

CHALLENGING APPLICATIONS FOR FT-NIR SPECTROSCOPY

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The feasibility of NIR spectroscopy as a quick and nondestructive method for quality control of uniformity of coating thickness of pharmaceutical tablets was investigated. Near infrared spectra of a set of pharmaceutical tablets with varying coating thickness were measured with a diffuse reflectance fiber optic probe connected to a Bruker IFS 28/N FT-NIR spectrometer. The challenging issues encountered in this study included: 1. The similarity of the formulation of the core and coating materials, 2. The lack of sufficient calibration samples and 3. The non-linear relationship between the NIR spectral intensity and coating thickness. A peak at 7184 cm^{-1} was identified that differed for the coating material and the core material when NIR spectra were collected at 2 cm^{-1} resolution (0.4 nm at 7184 cm^{-1}). The study showed that the coating thickness can be analyzed by polynomial fitting of the peak area of the selected peak, while least squares calibration of the same data failed due to the lack of availability of sufficient calibration samples.

Samples of coal powder and solid pieces of coal were analyzed by FT-NIR diffuse reflectance spectroscopy with the goal of predicting their ash content, percentage of volatile components, and energy content. The measurements were performed on a Bruker Vector 22N spectrometer with a fiber optic probe. A partial least squares model was constructed for each of the parameters of interest for solid and powdered sample forms separately. Calibration models varied in size from 4 to 10 PLS ranks. Correlation coefficients for these models ranged from 86.6 to 95.0%, with root-mean-square errors of cross validation comparable to the corresponding reference measurement methods. The use of FT-NIR diffuse reflectance measurement techniques was found to be a significant improvement over existing measurement methodologies in terms of speed and ease of use, while maintaining the desired accuracy for all parameters and sample forms.

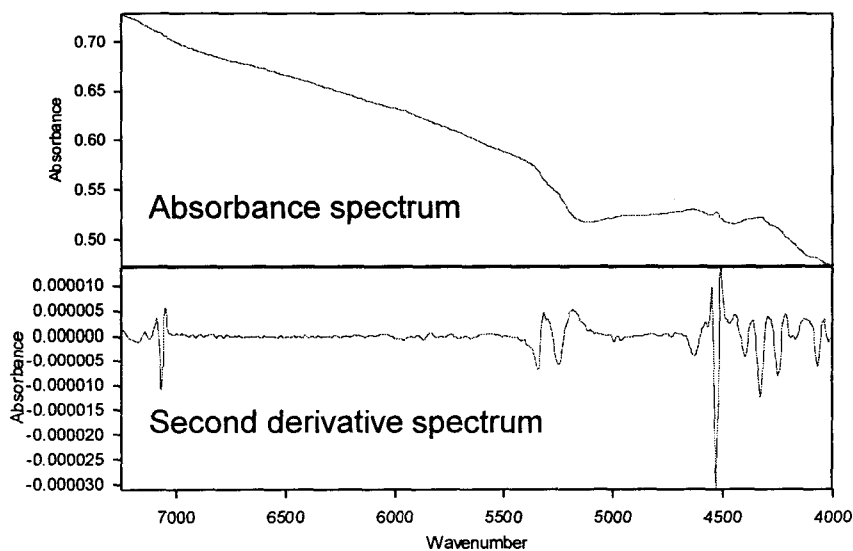


Figure 1. FT-NIR diffuse reflectance spectrum of powdered coal.