Application Note AN-NIR-022

近赤外分析計 (NIR) による石油製品の分析 (セタン指数、TAN、芳香族、硫黄なと)

Rapid determination of RON, MON, AKI, aromatic content, and density

In recent years, there has been a significant push to reduce the environmental impacts of fuels through improvements to fuel quality. This requires engines to be more efficient, along with increasing the octane content of fuel so higher compression engines can be utilized. The determination of key quality parameters of gasoline, namely research octane number (RON, ASTM D2699-19), motor octane number (MON, ASTM D2700-19), anti knock index (AKI), aromatic content (ASTM D5769-15), and density, conventionally requires several different analytical methods, which are laborious and need trained personnel. This application note demonstrates that the XDS RapidLiquid Analyzer, operating in the visible and near-infrared spectral region (Vis- NIR), provides a cost-efficient and fast solution for the multiparameter analysis of gasoline.

EXPERIMENTAL EQUIPMENT

Gasoline samples were measured with the XDS RapidLiquid Analyzer (RLA) in transmission mode over the full wavelength range (400–2500 nm). Reproducible spectrum acquisition was achieved using the built-in temperature controlled sample holder. For convenience, disposable vials with a path length of 8 mm were used, which made a cleaning procedure unnecessary. The Metrohm software package Vision Air Complete was used for data acquisition and prediction model development.

Figure 1. XDS RapidLiquid Analyzer and 8 mm disposable vial filled with a gasoline sample.

Table 1. Hardware and software equipment overview

Equipment	Metrohm number
XDS RapidLiquid Analyzer	2.921.1410
Disposable vials, 8 mm diameter, transmission	6.7402.000
Vision Air 2.0 Complete	6.6072.208

RESULTS

The obtained Vis-NIR spectra (Figure 2) were used to create prediction models for the determination of several key fuel parameters. The quality of the prediction models was evaluated using correlation diagrams, which display a correlation between the Vis-NIR prediction and primary method values. The respective figures of merit (FOM) display the expected precision of a prediction during routine analysis.

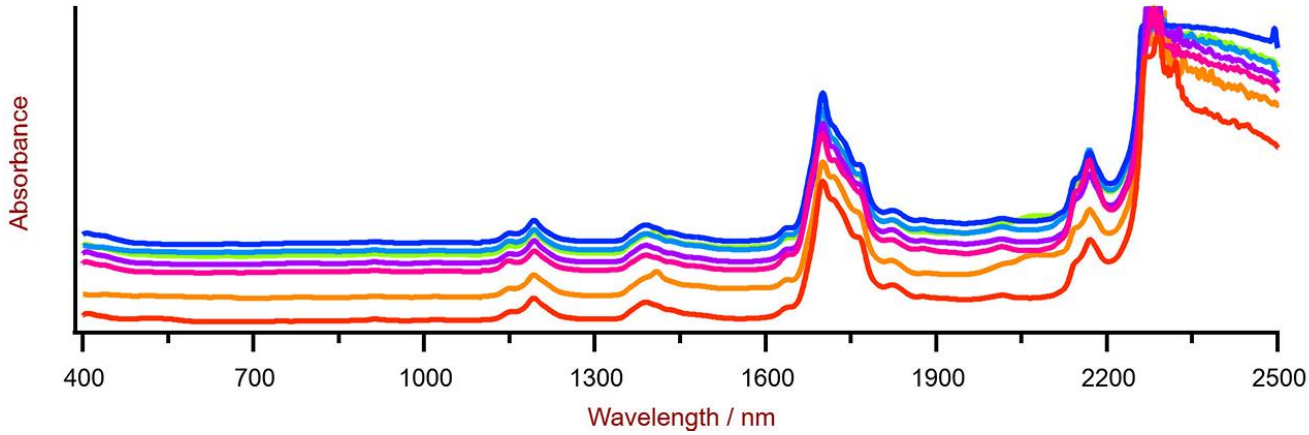

Figure 2. This selection of gasoline Vis-NIR spectra was obtained using a XDS RapidLiquid Analyzer and 8 mm disposable vials. For display reasons a spectra offset was applied.

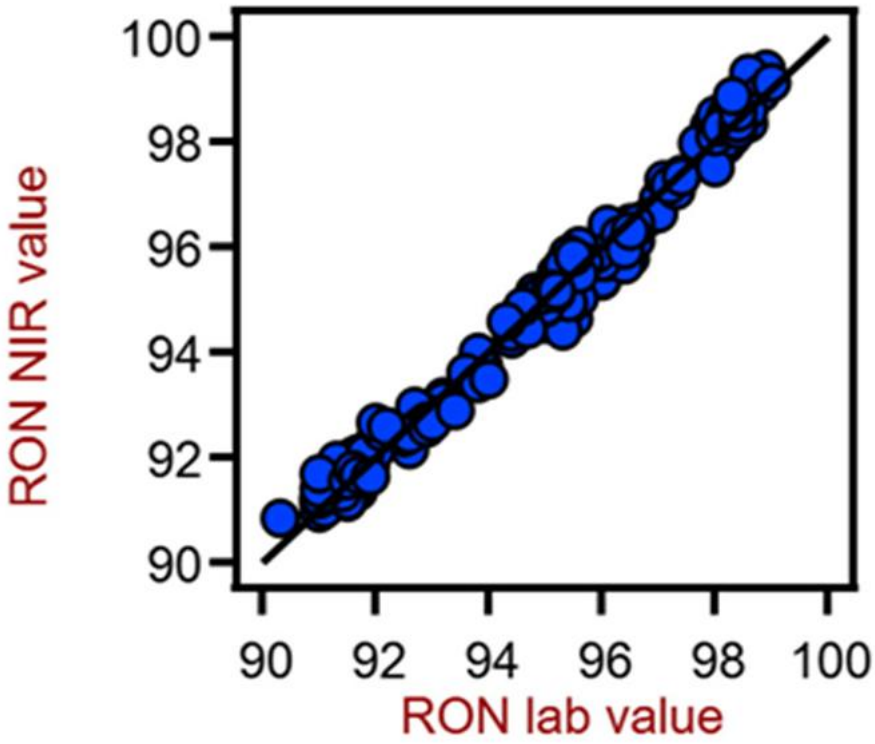

Figure 3. Correlation diagram for the prediction of the RON value in gasoline using a XDS RapidLiquid Analyzer. The reference lab values were determined according to CFR engine tests under controlled conditions.

Table 2. Figures of merit for the prediction of the RON value in gasoline using a XDS RapidLiquid Analyzer.

Figures of merit	Value
R^2	0.989
Standard error of calibration	0.26
Standard error of cross-validation	0.29

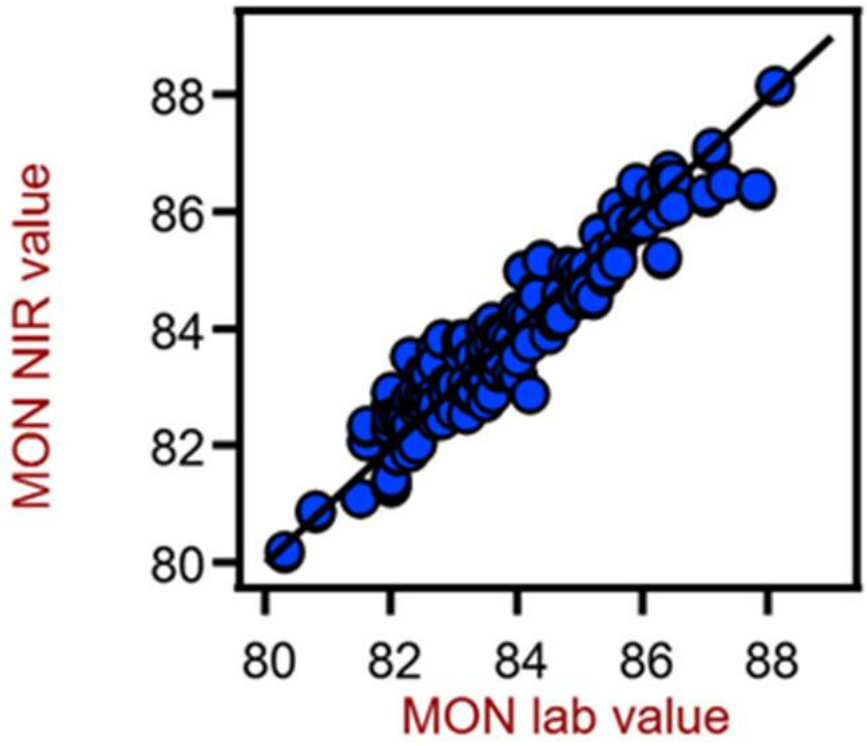

Figure 4. Correlation diagram for the prediction of the MON value in gasoline using a XDS RapidLiquid Analyzer. The reference lab values were determined according to CFR engine tests under controlled conditions.

Table 3. Figures of merit for the prediction of the MON value in gasoline using a XDS RapidLiquid Analyzer.

Figures of merit	Value
R^2	0.889
Standard error of calibration	0.50
Standard error of cross-validation	0.53

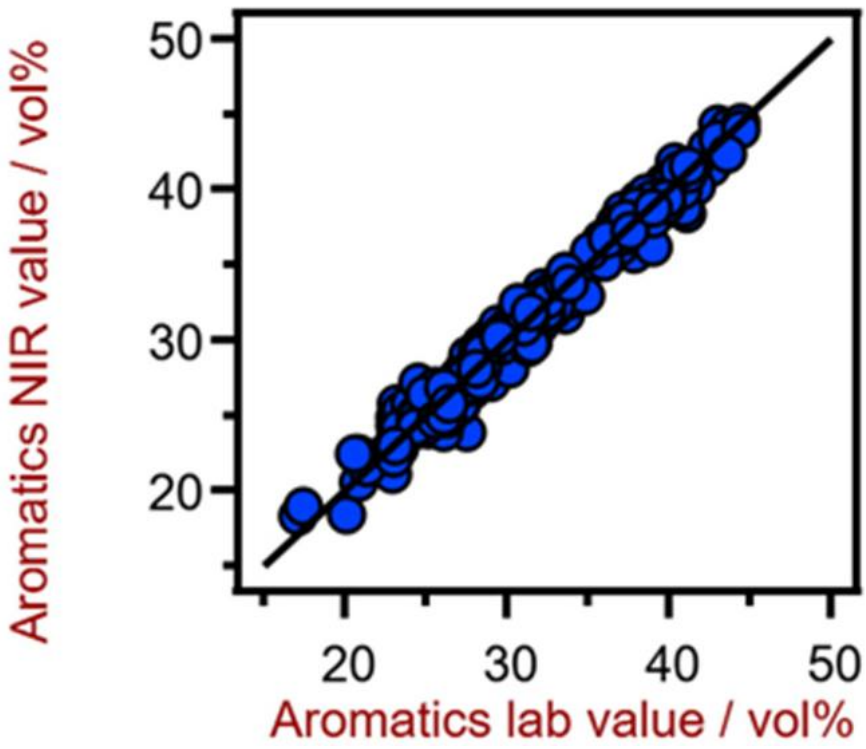

Figure 5. Correlation diagram for the prediction of the aromatics content in gasoline using a XDS RapidLiquid Analyzer. The lab values were determined with gas chromatography/mass spectrometry techniques.

Table 4. Figures of merit for the prediction of the aromatics content in gasoline using a XDS RapidLiquid Analyzer.

Figures of merit	Value
R^2	0.974
Standard error of calibration	0.97 vol%
Standard error of cross-validation	1.07 vol%

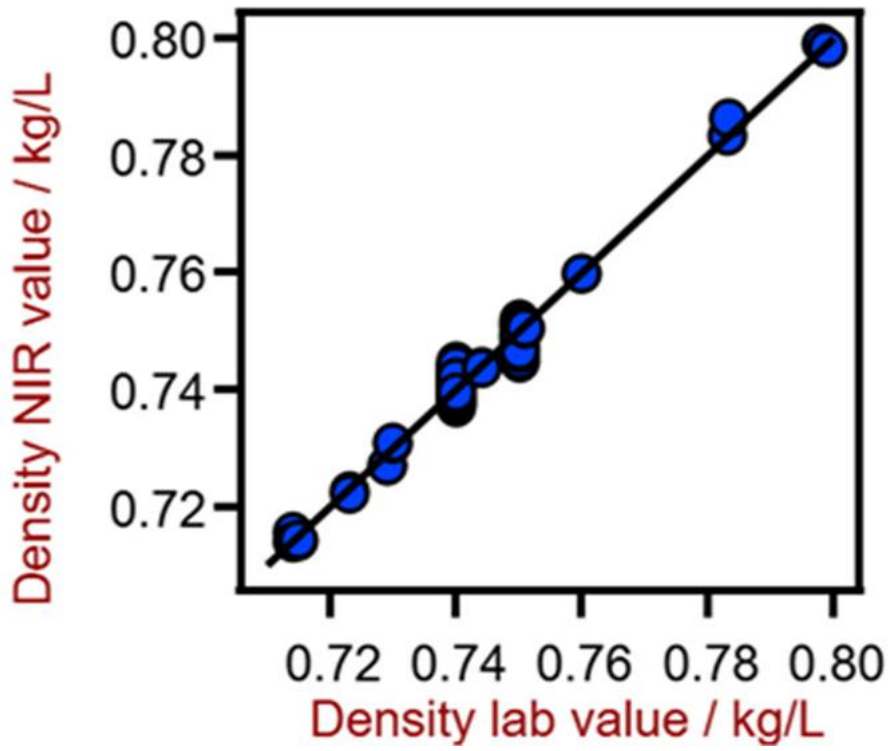

Figure 6. Correlation diagram for the prediction of gasoline density using a XDS RapidLiquid Analyzer. The lab values were determined using a density meter.

Table 5. Figures of merit for the prediction of gasoline density using a XDS RapidLiquid Analyzer.

Figures of merit	Value
R^2	0.973
Standard error of calibration	0.0021 kg/L
Standard error of cross-validation	0.0023 kg/L

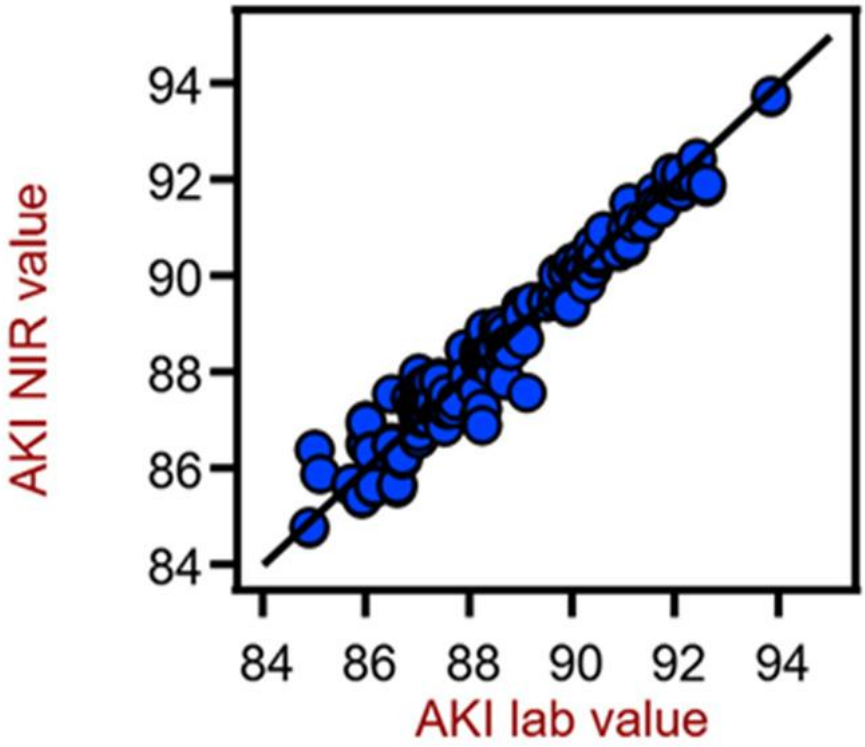

Figure 7. Correlation diagram for the prediction of AKI value in gasoline using a XDS RapidLiquid Analyzer. The reference lab values were determined according to CFR engine tests under controlled conditions.

Table 6. Figures of merit for the prediction of the AKI value in gasoline using a XDS RapidLiquid Analyzer.

Figures of merit	Value
R^2	0.945
Standard error of calibration	0.45
Standard error of cross-validation	0.46

CONCLUSION

This application note shows the feasibility of NIR spectroscopy for the analysis of RON, MON, AKI, aromatic content, and density. In comparison to wet chemical methods (Table 7), the time to result is a major advantage of NIR spectroscopy, since a single measurement is performed within one minute.

Table 7. Time to result with conventional testing methods

Parameter	Method	Time to result
RON	CFR engine test	~30 minutes per sample
MON	CFR engine test	~30 minutes per sample
AKI	CFR engine test	~30 minutes per sample
Aromatic content	Gas Chromatography	~45 minutes per sample

To view the information for all key parameters and to get the latest information, please check out our precalibrations:

Pre-calibrations

CONTACT

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NIRS XDS RapidLiquid Analyzer

あらゆる種類の液体および懸濁液の迅速て正確な分析。

NIRS XDS RapidLiquid Analyzerは、液体製剤および物質の迅速て正確な分析を可能にします。ホタンを押すたけて正確な測定結果か得られるため、NIRS XDS RapidLiquid Analyzerはラホおよひフロセスにおける品質管理のための信頼性か高くシンフルなソリューションてす。サンフルは、再使用可能な石英製キュヘットまたは使い捨てカラス製ハイアルに置かれます。温度調整されたサンフルコンハートメントは、再現性のある分析条件、およひそれによる正確な測定結果を保証します。

Vision Air 2.0 Complete

Vision Air - 汎用性に優れた分光法ソフトウェア。

Vision Air Complete は、規制環境下での使用のための、操作の容易な最新のソフトウェアソリューションてす。

Vision Air の利点の概要:

- 調整済みのユーザーインターフェースを伴う個別のソフトウェアアフリケーションにより、直観的かつ容易な操作か保証されます。
- 作業手順の容易な作成およびメンテナンス
- 安全かつ容易なテータ管理のための SQL テータへース

ハーション Vision Air Complete (66072208) には、可視近赤外分光法を用いた品質管理のための全てのアフリケーションか含まれています:

- 装置管理およびテータ管理のためのアフリケーション
- メソット開発のためのアフリケーション
- ルーチン分析のためのアフリケーション

その他の Vision Air Complete ソリューション:

- 66072207 (Vision Air Network Complete)
- 66072209 (Vision Air Pharma Complete)
- 66072210 (Vision Air Pharma Network Complete)