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.

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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.

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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**).
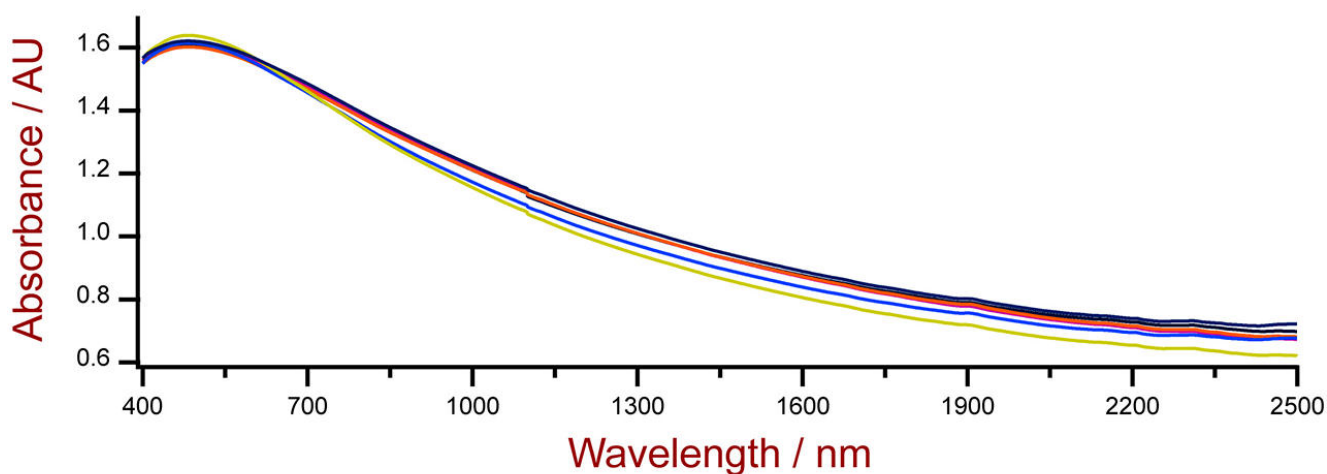

Figure 2. Selection of Vis-NIR spectra of coal samples analyzed on a DS2500 Solid Analyzer with the large sample cup.
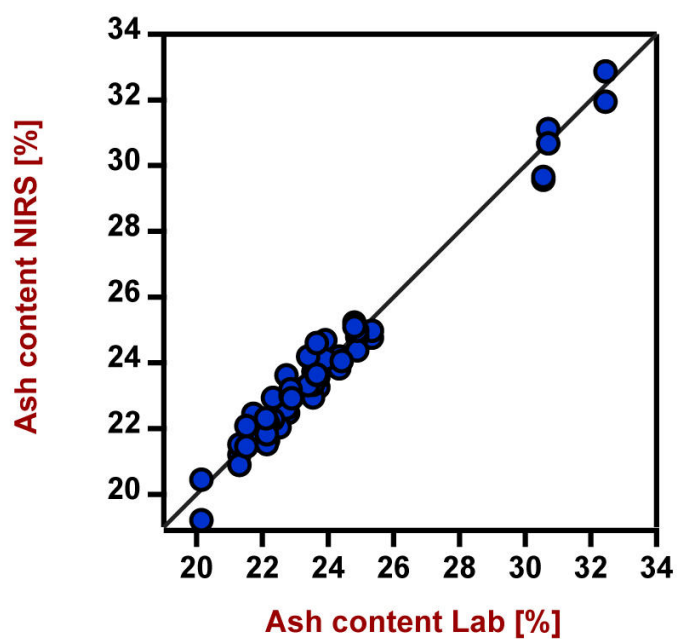
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Figure 3. Correlation diagram and the respective figures of merit for the prediction of ash content in coal using a DS2500 Solid Analyzer. The lab value was evaluated according to ASTM D3174.

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

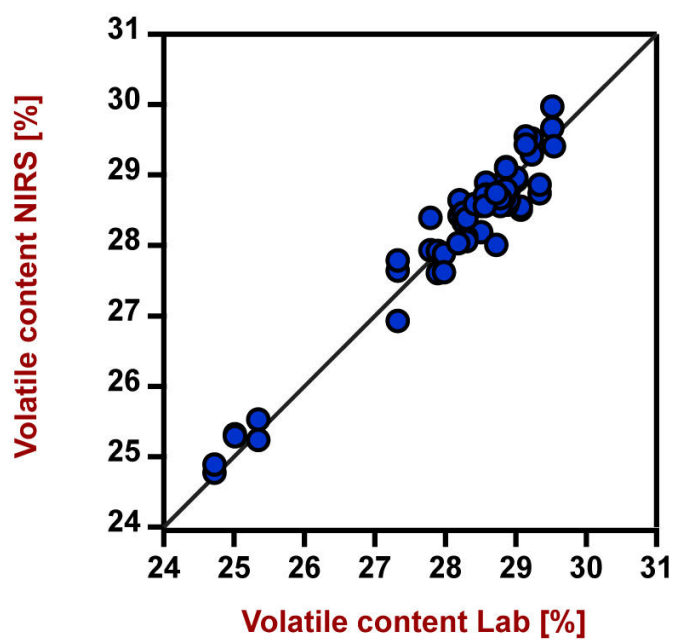Ω Metrohm

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%

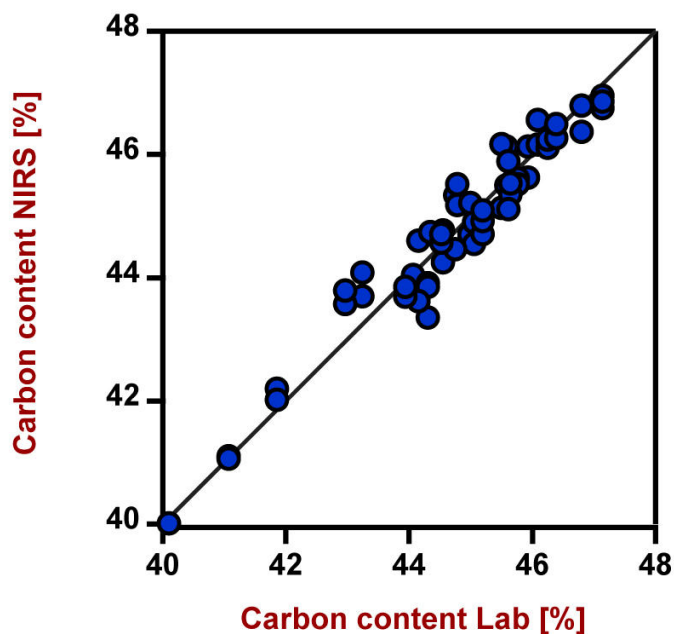Ω Metrohm

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%

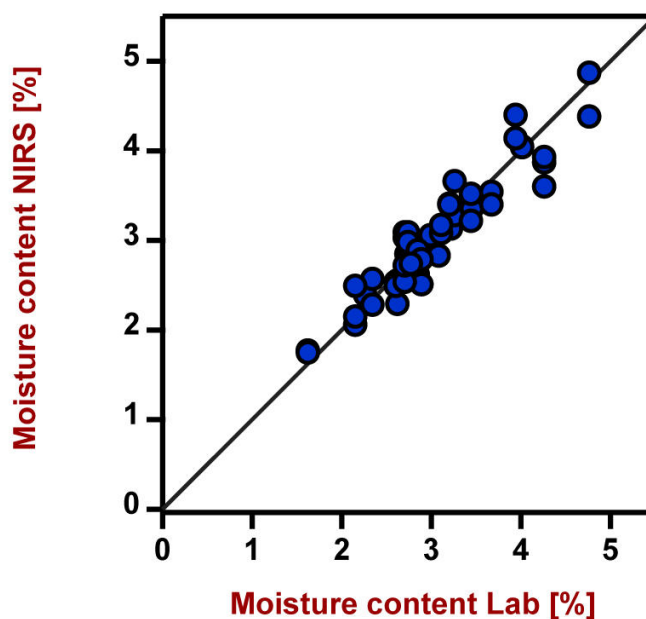Ω Metrohm

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.

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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
ラホおよひ生産環境における品質管理用の堅牢な近赤外分光法。
DS2500 Analyzerは、生産チェーン全体に沿った固形物、クリーム、およひオフションとしての液体のルーチン分析に実績のあるフレキシフルなソリューションてす。頑丈な仕様により、ＤＳ２５００ Analyzerは粉塵、湿気、振動や温度変動に強い為、過酷な生産環境ての使用に理想的てす。

DS2500は400～2500 nmのスヘクトル範囲全体をカハーし、1分以内に正確て再現性の高い結果を提供します。DS2500 Analyzerは製薬業界の要件を満たしており、簡単な操作により日常的な作業においてユーサーをサホートします。

装置に完全に適応した付属品により、顆粒のような粒の荒い固形物、またはクリームのような半固形液体サンフルなとのあらゆる困難なタイフのサンフルにおいても、最良の結果を得ることかてきます。固形物の測定においては、9つまてのサンフルのシリースの自動測定を可能にするMultiSample Cupを使用することて、生産性を高めることかてきます。

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