



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).

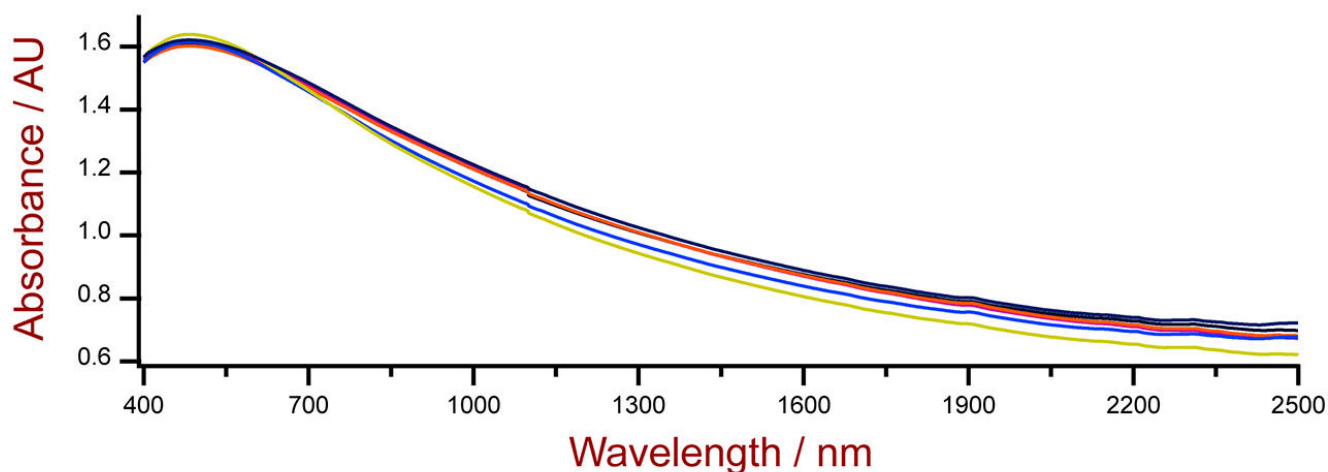


Figure 2. Selection of Vis-NIR spectra of coal samples analyzed on a DS2500 Solid Analyzer with the large sample cup.

RESULT ASH CONTENT

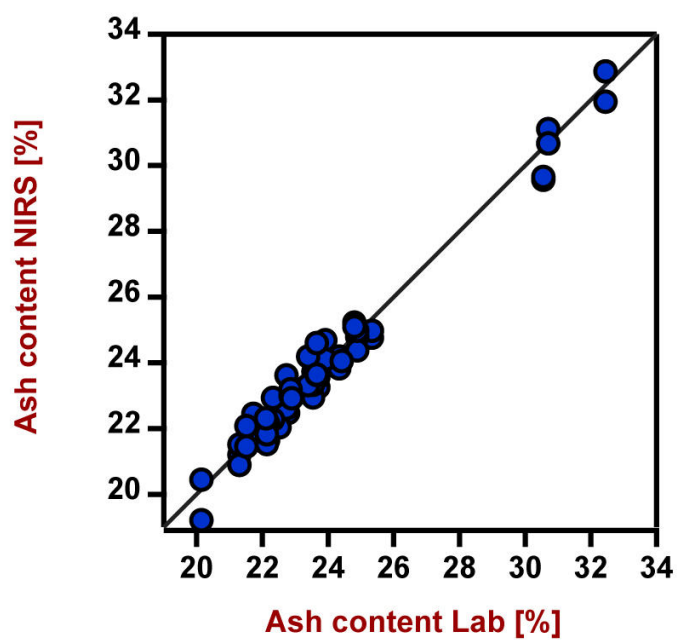


Figure 3. Correlation diagram and the respective figures of merit for the prediction of ash content in coal using a DS2500 Solid Analyzer. The lab value was evaluated according to ASTM D3174.

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

RESULT VOLATILE CONTENT

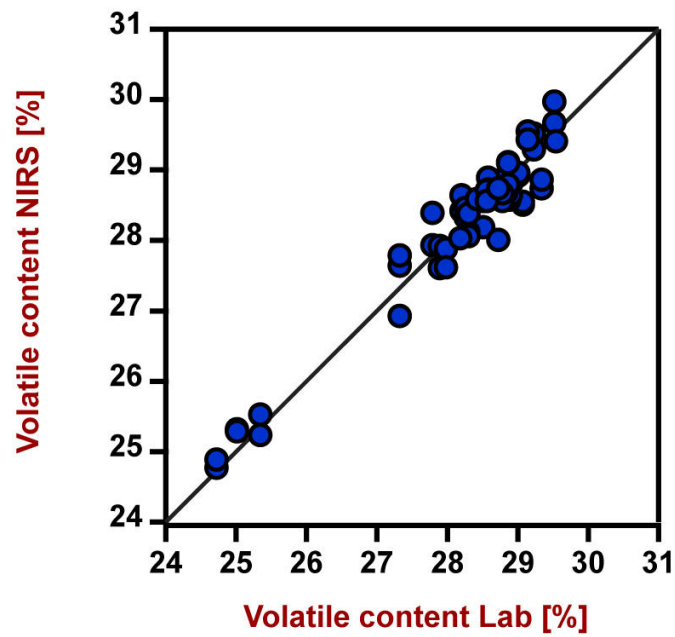


Figure 4. Correlation diagram and the respective figures of merit for the prediction of volatile content in coal using a DS2500 Solid Analyzer. The lab value was evaluated according to ASTM D3175.

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

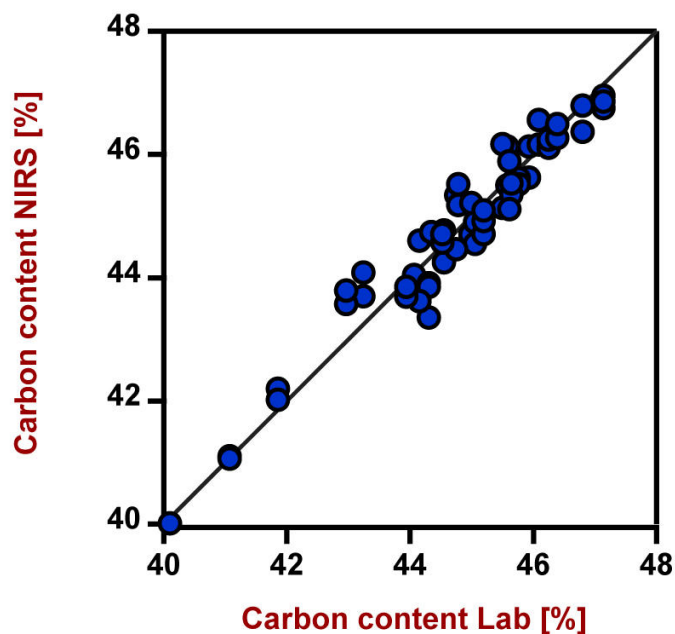


Figure 5. Correlation diagram and the respective figures of merit for the prediction of fixed carbon content in coal using a DS2500 Solid Analyzer. The lab value was evaluated according to ASTM D3172 (furnace combustion method).

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

RESULT WATER CONTENT

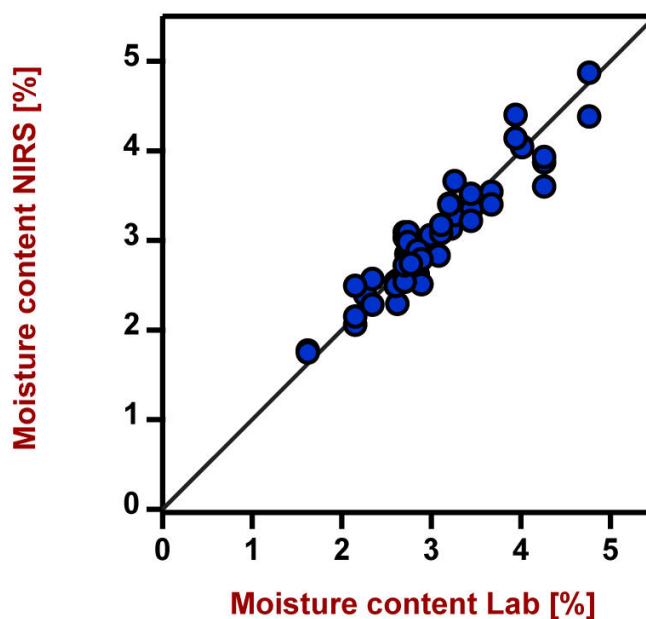


Figure 6. Correlation diagram and the respective figures of merit for the prediction of moisture content in coal using a DS2500 Solid Analyzer. The lab value was evaluated according to ASTM D3173 (furnace drying method).

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

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CONFIGURATION



DS2500 Solid Analyzer

Spectroscopie proche infrarouge robuste pour le contrôle de la qualité en laboratoire et en environnement de production.

L'analyseur DS2500 Analyzer est la solution éprouvée et souple destinée aux analyses de routine de matières solides, de crèmes et, en option, de liquides, tout au long de la chaîne de fabrication. Sa conception robuste fait du DS2500 Analyzer un appareil insensible à la poussière, à l'humidité, aux vibrations ainsi qu'aux variations de température, et donc particulièrement adapté aux rudes conditions d'un environnement de production.

Le DS2500 couvre l'ensemble de la gamme spectrale de 400 à 2 500 nm et fournit des résultats exacts et reproductibles en moins d'une minute. Le DS2500 Analyzer répond aux exigences de l'industrie pharmaceutique et représente une aide précieuse pour les opérations de routine quotidiennes grâce à sa simplicité d'utilisation.

Grâce à des accessoires parfaitement adaptés à l'appareil, il atteint des performances sans précédent avec tous les types d'échantillons, quel que soit le défi qu'ils opposent (matières solides à gros grains comme les granulats ou échantillons semi-solides ou liquides telles les crèmes). La productivité lors de mesures de matières solides peut encore être augmentée par l'utilisation du MultiSample Cup, lequel permet des mesures automatisées en série jusqu'à un maximum de 9 échantillons.