

Utilizing SIMPLISMA to Select Pure Variables for Classical Calibration

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A simple method for selecting the optimum frequency for univariate calibration in the presence of possible interfering species is described.

While excellent multivariate calibration tools are available, they are considered perplexing by many, and thus, some chemists still prefer the fast and intuitive classical calibrations. However, interfering species can seriously degrade non-multivariate calibration performance. As a result, it is critical to maximize knowledge of the interferences in order to avoid problems for univariate methods when selecting the analyte's optimum frequency. SIMPLISMA (1), a multivariate curve resolution technique, can help to easily find calibration wavelengths and regions that are free of interfering species.

Method

Both classical calibration and SIMPLISMA (SIMPLE-to-use Interactive Self-modeling Mixture Analysis) capabilities are built into the ACD/UV-IR Manager software. SIMPLISMA is valuable in calibration analysis because it can estimate the number of components in a mixture of unknowns, extract their pure spectra, and provide a semi-quantitative concentration profile for each. As input, SIMPLISMA requires a series of spectra for a mixture where the components are changing over time, such as a reaction profile or calibration training set. Pure component wavelengths with the maximum variance are detected without any *a priori* knowledge on the mixtures' composition by using a spectroscopic-like display tool, which only requires spectroscopic judgments to use. Pure variables are identified by the program where only a single component absorbs, to the exclusion of other components.

Experimental

Figure 1 shows a spectral series for a synthetic data set containing some components that can and cannot be treated in a univariate way. The pure variable corresponds to the maximum on the purity spectrum curve. Noise-like behavior or a minimum on the indicator function graph are used to determine the optimum number of components in the mixture.

In this case, three components were correctly detected and pure variables were found at 9, 38, and 73, for the red, blue, and green color pure spectra, respectively. Because of the overlap, and the nearby overcorrection leading to a negative absorbance around the pure variable value of 73, poor results would be expected with respect to calibration for the green component. In contrast, the red

Figure 1. Raw spectral series (top), purity spectrum for 4th component (middle), and resolved pure spectra (bottom).

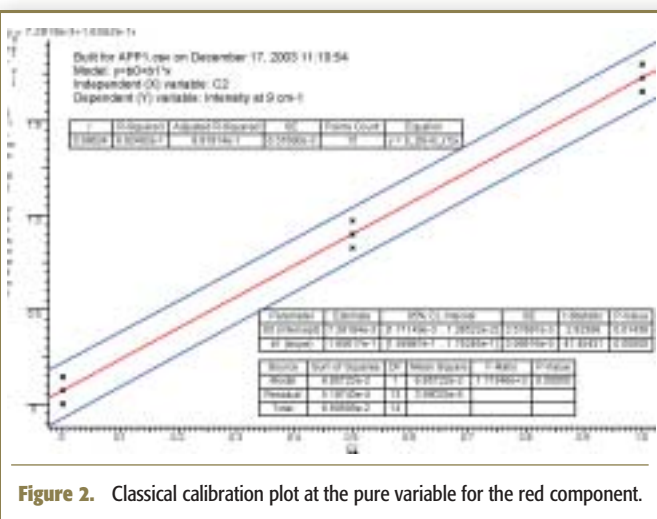
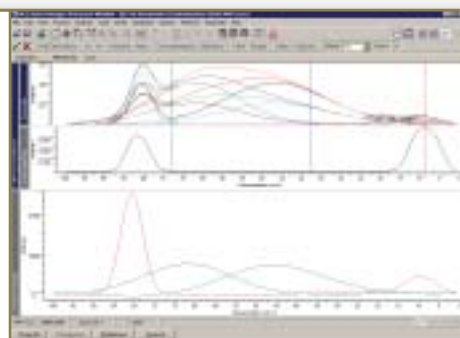


Figure 2. Classical calibration plot at the pure variable for the red component.

spectrum is problem free around its pure variable. Figure 2 shows a calibration curve plotted at the pure variable for the red component.

Conclusion

SIMPLISMA offers considerable insight into the feasibility of using classical calibration.

Reference

1. W. Windig and J. Guilment, *Anal. Chem.* **63**, 1425–1432 (1991).

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