



Application Note AN-NIR-080

柴油质量控制

Fast and straightforward determination of cetane index, flash point, CFPP, D95, and viscosity with NIRS

The cetane index (ASTM D613), flash point (ASTM D56), cold filter plug point (CFPP) (ASTM D6371), D95 (ISO 3405), and viscosity at 40 ° C (ISO 3104) are key parameters to determine for diesel quality. The primary test methods are labor intensive and challenging due to the need to use different analytical methods.

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 **simultaneous determination** of these key parameters in diesel. Vis-NIR spectroscopy allows for the analysis of diesel in **less than one minute** without sample preparation or using any chemical reagents.

EXPERIMENTAL EQUIPMENT

Diesel samples were measured in transmission mode with a XDS RapidLiquid Analyzer (RLA) over the full wavelength range (400–2500 nm). The built-in temperature controlled sample chamber was set to 30 ° C to provide a stable sample environment. For convenience reasons, disposable vials with a path length of 8 mm were used, which made a cleaning procedure obsolete. The Metrohm software package Vision Air Complete was used for data acquisition and prediction model development.



Figure 1. XDS RapidLiquid Analyzer with 8 mm disposable vial filled with a diesel 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 key diesel parameters. The quality of the prediction models was evaluated using correlation diagrams, which display the

correlation between Vis-NIR prediction and primary method values. The respective figures of merit (FOM) display the expected precision of a prediction during routine analysis.

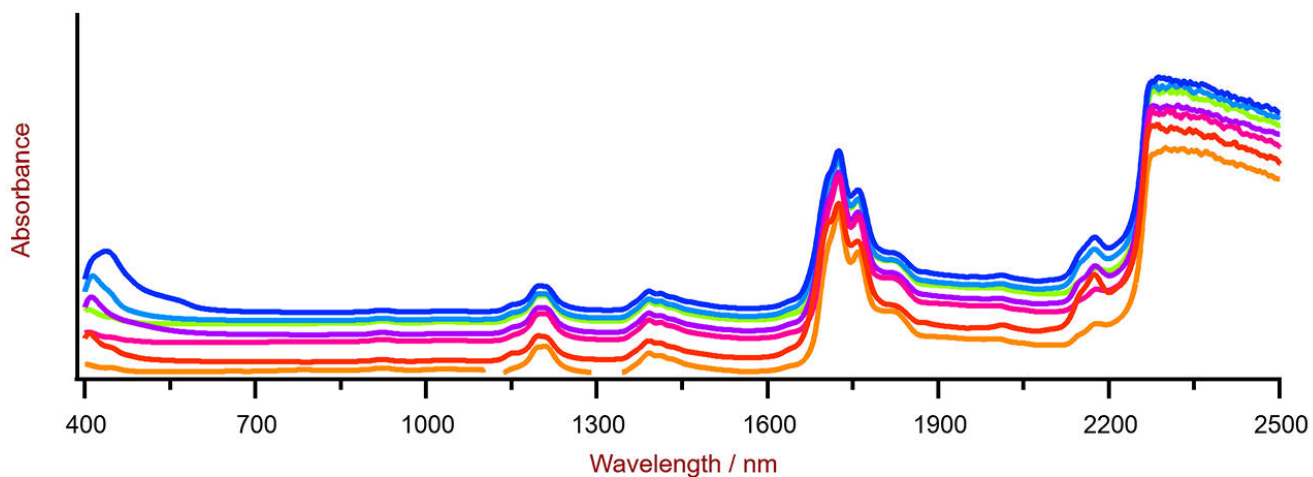


Figure 2. Selection of diesel Vis-NIR spectra obtained using a XDS RapidLiquid Analyzer and 8 mm disposable vials. For display reasons a spectra offset was applied.

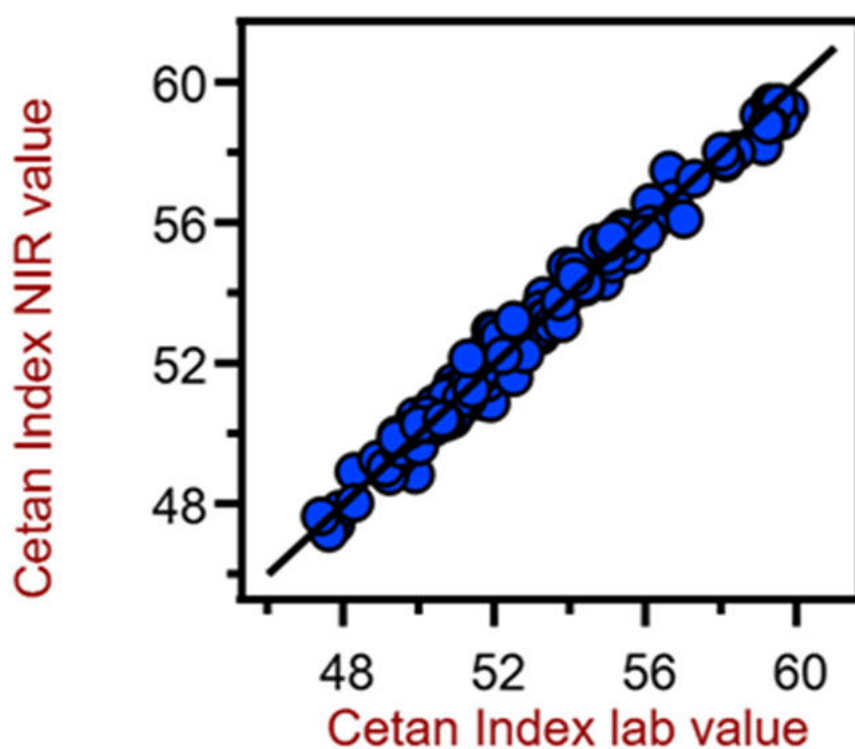


Figure 3. Correlation diagram for the prediction of the cetane index using a XDS RapidLiquid Analyzer. The cetane index lab value was calculated based on the density and distillation range.

Table 2. Figures of merit for the prediction of the cetane index using a XDS RapidLiquid Analyzer.

Figures of merit	Value
R^2	0.991
Standard error of calibration	0.093
Standard error of cross-validation	0.143

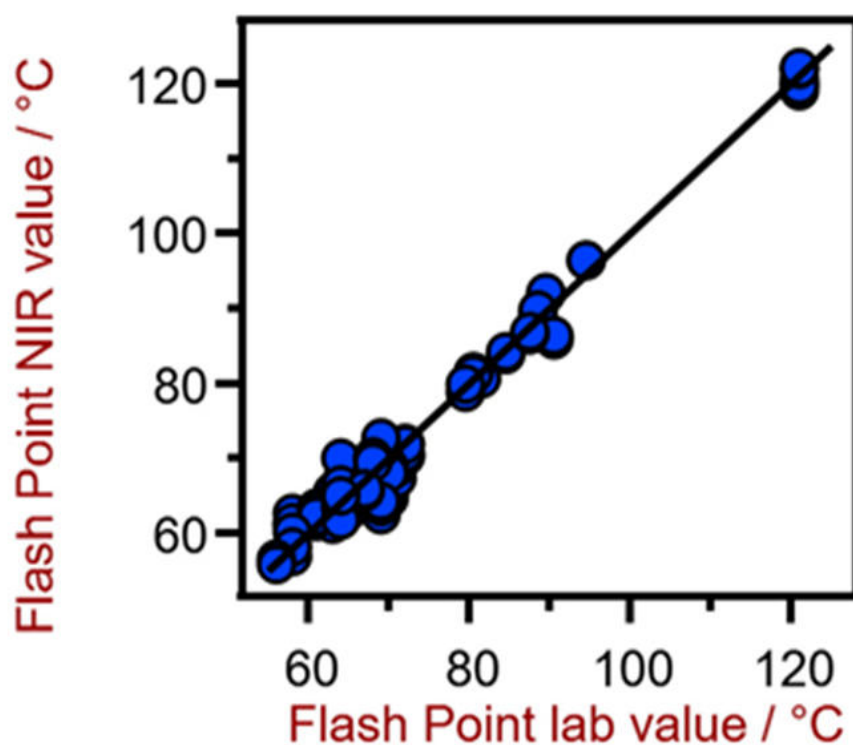


Figure 4. Correlation diagram for the prediction of the flash point using a XDS RapidLiquid Analyzer. The flash point lab value was evaluated using a dedicated flash point analyzer.

Table 3. Figures of merit for the prediction of the flash point using a XDS RapidLiquid Analyzer.

Figures of merit	Value
R^2	0.977
Standard error of calibration	2.22 ° C
Standard error of cross-validation	2.50 ° C

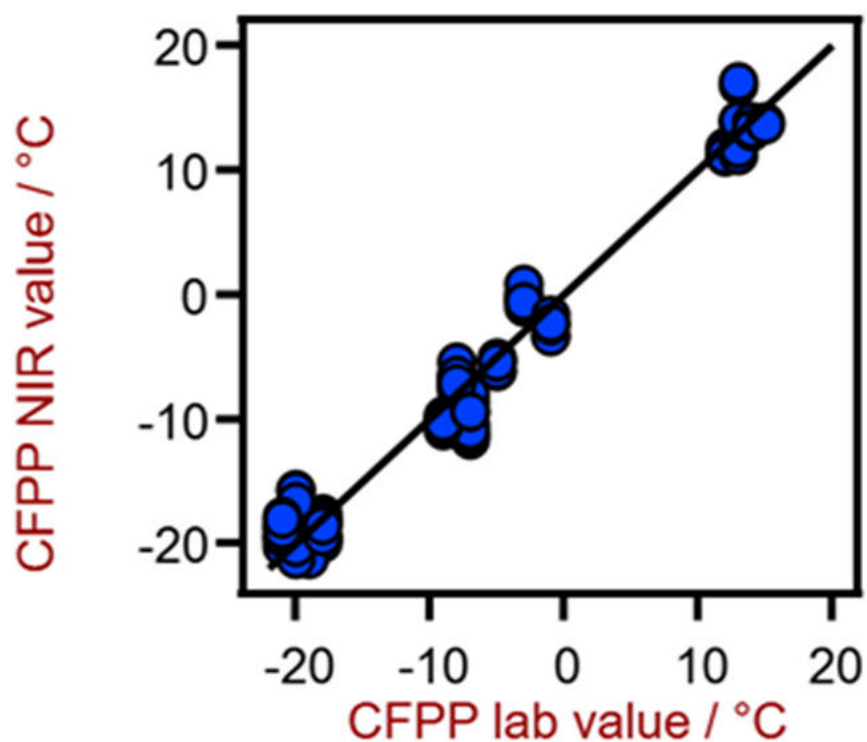


Figure 5. Correlation diagram for the prediction of CFPP using a XDS RapidLiquid Analyzer. The lab value was evaluated using flow meters.

Table 4. Figures of merit for the prediction of CFPP using a XDS RapidLiquid Analyzer.

Figures of merit	Value
R^2	0.973
Standard error of calibration	1.99 ° C
Standard error of cross-validation	2.24 ° C

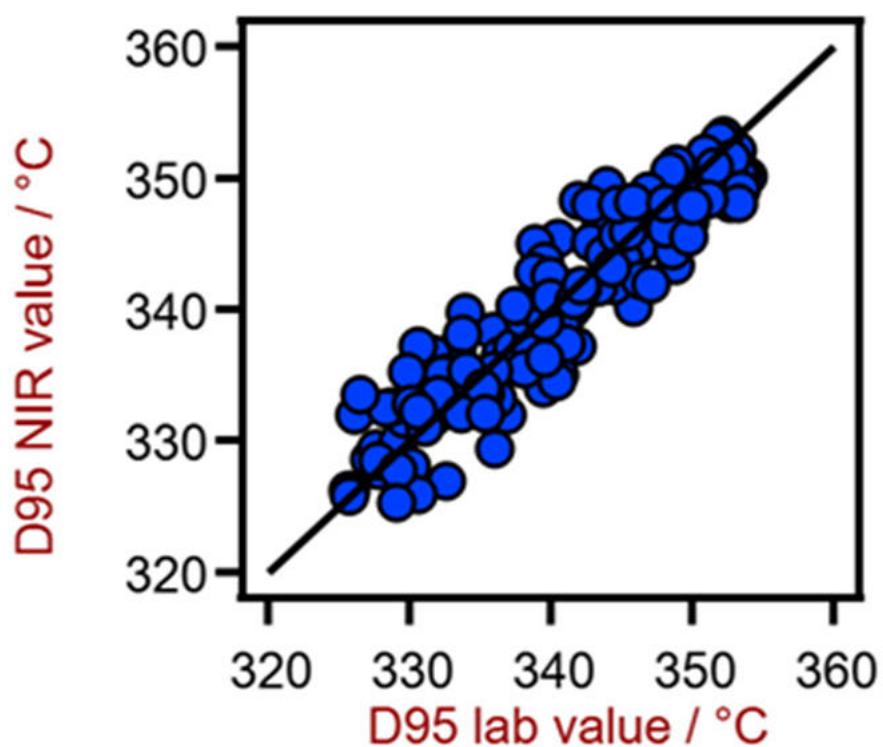


Figure 6. Correlation diagram for the prediction of D95 value using a XDS RapidLiquid Analyzer. The D95 lab value was evaluated using distillation.

Table 5. Figures of merit for the prediction of D95 using a XDS RapidLiquid Analyzer.

Figures of merit	Value
R^2	0.861
Standard error of calibration	3.07 °C
Standard error of cross-validation	3.47 °C

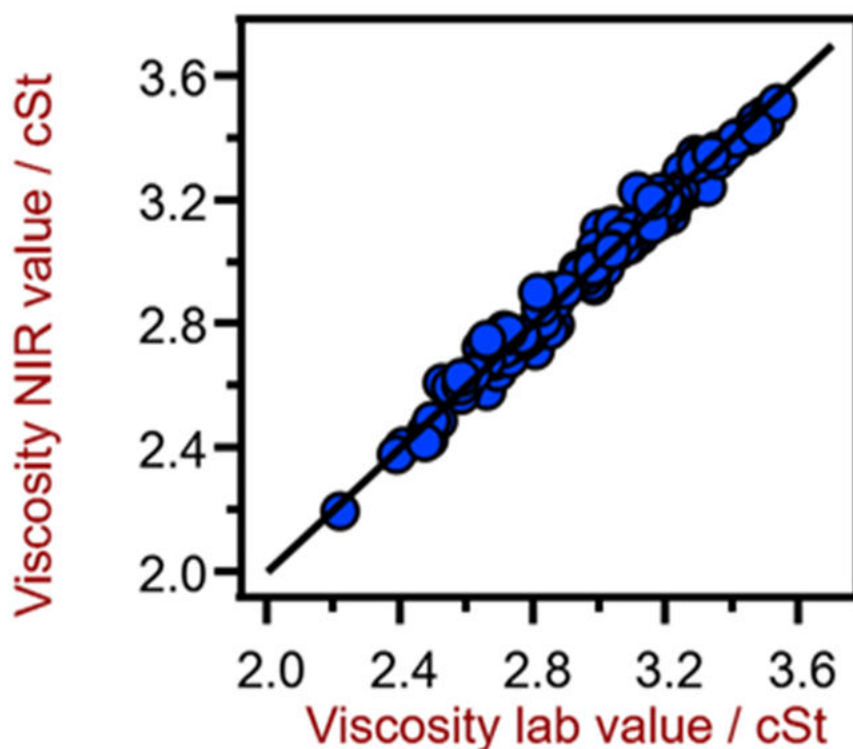


Figure 7. Correlation diagram for the prediction of the viscosity at 40 °C using a XDS RapidLiquid Analyzer. The viscosity lab value was evaluated using viscometry.

Table 6. Figures of merit for the prediction of the viscosity at 40 °C using a XDS RapidLiquid Analyzer.

Figures of merit	Value
R^2	0.983
Standard error of calibration	0.038 cSt
Standard error of cross-validation	0.047 cSt

CONCLUSION

This study demonstrates the feasibility of NIR spectroscopy for the analysis of the key parameters of diesel samples. In comparison to the standard methods, **no sample preparation is needed**. Samples are analyzed as they are, which allows for

simple operation when using NIR spectroscopy.

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)