

Self-Modeling Mixture Analysis of Time-Resolved Mass Spectra of a Three Component Mixture

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Introduction

The data analyzed in this study consist of time-resolved mass spectrometric analysis of a mixture of three photographic color-coupling components. Equal amounts of each component were mixed to make a sample with a total mass of 20 mg; the sample was then dissolved in 1 ml methanol. 1 μ l of the sample was deposited on a heated direct probe. The scanning rate was 1 spectrum/min.

The evaporation profiles of the three components were overlapping. As a result, there was no spectrum with a contribution of the only the middle component.

The goal of this analysis was to resolve the spectra of the pure components together with their evaporation profiles.

Results and Discussion

The data used in this analysis are a subset of the original data set. After a certain temperature has been reached, severe fragmentation occurs, which complicates the data set and is of no interest to the problem. The data set was truncated at the point where the fragmentation starts (1).

Application of PLS_Toolbox functions such as *purity*, *ALS*, or *MCR* results in the spectra displayed in Figure 1. The resolved components are displayed in order of evaporation time. Figure 1a shows the first resolved component; a reference spectrum for that component is shown in Figure 1b. In Figure 1c we see the spectrum with the highest relative amount of the second component, overlapped with spectra from the other two components. Figure 1d shows the resolved second component spectrum and Figure 1e the reference spectrum for that component. Comparing Figure 1c with Figure 1d clearly shows that self-modeling mixture analysis enables us to obtain the spectrum of a pure component, even if there is a severe overlap with other components. Figure 1f shows the spectrum of the third extracted

component with the relevant reference spectrum shown in Figure 1g.

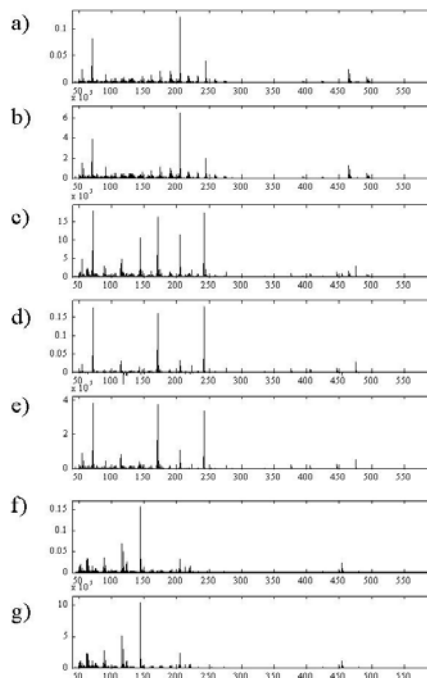


Figure 1. Resolved spectra (a,d,f) and reference spectra (b,e,g). In (c) we see the spectrum with the highest amount of the middle component as an example of the high overlap in the data.

The resolved contribution ('concentration') profiles of the three components are shown in Figure 2.

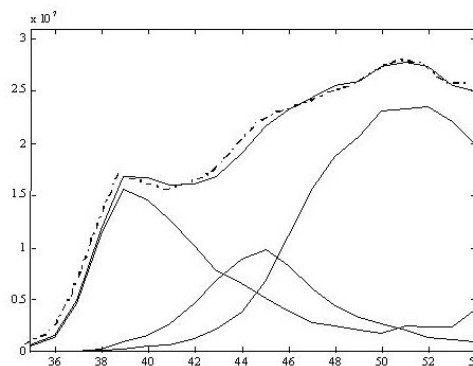


Figure 2. Resolved contribution profiles and their sum (solid line). The dashed line is the original total ion current of the data file.

The sum of these three components, the reconstructed total ion current (TIC) and the original TIC of the mass spectra file are overlaid over the three contribution profiles of the resolved components. The high similarity between the reconstructed TIC and the original TIC shows that the data set is well-represented by three components. It is clear from the resolved contribution profiles that there is indeed a high overlap of the middle component with the two other components, as we had already observed in Figure 1c.

Conclusion

This example showed that it was possible to effectively resolve spectra with overlapping evolution profiles. Resolution of overlapping data is not limited only to time-resolved data, such as these, but to any set of mixture spectra.

Literature

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