Three-component decomposition of coal spectrum in R

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R with its CRAN is an excellent tool for building automated high-accuracy tests of spectroscopic data in Diffuse Reflectance Infrared Fourier Transform (DRIFT) spectrometry of coals. R’s power is revealed by mix of truly ease in deployment of complex algorithms and its code clarity. That is why, R is chosen as a language and development environment for building Spectrotest-SDK – the special development kit, which provides functions and S3-classes for rapid automation of DRIFT-data processing tasks.

The identification and further interpretation of broad bands in DRIFT-spectra of coals has a long-term story, which arises from various hypotheses of coal structure. Given these circumstances we searched for simple, yet effective approach to divide spectral data into strictly localized and mainly delocalized parts. We found the non-quadratic cost function technique [1] to be the starting point to fit a polynomial as the delocalized part, i.e. the background. As a result, we authored R-function fons included in Spectrotest-SDK to programmatically realize the “coal-oriented” modification of the proposed technique. Herewith, the R-code of the authored function looks rather plain and simple due to function pseudoinverse located in the remarkable package copcor.

Thoroughly looking through numerous combinations of tuning parameters for the function fons, we found those values that assisted in three-component decomposition of DRIFT-spectra of more than 100 coals at different metamorphic stages. Those components may be consecutively treated as spectra of monomer (localized) and polymer (delocalized) parts of chemical structure and methodical background.

So, we will describe the latest practical experience of implementing this decomposition in the light of application of chemometric tools for coal calibration in R [2].

References