Abstract

Three-way analysis of a phenol formaldehyde curing reaction using spectral information from near infrared and infrared spectroscopy

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Introduction

The polymerisation reaction of phenol formaldehyde is studied using spectral information from two different spectroscopic techniques; NIR hyperspectral imaging and infrared (IR). An experimental design is followed over time using the spectra as responses which leads to three-way data arrays. A comprehensive understanding of the current reaction is very important for industrial on-line applications.

Materials and methods

The design: six runs of samples, using three different types of backing material were coated with phenol formaldehyde adhesive and cured for a total of 8 hours in two different temperature profiles. Responses: each sample was measured with a sisuChema NIR line-by-line scanning camera and a PerkinElmer FTIR-1000 instrument (diamond ATR cell) up to 8 hours, giving a total of 72 NIR-images and IR-spectra. The acquired images had 239 spectral bands with a spectral resolution of approximately 6 nm in the NIR region (1000–2498 nm). The IR-spectra were measured between 4000 and 660 cm^{-1} with a spectral resolution of 2 cm^{-1}. The collected spectra were reorganised into three-way arrays, run × time × wavelength, and analysed using three-way methods.

Results and Discussion

The IR/NIR data gave PARAFAC loadings that allowed interpretation of the design, the time profiles and the spectral properties of the reagents and polymer. The NIR data allowed hyperspectral image and multiway analysis. A comparison of PARAFAC loadings from NIR and IR data gave useful insights into similarities and differences between the methods. A comparison with two-way data analysis from Raman spectra measured in a test tube was also made. The curing time was determined for each run (6-8 hours).

Conclusion

NIR hyperspectral imaging is extremely fast, even faster than bulk NIR measurement, when acquiring a spectrum in each pixel. The IR PARAFAC and the NIR PARAFAC loadings combined with hyperspectral image analysis gave valuable information about the design, the reaction and the curing time. The spectral interpretation of the IR data simplified the corresponding interpretation of the NIR loadings.

Reference paper as:
Lillhonga, T., Dahlbacka, J. and Geladi, P. (2012). Three-way analysis of a phenol formaldehyde curing reaction using spectral information from near infrared and infrared spectroscopy (abstract), in: Proceedings of the 15th International Conference on Near Infrared Spectroscopy, Edited by M. Manley,C.M. McGoverin, D.B. Thomas and G. Downey, Cape Town, South Africa, p. 96.