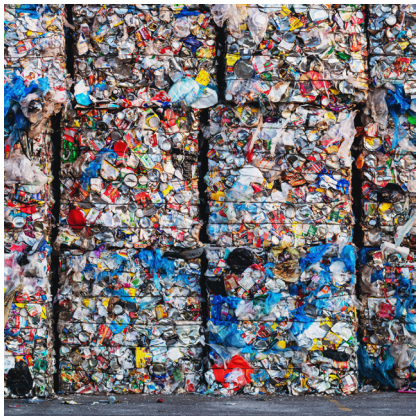
Detection of Polymer Impurities in Recycled Plastics using Chemometric analysis of ATR Spectroscopy

In this note: learn how the Specac Quest can be used to quickly idenitfy impurities in your plastic materials.

As concern grows over the amount of waste we send to landfill, demand for the ability to recycle has increased - particularly for plastic waste. Separating different types of polymers is essential to ensure the recycled product is suitable for reuse. Although every effort is made to ensure a pure recycled plastic is obtained, contamination is inevitable and therefore methods are required to quantify impurities. Here we have used FTIR spectroscopy coupled chemometric analysis to analyze polypropylene (PP) impurities in polyethylene (PE).

Chemometrics is the application of statistical tools to the measurement of chemical properties [1]. One of these tools is Partial Least Squares (PLS) analysis, a method to find the fundamental relationship between two related matrices. In our case the first matrix is comprised of the ATR-FTIR spectra, whilst the second matrix is the sample composition data. A model is first constructed using spectra of known composition. The model is validated against further spectra of known composition and once validated the model can then be applied to swiftly determine the composition of unknown real-world samples.



Discarded consumer plastics bundled and awaiting recycling.

Experimental

In order to compare the spectra of PP impurities in PE, blends of the two polymers were prepared by melt-blending the two polymers at 160 °C. To minimize potential sample inhomogeneity, five aliquots were taken from each blend, a spectrum of each recorded and then averaged together. Spectra were recorded on a commercially available spectrometer equipped with a Specac Quest™ ATR, with 32 scans co-averaged together at a resolution of 4 cm^{-1}. Chemometric modelling was conducted using a commercially available software package. Spectra were preprocessed by obtaining the second derivative to accentuate differences in the spectra, and minimize the effect of baseline variation. Ten blended and two pure PP/PE samples were prepared and used to build the PLS model. In order to validate the model an additional eight blends and two pure samples were prepared and the known sample concentration compared to the predicted composition from the PLS model.

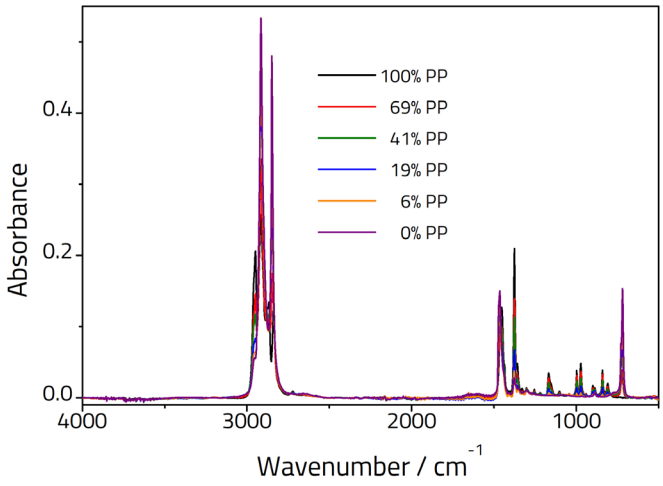


Figure 1: *ATR-FTIR Spectra of polymer blends with varying proportions of PP and PE.*

Results and Discussion

Figure 1 compares the average spectra recorded of various blends of PP/PE. The finger print region is shown in more detail in Figure 2. PP has a number of bands between 800-1200 cm^{-1} that are absent for PE, whilst PE has a band at 720 cm^{-1} that is absent for PP. Bands at 1360 and 1375 cm^{-1}, assigned to CH_3 bending vibrations, are significantly more intense for the PP sample relative to the PE sample due to the presence of a methyl pendant group on each monomer repeat unit which is absent for the PE polymer. The band at 1454 cm^{-1} in PP (assigned to C-H bends) shifts to 1464 cm^{-1} for the pure PE sample. Additional changes are also observed in the C-H stretching region.

It should be noted that ATR is only semi-quantitative since sample contact with the crystal will affect the intensity of the peaks. Nonetheless the relative peak intensities can be used for determining sample composition. It is possible to take the ratio of two peaks, one from each compound. However, as the two components will change relative to one another linearity would only be expected over a narrow range.

Therefore, we have modelled the data using PLS regression analysis. Twelve spectra of variable composition (0-100 % PP) were used to create the model and then a further ten spectra of different samples of known composition were used to validate the model. Two PLS component factors were chosen to fit the data to in order to obtain a good fit. Additional components were avoided in order to prevent overfitting.

The comparison of actual vs. PLS predicted is shown in Figure 3. A relatively low Root Mean Standard Error of Cross Validation (RMSECV) and Root Mean Standard Error of Prediction (RMSEP) were obtained indicating a good fit to the data. Further improvements to the model, particularly for low concentrations of impurities, may be possible using the Specac Constant Thickness Film Maker, however care should be used to ensure that the regions chosen for the model are not over absorbed.

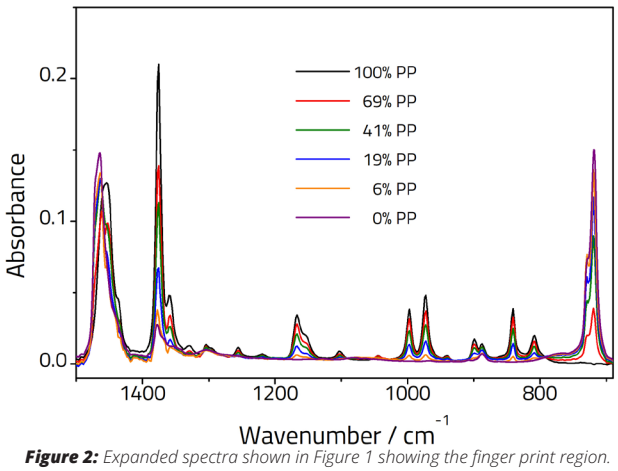


Figure 2: *Expanded spectra shown in Figure 1 showing the finger print region.*

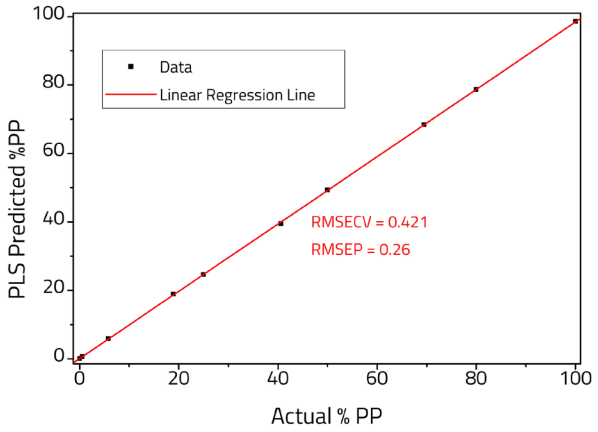


Figure 3: *Validation data comparing actual % of PP with the composition data predicted by the PLS model fit to the FTIR data.*

Conclusion

ATR measurements have been used to successfully monitor changes in composition of a PE/PP blend. Chemometric modeling enables the operator to extract the maximum possible information from their spectral dataset. The same technique could be applied to the detection of many different types of impurities in recycled plastics enabling rapid screening via the use of the quest ATR accessory.

References

1. Biancolillo, A., Marini, F. Front. Chem., 6, (2018), 576

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