

Application Note AN-NIR-096

Water in diesel with NIRS

Moisture in diesel fuel within seconds using NIR spectroscopy

Fuels can incorporate traces of water during the production process, in transport, and while in storage. Excessive water in fuels leads to several problems. For example, elevated water content in diesel fuel promotes biological growth in storage fuel tanks, which could lead to metal corrosion and formation of sludge and biofilms. This in turn clogs filters in fuel systems and results in damage to diesel engines.

The standard specification for diesel fuel quality includes multiple parameters, but dissolved water is the biggest risk factor. According to the European Committee for Standardization, the maximum acceptable amount of water in diesel fuel for commercialization is 200 mg/L (ppm) (EN 590). Usually, this is determined by Karl Fischer (KF) titration, yet this method requires chemicals and takes about five minutes to perform. This Application Note describes how near-infrared spectroscopy (NIRS) is a faster and more cost-efficient alternative to KF titration for the **prediction of water content** in diesel fuel.

EXPERIMENTAL EQUIPMENT

Samples of diesel with varying water content (from 66 to 362 mg/L) were measured with an OMNIS NIR Analyzer Liquid in transmission mode (1000–2250 nm). Reproducible spectrum acquisition was achieved using the built-in temperature control. For convenience, disposable vials with a pathlength of 8 mm were used, which made cleaning of the sample vessels unnecessary. The OMNIS software was used for all data acquisition and prediction model development.



Figure 1. OMNIS NIR Analyzer and a sample filled in a disposable vial.

Table 1. Hardware and software equipment overview.

Equipment	Article number
OMNIS NIR Analyzer Liquid	2.1070.0010
Holder OMNIS NIR, vial, 8 mm	6.07401.070
Disposable vial, 8 mm, transmission	6.7402.240
OMNIS Stand-Alone license	6.06003.010
Quant Development software license	6.06008.002

RESULT

The NIR spectra (**Figure 2**), along with the corresponding reference values, were used to create a prediction model for quantification of the moisture content in diesel samples. The quality of the prediction model was evaluated using the correlation diagram shown in **Figure 3** which displays a very high correlation between the NIR prediction and the measured values of water content using KF titration (reference values). The respective figures of merit (FOM) display the expected precision of a prediction during routine analysis.

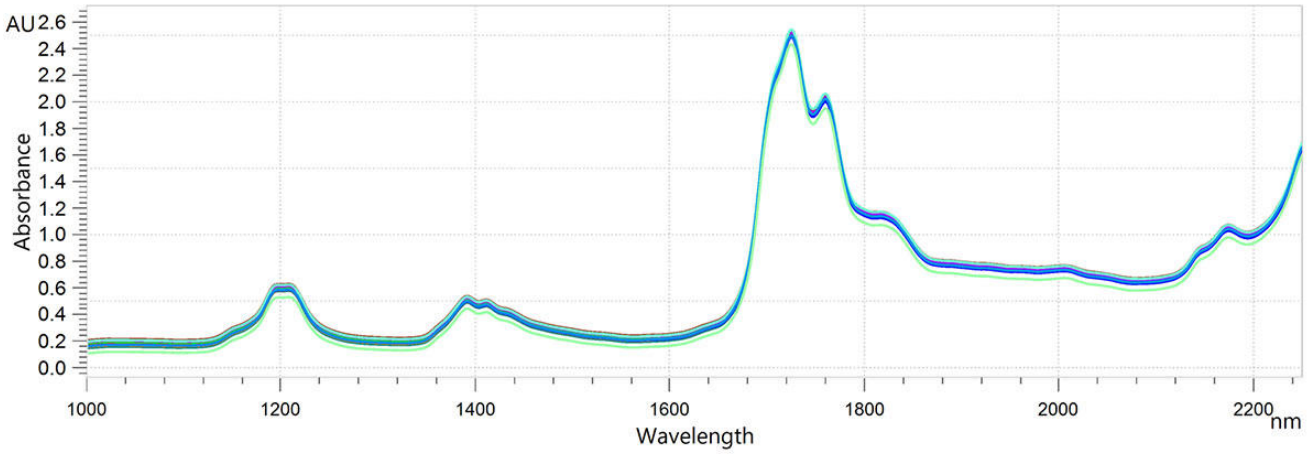

Figure 2. Stacked collection of NIR spectra from diesel samples analyzed with the OMNIS NIR Analyzer Liquid.

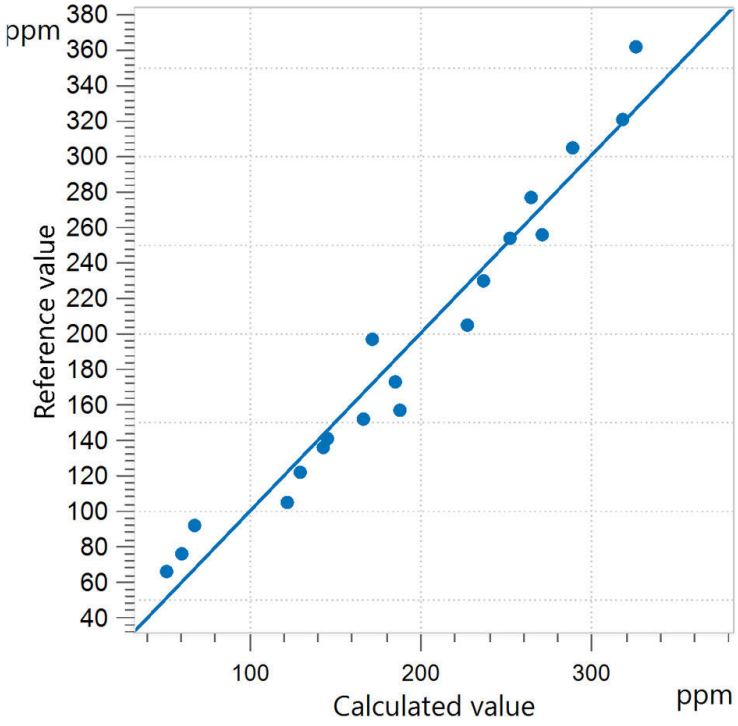

Figure 3. Correlation diagram and the respective figures of merit for the prediction of water content in diesel using an OMNIS NIR Analyzer Liquid. The lab values were evaluated using KF titration.

R^2	SEC (mg/L)	SECV (mg/L)
0.957	12	17

CONCLUSION

This Application Note demonstrates the feasibility to determine a key parameter for the quality control of diesel fuel – water content – with NIR spectroscopy. The main advantages of NIR spectroscopy over wet chemical methods like KF titration are that running costs are significantly lower and time-to-result is significantly reduced to a few seconds. Additionally, no chemicals are required, and the technique is non-destructive to samples.

Table 2. Time to result overview for KF titration.

Parameter	Method	Time to result
Water	Karl Fischer titration	5 minutes

Internal reference: AW NIR CH-0064-112021

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CONFIGURATION



OMNIS NIR Analyzer Liquid
用于液体样品的近红外光谱仪。
OMNIS NIR Analyzer 按照瑞士质量标准开发和制造,是用于整个生产链中常规分析的近红外光谱解决方案。最新技术的应用以及与现代 OMNIS Software 的集成,体现在这款 NIR 光谱仪的速度、操作性和灵活应用上。
OMNIS NIR Analyzer Liquid 的优势概览:

- 液体样品测量时间小于 10 秒
- 样品温度调节范围为 25–80 °C
- 自动检测样品容器的放入和移除
- 可轻松集成至自动系统,或与其它分析技术(滴定)联用。
- 支持多种不同路径长度的样品容器



OMNIS NIR8 mm

适合 8 mm 一次性小管的 OMNIS NIR Analyzer 的小管支架 (6.7402.240)。



8 mm 100

100 个玻璃(硼硅)一次性样品瓶,具有 8 mm 的光路长度,适用于分析透射中的液体。一次性样品瓶交付时带有所属的螺旋塞(件数 = 100)。

兼容:

- 支架 OMNIS NIR,小管,8 mm (**6.07401.070**)
- DS2500 支架适用于 8 mm 一次性样品瓶 (**6.7492.020**)

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Quant Development

用于在独立 OMNIS Software 安装套件中编写和编辑量化模型的软件许可证。