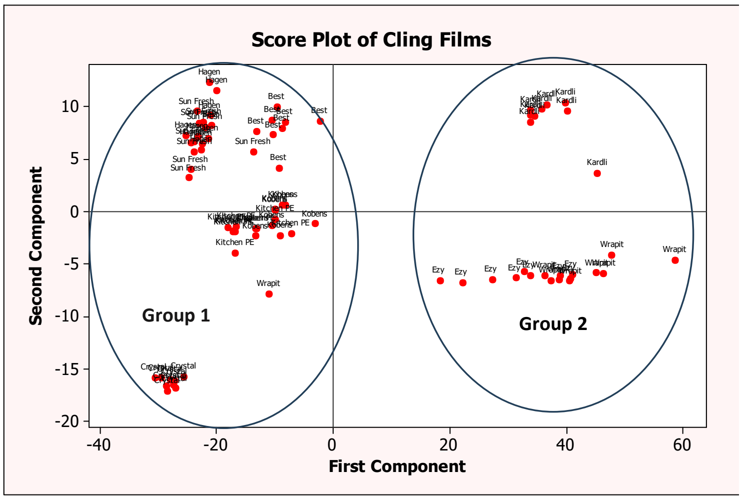

Figure 4. 2D PCA model for discrimination of cling film. Scores on PC 1 (83.1%), and PC 2 (7.1%)

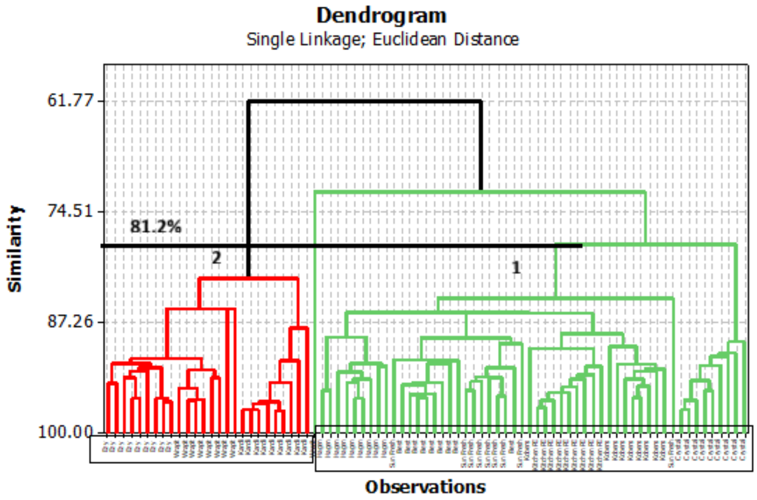

Figure 5. Dendrogram of cling samples (PVC and LDPE)

HCA

At a similarity level of 81.20%, the dendrogram of the cling film samples shown in **Figure 5** displays two main groups: Group 1 = LDPE samples and Group 2 = PVC samples. Both groups are aligned with PCA grouping in the previous section. This figure further evidences the observable effect on the clear separation of PCA analysis, where HCA revealed two main groups based on similarities in their ATR-FTIR spectra and the nature of their type (PVC or LDPE). **Figure 5** illustrates the HCA classification using single linkage and Euclidean distance in classifying cling film. As for the single linkage method, the minimum distance (nearest neighbour) between samples was used as the clustering strategy.

Simulated forensic case scenario

In many forensic cases, cling film is often used to hold and transport drugs, such as heroin and methamphetamine, in small quantities for sale [3]. Therefore, the source correspondence of polymers used for wrapping and transporting drugs must be further analysed as it will reveal valuable clues to link a questioned drug to a known cling film. This study tested seven (7) unknown cling films for source correspondence to understand the performance of the PCA method for discrimination purposes. All of these samples were correctly associated with the true class they belonged to, as shown in **Figure 6**. 100% correct prediction of the unknown PVC and LDPE samples is shown in **Table 4**, reinforcing the high predictive power and accuracy of the PCA model for distinguishing between cling film in real forensic cases.

Several studies have demonstrated the use of destructive techniques for discrimination of polymers of cling film. For instance, Nissen et al. [19], Sajwan et al. [5], Causin et al. [1], and Roux et al. [3] evaluated the composition of cling film using the discrimination power (DP) method. Meanwhile, the majority of work done between 1991 until 2018 [14-18] employed non-destructive methods to maintain the sample's integrity of evidence (Table 5). 90% of these studies focused on the examination of cling film using merely discriminating power method and no statistics. On the other hand, the remaining 10% includes a study by Telford et al. [20], which utilised ATR-FTIR coupled with chemometrics (PCA and LDA) focusing on LDPE-based cling film without the use of PVC samples for further comparison. They employed both ATR-FTIR and chemometrics to analyse nine rolls of five LDPE cling film brands. However, Principal Component Analysis (PCA) and Linear Discriminant Analysis (LDA) were not used for the prediction of unknown classification models to be applied in forensic scenario. This study addressed such gap by expanding the work with larger samples (i.e. 81 samples) for discrimination purposes. More importantly, the proposed PCA model was applied in simulated forensic case scenario with a number of unknown samples for prediction purposes.

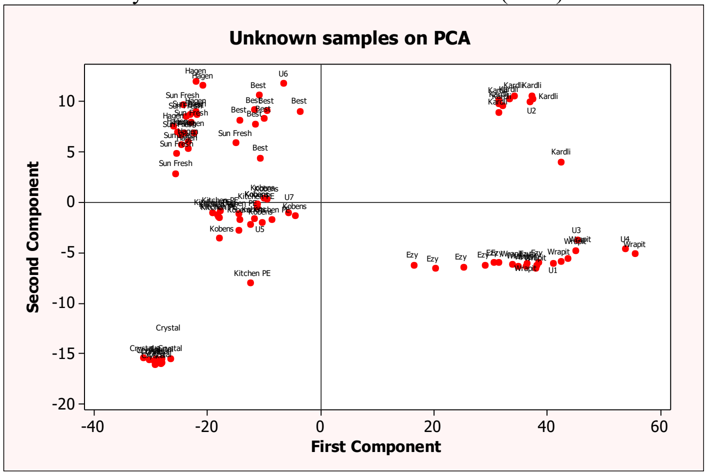

Figure 6. Unknown samples on PCA

Table 4. Actual and predicted types of the seven unknown samples of cling films. Note that the type of each unknown is 100% correctly predicted

Sample ID	Actual Type	Predicted Type
U1	PVC	PVC
U2	PVC	PVC
U3	PVC	PVC
U4	PVC	PVC
U5	LDPE	LDPE
U6	LDPE	LDPE
U7	LDPE	LDPE

Table 5. Comparison of our study with different techniques from previous studies

No.	Analytical Technique	Nature of Work	Statistical Technique	References
1	FTIR	Non-destructive	No statistics No chemometric methods reported	[14]
2	FTIR	Non-destructive	PVC samples only No chemometric methods reported	[15]
3	FTIR	Non-destructive	PVC samples only No statistics	[16]
4	FTIR	Non-destructive	No statistics No chemometric methods reported	[17]
5	FTIR	Non-destructive	Low density polyethylene (LDPE) No statistics	[18]
6	Optical examination, UVVis spectroscopy, and FTIR spectroscopy	Non-destructive and Destructive	Optical examination, UVVis spectroscopy, and FTIR spectroscopy	[3]
7	Differential Scanning Calorimetry infrared spectroscopy	Destructive/ Non-destructive	Fifty shopping bags No statistics No chemometric techniques reported	[1]
8	Differential Scanning Calorimetry	Destructive	No statistics No chemometric techniques reported	[5]
9	ICP-MS	Destructive	Detection ofelements in plastic film No statistics No chemometric techniques	[19]
10	FTIR	Non-destructive	LDPE samples only Limited samples only PCA/LDA	[20]
11	ATR-FTIR	Non-destructive	PCA/HCA Larger samples Unknown samples were applied in forensic cases	Present work

Conclusion

This work demonstrates the use of ATR-FTIR spectroscopy for discrimination and source correspondence of cling film (PVC and LDPE) as trace evidence commonly found in forensic investigations. 81 cling film samples were analysed using the ATR-FTIR technique, followed by the chemometric analysis of PCA and HCA. Once discriminated through visual inspection via ATR-FTIR, the chemometrics analysis of PCA was used to segregate the cling film class. Similar trends were observed in HCA where all samples (100%) were correctly segregated into two classes. The study further investigated the potential usage in simulated forensic case scenario where the obtained spectra from the unknown cling film were analysed on a trained PCA model. The results indicated that the PCA model recorded 100% accuracy in prediction unknown samples into their respective classes. Nevertheless, the spectral changes in contaminated and degraded samples over a longer time period should be investigated as potential work in the future.

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