



Application Note AN-NIR-117

利用近红外光谱分析煤炭中的水分、灰分、碳和挥发物含量

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**).

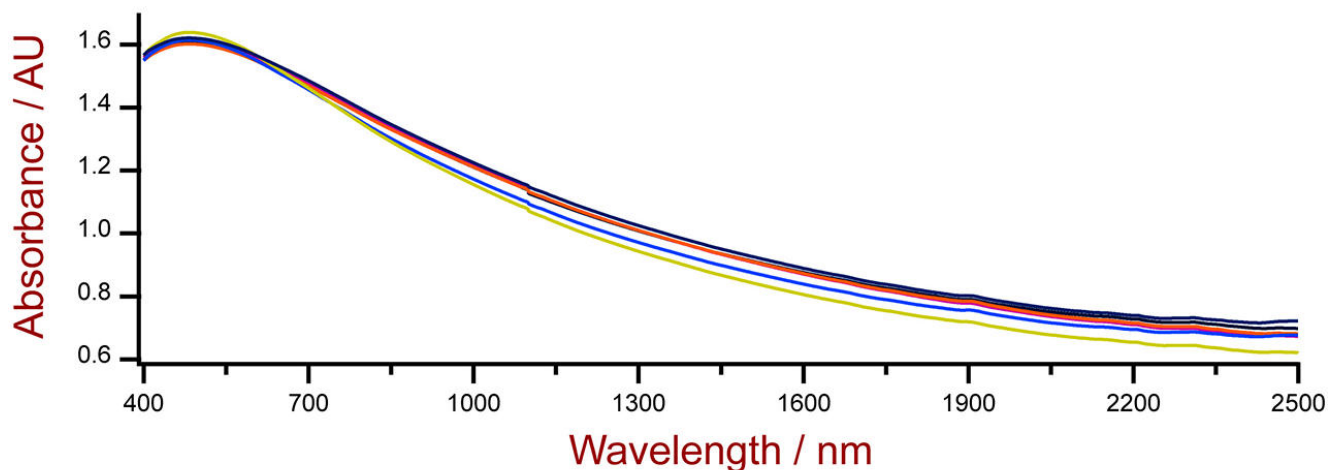


Figure 2. Selection of Vis-NIR spectra of coal samples analyzed on a DS2500 Solid Analyzer with the large sample cup.

RESULT ASH CONTENT

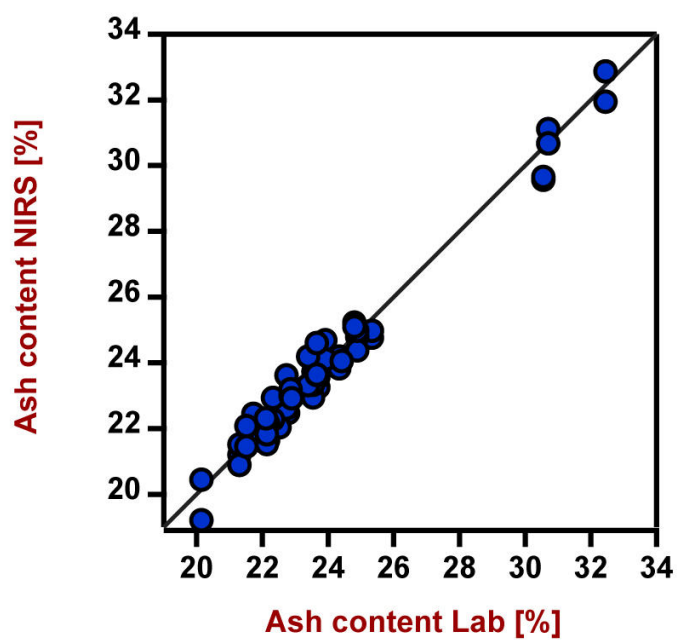


Figure 3. Correlation diagram and the respective figures of merit for the prediction of ash content in coal using a DS2500 Solid Analyzer. The lab value was evaluated according to ASTM D3174.

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

RESULT VOLATILE CONTENT

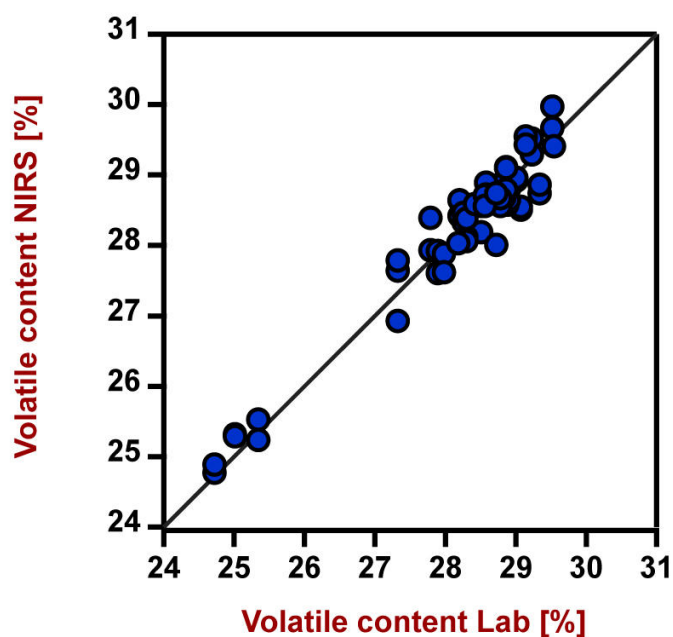


Figure 4. Correlation diagram and the respective figures of merit for the prediction of volatile content in coal using a DS2500 Solid Analyzer. The lab value was evaluated according to ASTM D3175.

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

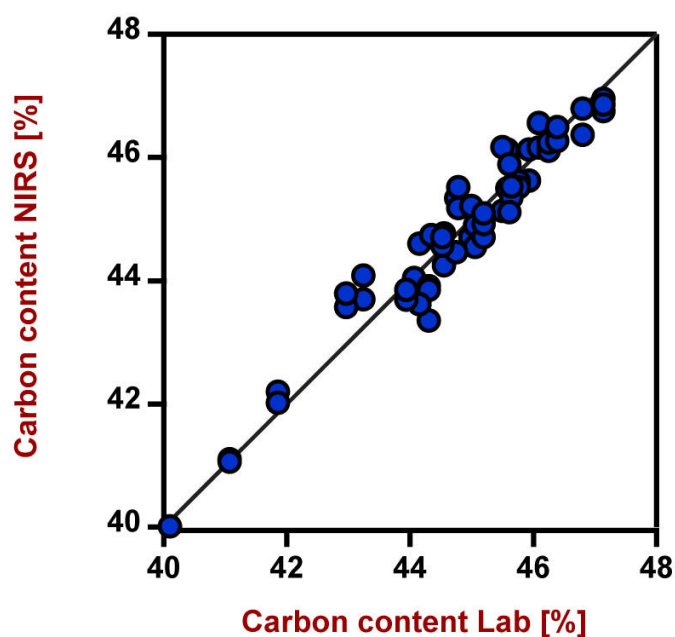


Figure 5. Correlation diagram and the respective figures of merit for the prediction of fixed carbon content in coal using a DS2500 Solid Analyzer. The lab value was evaluated according to ASTM D3172 (furnace combustion method).

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

RESULT WATER CONTENT

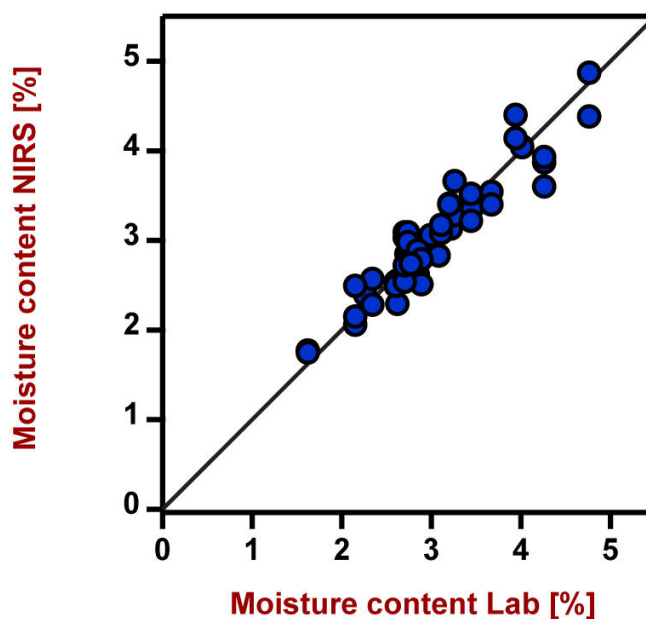


Figure 6. Correlation diagram and the respective figures of merit for the prediction of moisture content in coal using a DS2500 Solid Analyzer. The lab value was evaluated according to ASTM D3173 (furnace drying method).

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

坚固结实的近红外光谱仪,用于生产环境和试验室中的质量检查。

DS2500 分析仪是经过验证的灵活解决方案,用于对整个生产链过程中的固体、乳膏和液体进行常规分析。其坚固结实的设计使 DS2500 Analyzer 分析仪不受灰尘、湿度、振动和温度波动的影响,因此非常适用于在恶劣的生产环境中使用。

DS2500 涵盖了从 400 到 2500 nm 的整个光谱范围,并能在不到一分钟时间内提供准确和可再现的结果。

DS2500 Analyzer 满足制药行业的要求,并由于操作简便而能帮助用户完成其日常工作任务。

由于与设备匹配,附件可以承受任何具有挑战性的样品类型,例如:粒料之类的粗颗粒固体或乳膏之类的半固体样品,可获得结果。测量固体的时候,使用 MultiSample Cup 可以提高生产率,可以自动批量测量多 9 个样品。