BULK MINERALOGICAL CHARACTERISATION OF RESERVOIR ROCKS AND SANDSTONES USING DIFFUSE REFLECTANCE INFRARED FOURIER TRANSFORM SPECTROSCOPY AND PARTIAL LEAST SQUARES ANALYSIS

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Within the oil industry, knowledge of the mineralogical composition of sandstone-based reservoir rocks is very important especially when complex multicomponent treatment fluids are applied to the reservoirs in order to enhance the oil extraction process (Borling et al., 1994). Other industrial areas interested in such analysis include: geophysics, construction, water industries and ceramics. Current bulk mineralogical analysis relies heavily on X-ray diffraction (XRD) and tends to be supported by infrared spectroscopy, chemical analysis and electron microscopy (Środoń, 2002). Combination of these techniques is time consuming and expensive yet still only 3–5wt% accurate.

Here, a Partial Least Squares Analysis (PLS) model created from Diffuse Reflectance Infrared Fourier Transform Spectroscopy (DRIFTS) spectra of mineral mixtures has been formulated and is able to quantify each mineral component in an independent mineral mixture within 1.0wt% accuracy. An improved method for obtaining highly reproducible DRIFTS spectra was used, which was essential for accurate quantification within the PLS models. This methodology could also be applied to a variety of powdered samples including cements, soils, coals and minerals, which are also routinely analysed by DRIFTS (Kelvey and Britt, 1996). PLS is a multivariate statistical technique based on the PLS algorithm that can be used to quantify analyte components in infrared spectra, without the use of the Beer-Lambert Law (or its Kubelka-Munk equivalent for diffuse reflectance) (Beebe and Kowalski, 1987). This technique is especially appropriate when analysing complex multiple-component spectra, which contain many broad and overlapping bands. In essence the PLS algorithm examines regions of the spectra to determine which areas vary as a function of component concentration.

The seven mineral standards used in the PLS model of mineral mixtures were chosen to represent those typically en-

countered in sandstone-type rocks: quartz, dolomite, montmorillonite, illite, kaolinite, chlorite and albite. The results obtained from applying the PLS model of mineral standard mixtures to several sandstone-type quarry rocks and a suite of reservoir rocks from various depths of an oilfield were much better than anticipated given that the model did not describe the total variance of mineral components crystallinity expected in the rocks. The model was unable to differentiate between montmorillonite and illite due to their similar spectra, but was able to quantify their combined amounts. However, it was able to quantify the amount of albite in the quarry rocks in the presence of K-feldspar even though their spectra were very similar. A separate PLS model constructed using the DRIFTS spectra of the reservoir rocks showed that calcite and dolomite could be individually quantified despite their similar DRIFTS spectra. The model was also able to identify the type of clay present in the rock as montmorillonite and illite.

This feasibility study clearly demonstrated the high potential of a quick, accurate alternative method of quantifying bulk mineralogy in a sandstone-type rock by applying PLS analysis to their DRIFTS spectra. Moreover, the potential to improve quantification could be achieved by extending the model to include larger numbers of standards and real samples with data that covers all the expected variance in the rocks.

References

BEEBE, K. R., KOWALSKI, B. R. (1987): Analytical Chemistry, 59, 1007–1017A.

BORLING, D. et al. (1994): Oilfield Review – Schlumberger Cambridge Research, April, 44–58.

KELVEY, M. L., BRITT, T. R. (1996): Analytical Chemistry, 127R-128R.

ŚRODOŃ, J. (2002): Mineralogical Magazine, 66, 677–687.