Temperature Correction of UV Spectra by Loading Space Standardisation

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Temperature can significantly affect spectroscopic-based methods for *in situ* monitoring of processes. As the use of temperature is inherent to many processes, such as cooling crystallisation, changes in temperature cannot be avoided. Therefore, removal of the effects of temperature from spectroscopic data is required and many advanced temperature correction algorithms have been developed for this purpose. Amongst these, a comparatively simple algorithm to implement is loading space standardisation (LSS).[1,2]

Construction of an LSS model requires a dataset comprising multiple samples (concentration) at a number of temperatures. To collect spectral calibration data relevant to many processes, such as cooling crystallisation, there are likely to be unobtainable concentration/temperature combinations.[3,4] A model system of L-ascorbic acid (LAA) was selected for the study. Spectral data were collected for the construction of a calibration model to predict the solute concentration of LAA by UV-visible spectrometry. An LSS temperature correction model was constructed using a subset of the calibration samples and subsequently applied to correct all of the spectra within the calibration set as though they were collected at a single temperature (Figure 1). Compared to a partial least squares (PLS) model constructed without LSS correction, the PLS model constructed from the LSS corrected spectra required fewer latent variables and demonstrated improved model predictive performance.

A slurry of LAA was prepared and held at a number of temperatures using a stepped heating profile, with UV monitoring present. Solubility values at each hold temperature were obtained using PLS models constructed from data with and without LSS correction and compared to gravimetrically obtained solubility values. Correction with LSS gave rise to solubility predictions that were closer to the gravimetrically determined solubility value.
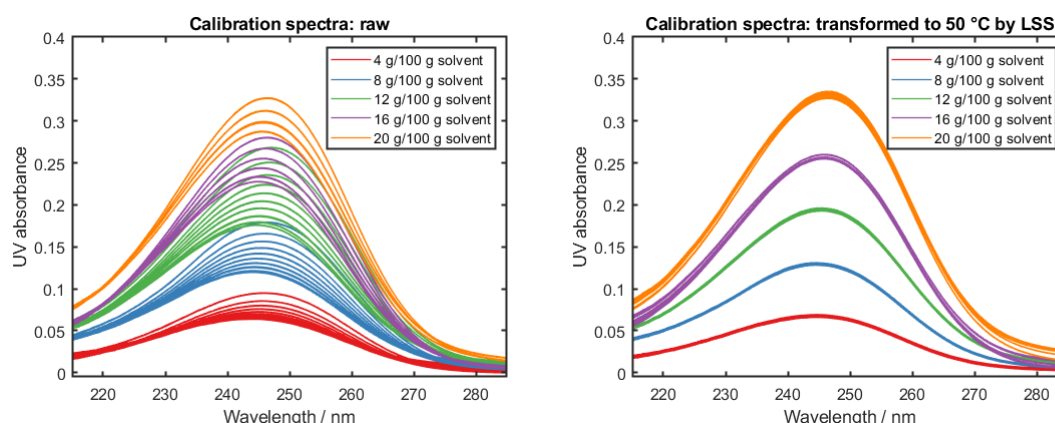

Figure 1. UV calibration spectra of LAA, before and after temperature correction by LSS.

References

1   Z.-P. Chen, J. Morris and E. Martin, *Anal. Chem.*, 2005, **77**, 1376-1384.
2   Z.-P. Chen and J. Morris, *Analyst*, 2008, **133**, 914-922.
3   Z. P. Chen, J. Morris, A. Borissova, S. Khan, T. Mahmud, R. Penchev and K. J. Roberts, *Chemom. Intell. Lab. Syst.*, 2009, **96**, 49-58.
4   T. Chen and E. Martin, *J. Chemometrics*, 2007, **21**, 198-207.