

Application Note AN-NIR-117

# Analysis of moisture, ash, carbon, and volatile content in coal by NIRS

## Near-infrared spectroscopy (NIRS) offers results in seconds

Moisture, ash, fixed carbon, and volatile content are the most important parameters regarding coal analysis. The standard methods to measure these parameters involves combustion in special furnaces. Prior to combustion, the coal samples need to be pulverized and weighed. To determine the volatile content in coal, combustion needs to be performed under a controlled atmosphere of pure nitrogen at temperatures over 900 °C.

Conventional methods used to determine the key quality parameters for coal samples are time consuming and, based on the nitrogen consumption, cost intensive. Near-infrared (NIR) spectroscopy is an excellent alternative method to simultaneously determine all four quality parameters in less than one minute without any sample preparation. This Application Note demonstrates that the Metrohm NIRS DS2500 Solid Analyzer operating in the visible and near-infrared spectral region (Vis-NIR) offers users an easier way to perform coal quality analysis.

## EXPERIMENTAL EQUIPMENT

Different pulverized coal samples (n = 30) with a particle size of 0.2 mm were measured on the Metrohm NIRS DS2500 Solid Analyzer (Figure 1). All measurements on the DS2500 Solid Analyzer were performed in rotation using a large sample cup to average the subsample spectra. This sample setup reduces the influence of the particle size distribution of the coal particles. Data acquisition and prediction model development were performed with the software package Vision Air Complete.

**Table 1.** Hardware and software equipment overview.

| Equipment | Article number |
|---|---|
| DS2500 Solid Analyzer | 2.922.0010 |
| DS2500 large sample cup | 6.7402.050 |
| Vision Air 2.0 Complete | 6.6072.208 |




**Figure 1.** Metrohm NIRS DS2500 Solid Analyzer with the DS2500 large sample cup for measuring coal samples in rotation.

## RESULT

All measured Vis-NIR spectra (Figure 2) were used to create a prediction model for quantification of the calibration models. The quality of the prediction model was evaluated using correlation diagrams which display a high correlation ($R^2$ > 0.89) between the Vis-NIR prediction and the reference methods for all parameters. The respective figures of merit (FOM) display the expected precision and confirm the feasibility during routine analysis (Figures 3–6).

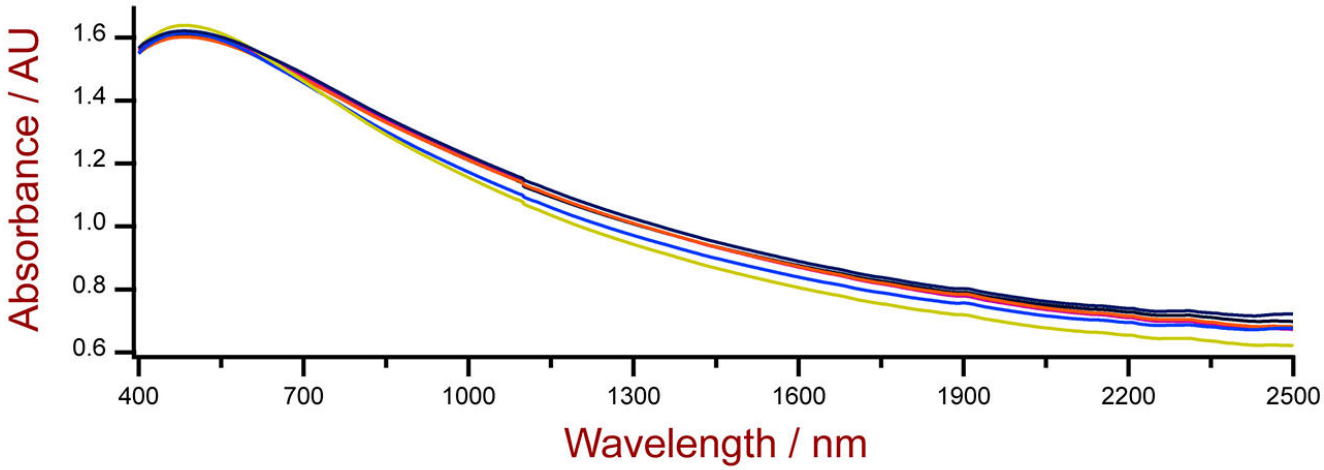



**Figure 2.** Selection of Vis-NIR spectra of coal samples analyzed on a DS2500 Solid Analyzer with the large sample cup.

## RESULT ASH CONTENT

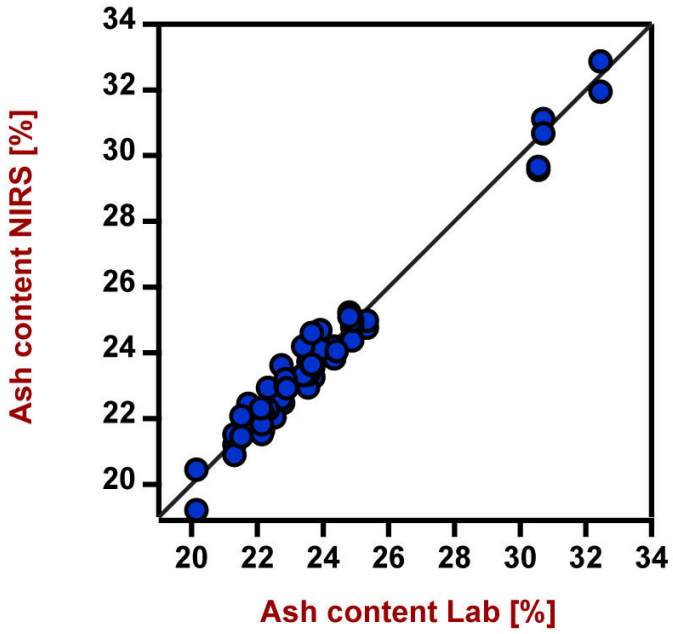



**Figure 3.** Correlation diagram and the respective figures of merit for the prediction of ash content in coal using a DS2500 Solid Analyzer. The lab value was evaluated according to ASTM D3174.

| Figures of Merit | Value |
|---|---|
| $R^2$ | 0.973 |
| Standard Error of Calibration | 0.48% |
| Standard Error of Cross-Validation | 0.73% |

## RESULT VOLATILE CONTENT

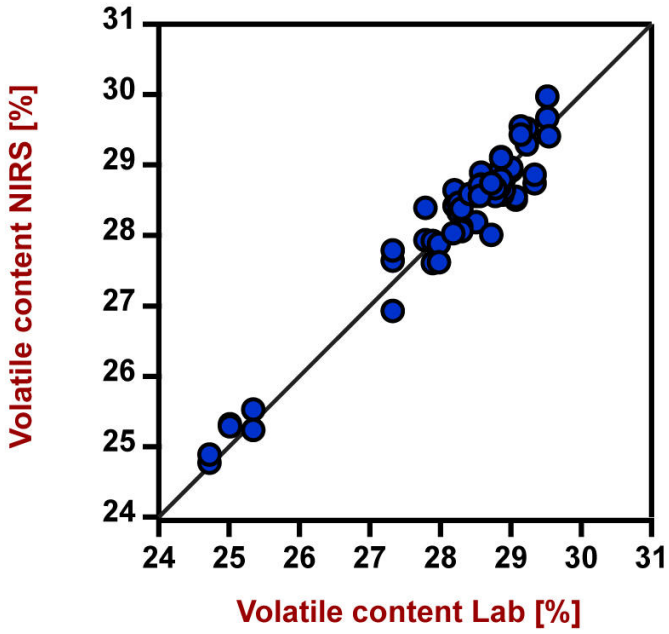



**Figure 4.** Correlation diagram and the respective figures of merit for the prediction of volatile content in coal using a DS2500 Solid Analyzer. The lab value was evaluated according to ASTM D3175.

| Figures of Merit | Value |
|---|---|
| $R^2$ | 0.944 |
| Standard Error of Calibration | 0.29% |
| Standard Error of Cross-Validation | 0.38% |

## RESULT FIXED CARBON CONTENT

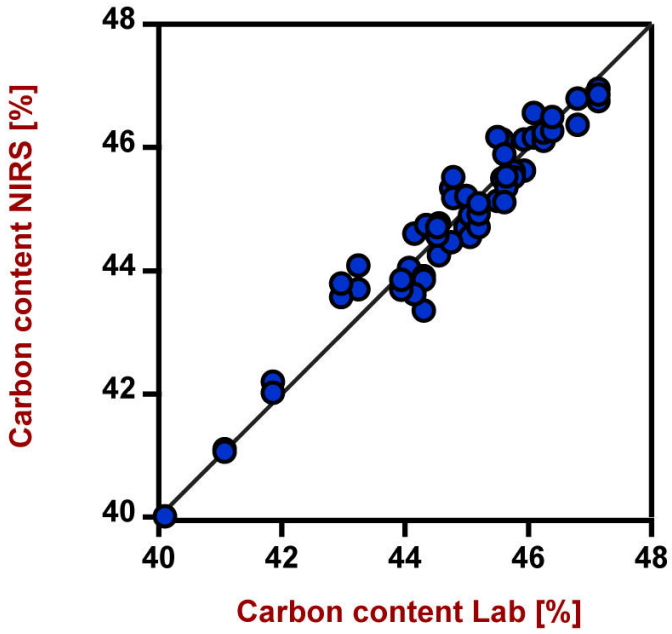



**Figure 5.** Correlation diagram and the respective figures of merit for the prediction of fixed carbon content in coal using a DS2500 Solid Analyzer. The lab value was evaluated according to ASTM D3172 (furnace combustion method).

| Figures of Merit | Value |
|---|---|
| $R^2$ | 0.937 |
| Standard Error of Calibration | 0.40% |
| Standard Error of Cross-Validation | 0.52% |

## RESULT WATER CONTENT

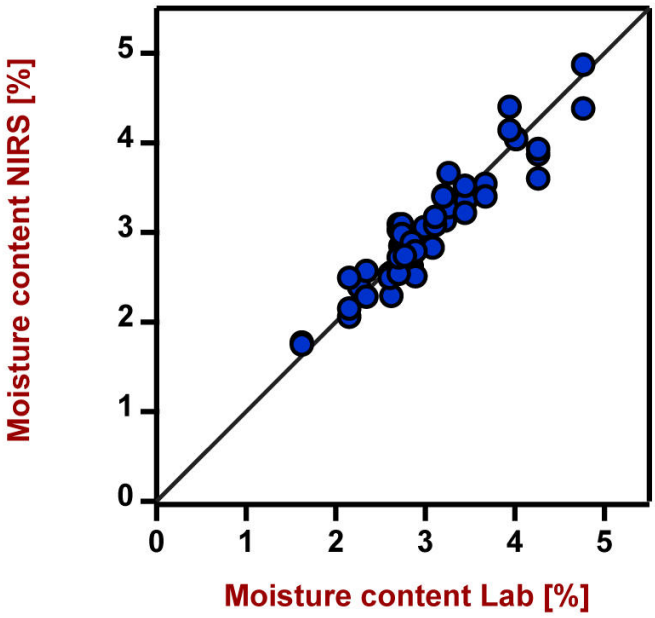



**Figure 6.** Correlation diagram and the respective figures of merit for the prediction of moisture content in coal using a DS2500 Solid Analyzer. The lab value was evaluated according to ASTM D3173 (furnace drying method).

| Figures of Merit | Value |
|---|---|
| $R^2$ | 0.896 |
| Standard Error of Calibration | 0.23% |
| Standard Error of Cross-Validation | 0.28% |

## CONCLUSION

This Application Note demonstrates the feasibility of the Metrohm NIRS DS2500 Solid Analyzer for the determination of ash, moisture, fixed carbon, and volatile content in coal. Vis-NIR spectroscopy enables fast determination (Table 2) without any sample preparation. In addition, the use of nitrogen gas is obsolete which reduces analysis cost.

**Table 2.** Time to result overview for different coal quality parameters using standard analysis methods.

| Parameter | Method | Time to result |
|---|---|---|
| Ash content | Volatile matter furnace | 1–2 h: grinding, weighing, combustion |
| Volatile content | Volatile matter furnace | 0.5 h: grinding, weighing, combustion |
| Fixed carbon content | Volatile matter furnace | 0.5 h: grinding, weighing, combustion |
| Moisture content | Volatile matter furnace | 0.5 h: grinding, weighing, combustion |

## CONTACT

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## CONFIGURATION



DS2500 Solid Analyzer

Robust near-infrared spectroscopy for quality control, not only in laboratories but also in production environments.

The DS2500 Analyzer is the tried and tested, flexible solution for routine analysis of solids, creams, and optionally also liquids along the entire production chain. Its robust design makes the DS2500 Analyzer resistant to dust, moisture, vibrations, and temperature fluctuations, which means that it is eminently suited for use in harsh production environments.

The DS2500 covers the full spectral range from 400 to 2500 nm and delivers accurate, reproducible results in less than one minute. The DS2500 Analyzer meets the demands of the pharmaceutical industry and supports users in their day-to-day routine tasks thanks to its simple operation.

Thanks to accessories tailored perfectly to the instrument, optimum results are achieved with every sample type, no matter how challenging it is, e.g. coarse-grained solids such as granulates or semi-solid samples such as creams. The MultiSample Cup can help improve productivity when measuring solids, as it enables automated measurements of series containing up to 9 samples.