

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 (<u>reference</u> <u>values</u>). The respective figures of merit (FOM) display the expected precision of a prediction during routine analysis.



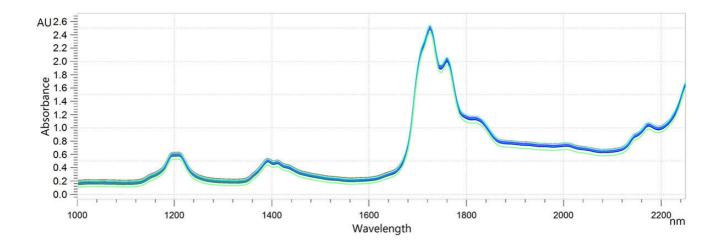


Figure 2. Stacked collection of NIR spectra from diesel samples analyzed with the OMNIS NIR Analyzer Liquid.

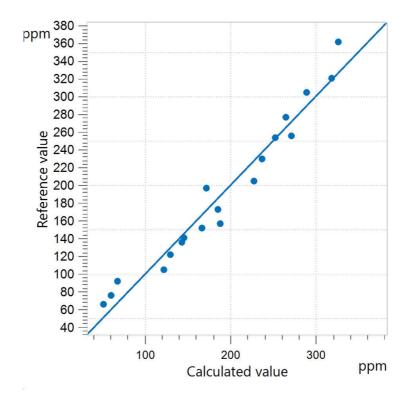


Figure 3. Correlation diagram and the respective figures of merit for the prediction of water content in diesel using an OMNIS NIR Analyzer Liquid. The lab values were evaluated using KF titration.

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

CONTACT

メトロームジャパン株式会 社 143-0006 東京都大田区平 和島6-1-1 null 東京流通センター アネックス9階

metrohm.jp@metrohm.jp



CONFIGURATION





液体サンフルのための近赤外スヘクトロメーター。

OMNIS NIR Analyzer は、スイスの品質基準に従って開発・製造された、生産チェーン全体に沿ったルーチン分析のための近赤外分光法 (NIRS) ソリューションです。最新技術の適用と最新の OMNIS Software への統合は、この NIR スヘクトロメーターの速度、ユーサヒリティ、柔軟な使用に反映されています。

OMNIS NIR Analyzer Liquid の利点の概要:

- 10 秒未満て液体サンフルを測定
- 25° C~80° Cのサンフルの温度制御
- サンフル容器の取り付けと取り外しの自動検出
- オートメーションシステムへの統合、またはそ の他の分析技術 (滴定) との連結か容易
- 様々な光路長を有する多数のサンフル容器に対応



OMNIS NIR8 mm

8 mm 使い捨てハイアル (6.7402.240) のための OMNIS NIR Analyzer 用ハイアルホルター。



8 mm100

透過した液体を分析するための光学的距離 8 mm のカラス製 (ホウケイ酸塩) 使い捨てハイアル 100 個。使い捨てハイアルには閉し蓋 (個数 = 100) か付属されています。

次の製品と互換性かあります:

- ホルター OMNIS NIR、ハイアル、8 mm (6.07401.070)
- 使い捨てハイアル 8 mm 用の DS2500 ホルタ - (6.7492.020)



OMISS A WHOLE NEW LEVEL OF PERFORMANCE



OMNIS

WindowsTMコンヒューター上のOMNISソフトウェアをスタントアローン操作することか可能になります。

特徴:

- ライセンスには、既に1つのOMNISテハイスライセンスか含まれています。
- メトローム・ライセンシンクホータルにて、ア クティフ化する必要かあります。
- 他のコンヒューターに移行することはてきません。

Quant Development

スタントアロン型 OMNIS Software のインストールにおける定量化モテルの作成と編集のためのソフトウェアライセンス。

