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Self-modeling Mixture Analysis of FTIR Microscopy Spectra of a Polymer Laminate

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Key words: FTIR microscopy; lab analysis; self-modeling mixture analysis; polymer laminate; purity

Introduction: The data analyzed in this study consists of FTIR microscopy spectra of a 240 μm thick polymer laminate, shown schematically in Figure 1. The laminate has three layers: a top layer of polyethylene (PE), a middle layer of isophtalic polyester (IPE) and a bottom layer of polyethylene terepthalate. (PET). At the beginning of this study, the identity of the IPE layer was unknown but of great interest.

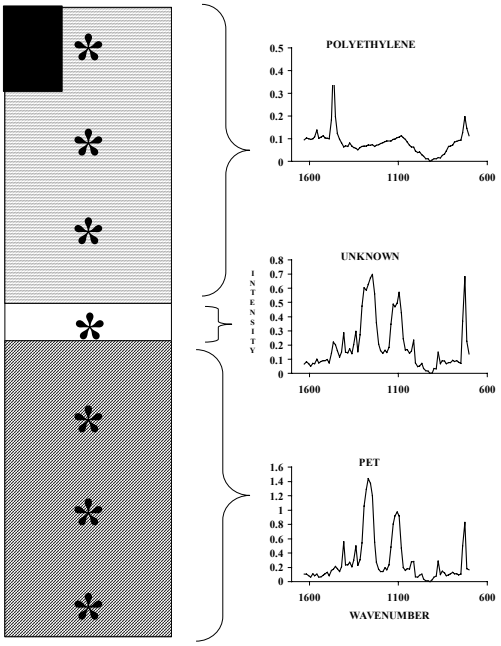

Figure 1. Schematic representation of the polymer laminate and representative spectra.

The spatial resolution of the instrument (i.e. the physical area observed in a single measurement) is indicated with the dark rectangle. Measurements were taken at various points along a cross-section of the polymer. The center of each measurement point is indicated by a star in Figure 1. The insets next to the schematic show the spectra taken at the top, middle, and bottom layers. Although the top and bottom spectra match PE and PET fairly well, the spectrum of the middle layer has contributions from both of the other layers because the thickness of the middle layer (2-3 μm) is beyond the 10 μm spatial resolution of the spectroscopic method.

The goal of this analysis was to resolve the spectrum of the middle layer in order to determine its identity with library search.

Results and Discussion: In order to obtain the correct spectrum for the middle layer, one can use self-modeling mixture analysis. With self-modeling mixture analysis techniques, spectral mixture data can be resolved into the spectra of the pure components and their contributions ("concentrations").

A successful analysis should result in one component with high contributions in the top layer but none in the middle or bottom layers. A second component should exhibit no contributions in the top and middle layers but high contributions for the bottom layer. Finally, the unknown component (IPE) should show contributions in the middle layer but none in the top and bottom layers.

Application of PLS_Toolbox function `purity` results in Figure 2 and 3.

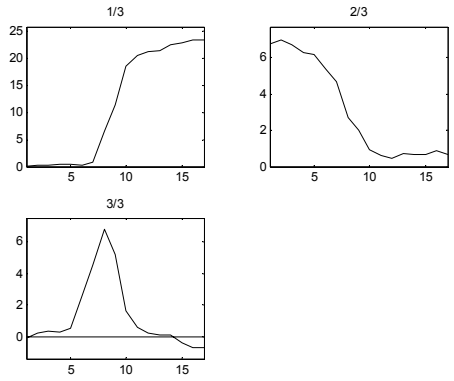

Figure 2. Resolve contribution ("concentration") profiles of polymer laminate

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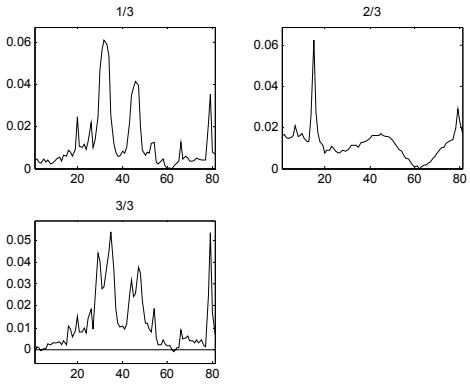

Figure 3. Resolved spectra of polymer laminate.

The resolved contributions in Figure 2 indicate that the expected contribution profiles were obtained. The most important part of this result is the spectrum of interest in Figure 3 (3rd spectrum). This spectrum could be identified correctly as isophtalic polyester. For more information about this data, see references 1 and 2.

Concluding remarks.

This example showed that it was possible to effectively enhance the resolution of the spectroscopic analysis using chemometrics. Related applications include spectra micro-inclusions in coated polymers which are very difficult to isolate by mechanical means. An alternative is FTIR microscopy, but the micro inclusion is generally smaller that the observation area of the microscope. This type of problem can be a show-stopper in manufacturing. This combination of spectroscopy and chemometrics has been crucial is solving such manufacturing problems.

Literature:

1) J. Guilment, S. Markel, W. Windig, Infrared chemical micro-imaging assisted by interactive self-modeling multivariate analysis, Appl. Spectr., 48, 1994, 320-326.

2) W. Windig, S. Markel, Simple-to-use interactive self-modeling mixture analysis of FTIR microscopy data, Journal of Molecular Structure, 292, 1993, 161-170.