



Application Note AN-NIR-022

汽油质量控制

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.

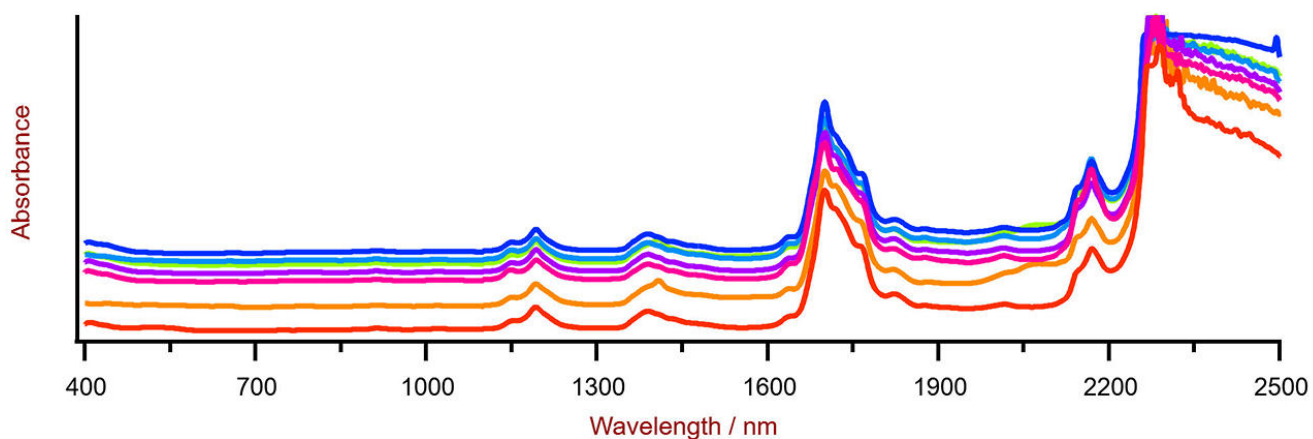


Figure 2. This selection of gasoline Vis-NIR spectra was obtained using a XDS RapidLiquid Analyzer and 8 mm disposable vials. For display reasons a spectra offset was applied.

RESULTS

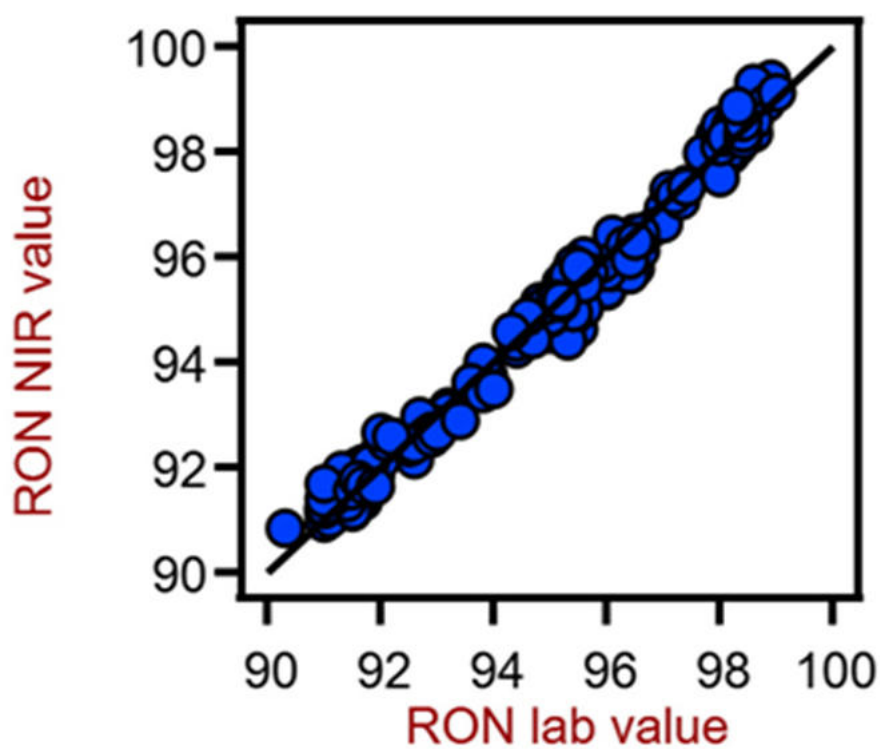


Figure 3. Correlation diagram for the prediction of the RON value in gasoline using a XDS RapidLiquid Analyzer. The reference lab values were determined according to CFR engine tests under controlled conditions.

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

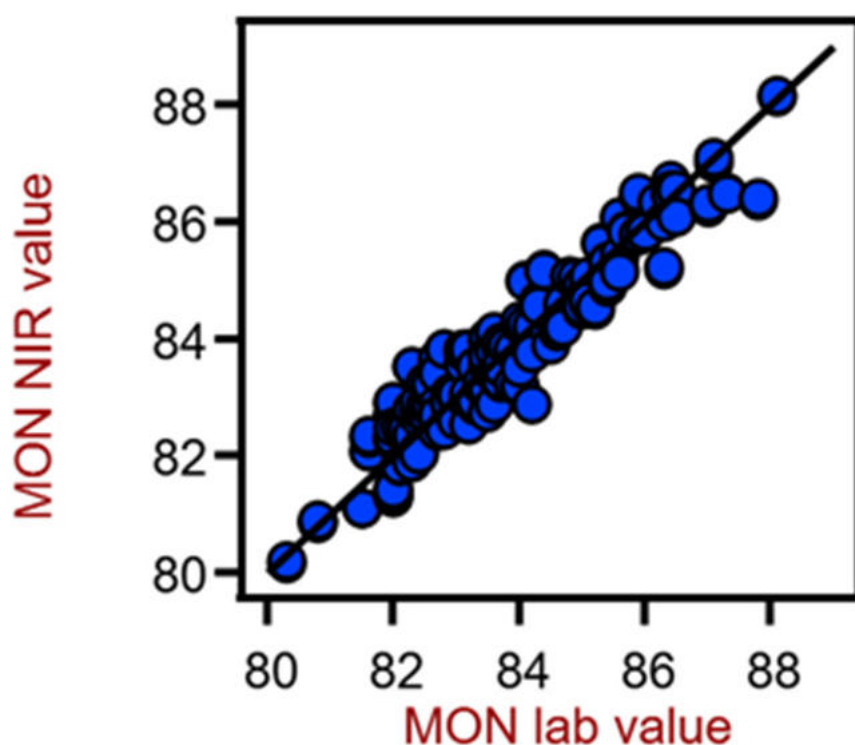


Figure 4. Correlation diagram for the prediction of the MON value in gasoline using a XDS RapidLiquid Analyzer. The reference lab values were determined according to CFR engine tests under controlled conditions.

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

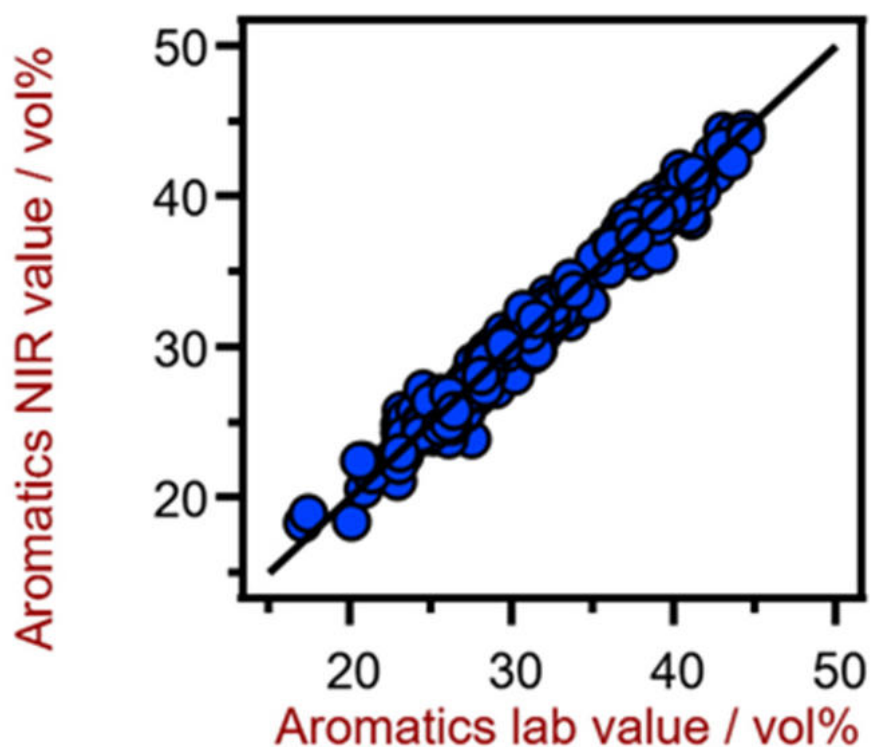


Figure 5. Correlation diagram for the prediction of the aromatics content in gasoline using a XDS RapidLiquid Analyzer. The lab values were determined with gas chromatography/mass spectrometry techniques.

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%

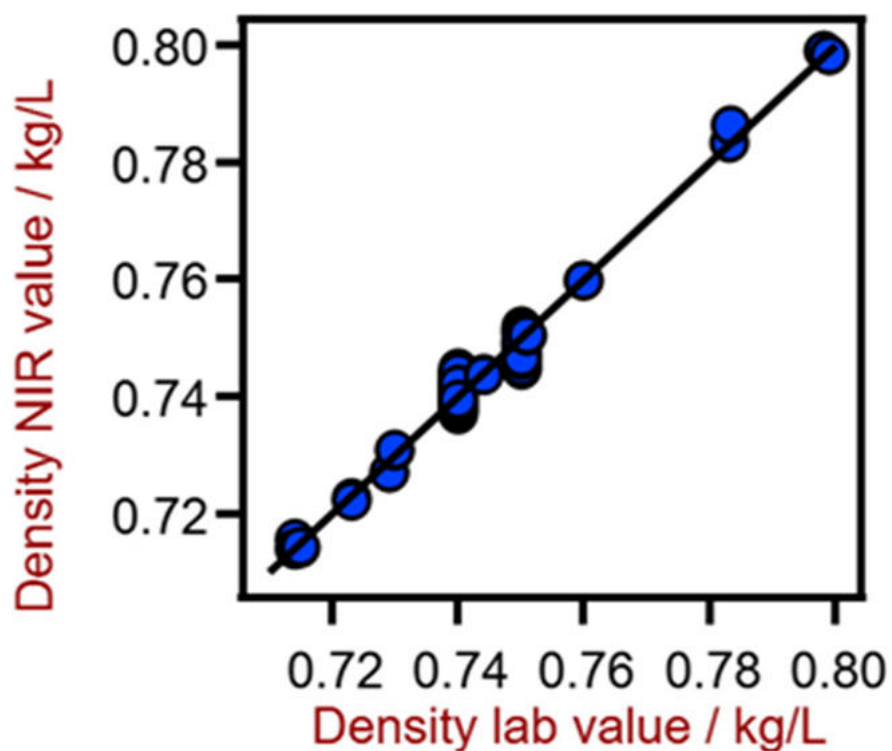


Figure 6. Correlation diagram for the prediction of gasoline density using a XDS RapidLiquid Analyzer. The lab values were determined using a density meter.

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

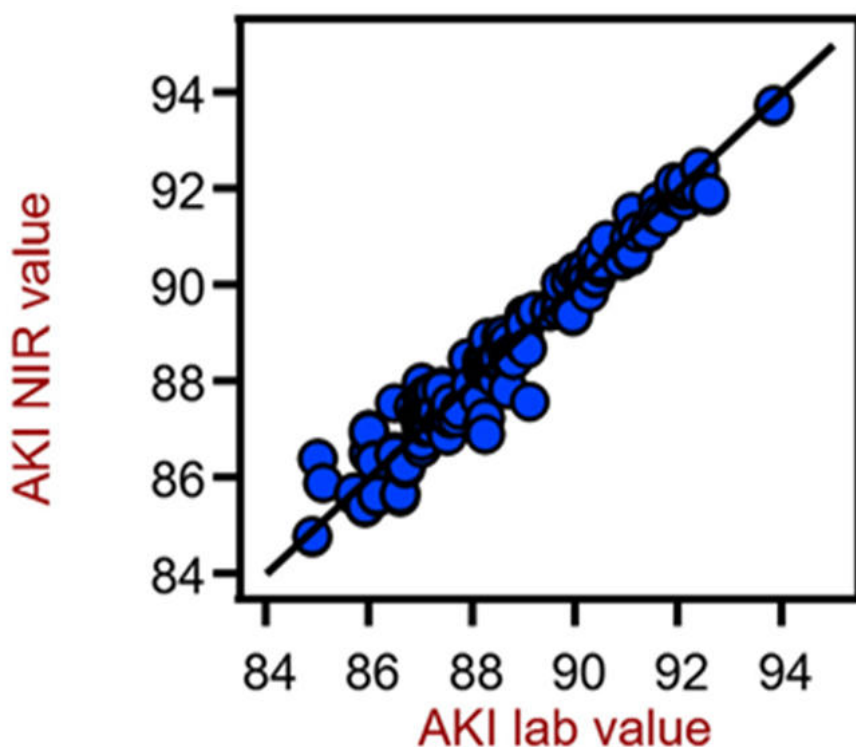


Figure 7. Correlation diagram for the prediction of AKI value in gasoline using a XDS RapidLiquid Analyzer. The reference lab values were determined according to CFR engine tests under controlled conditions.

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](#)

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NIRS XDS RapidLiquid Analyzer 快速精确地分析各种液体和悬浮液.

NIRS XDS RapidLiquid Analyzer 分析仪可快速精确地分析液体制剂和物质。按下按钮即可得到精确的测量结果,NIRS XDS RapidLiquid Analyzer 是适用于实验室和工艺过程中质量控制的可靠且方便的解决方案。样品将被预置在可重复使用的石英比色皿或一次性玻璃瓶中;可控制温度的样品室确保可重现的分析条件,由此得到精确的测量结果。



Vision Air 2.0 Complete

Vision Air – 通用的光谱分析软件。

Vision Air Complete 是用于监管规范环境的先进易用的软件解决方案。

Vision Air 优点一览:

- 便捷的软件应用和经过适配的用户界面保证了直观简单的操作方式
- 操作过程的创建与维护方式简单
- SQL 数据库,可安全且简单地管理数据

Vision Air Complete (66072208) 版本包含所有用于可见近红外光谱分析质量保证过程的应用:

- 仪器和数据管理应用
- 方法开发应用
- 常规分析应用

其它 Vision Air Complete 解决方案:

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