



Application Note AN-NIR-096

# Quality Control of Diesel

## Moisture determination within one minute using NIRS

Fuels can incorporate traces of water during the production process, in transport, and while in storage. Excessive water in fuels poses several problems. For example, elevated water content in diesel fuel promotes biological growth in storage tanks, which could lead to metal corrosion and formation of sludge and biofilms. This in turn can cause blockage of fuel filters and therefore damage vehicle fuel injection systems. The standard specification for diesel fuel quality includes multiple parameters, but water contamination is the biggest risk factor.

According to the European Committee for Standardization, the maximal acceptable amount of water in diesel 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 contents (from 103 to 379 mg/L) were measured with a DS2500 Liquid Analyzer in transmission mode (400–2500 nm). Reproducible spectrum acquisition was achieved using the built-in temperature control at 40 ° C. For convenience, disposable vials with a pathlength of 8 mm were used, which made cleaning of the sample vessels unnecessary. The Metrohm software package Vision Air Complete was used for all data acquisition and prediction model development.



**Figure 1.** DS2500 Liquid Analyzer and a sample filled in a disposable vial.

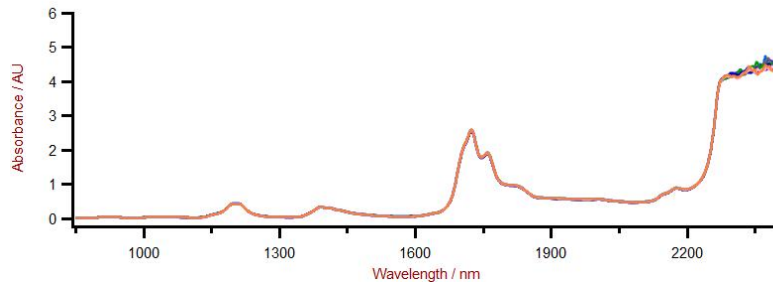
**Table 1.** Hardware and software equipment overview

Equipment	Metrohm number
DS2500 Liquid Analyzer	2.929.0010
DS2500 Holder 8 mm vials	6.7492.020
Disposable vials, 8 mm	6.7402.000
Vision Air 2.0 Complete	6.6072.208

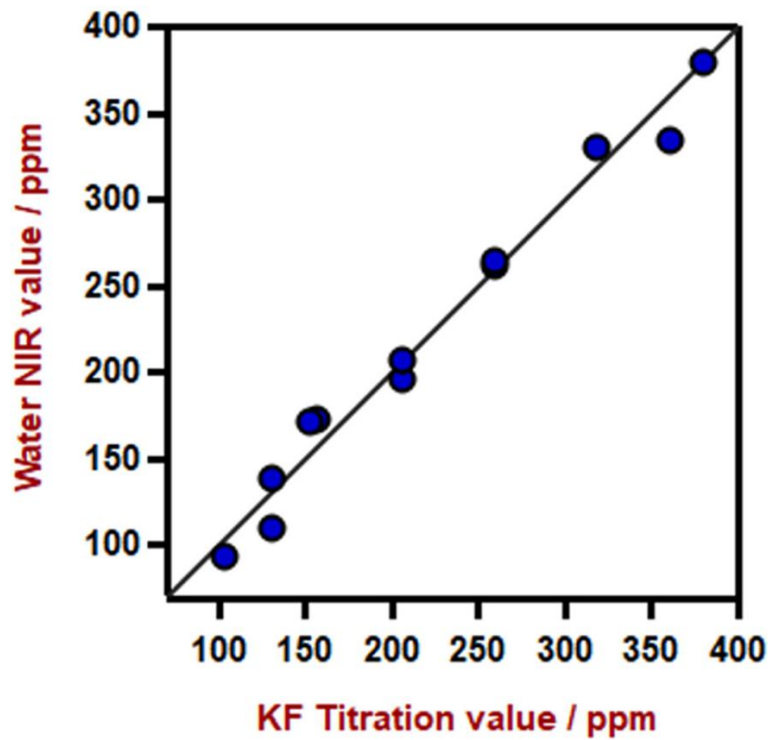
## RESULT

The obtained Vis-NIR spectra (**Figure 2**) 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, which

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



**Figure 2.** Vis-NIR spectra of diesel samples analyzed on a DS2500 Liquid Analyzer.



**Figure 3.** Correlation diagram for the prediction of water content in diesel using a DS2500 Liquid Analyzer. The lab value was evaluated using KF titration.

**Table 2.** Figures of merit for the prediction of water content in diesel using a DS2500 Liquid Analyzer.

Figures of merit	Value
$R^2$	0.9776
Standard error of calibration	16 ppm
Standard error of cross-validation	21 ppm

## CONCLUSION

This application note demonstrates the feasibility to determine a key parameter of the quality control of diesel fuel (water content) with NIR spectroscopy. The main advantages of Vis-NIR spectroscopy over wet chemical methods

are that running costs are significantly lower and time-to-result is significantly reduced. 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

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### DS2500 Liquid Analyzer 固耐用的近外光,用于生境和室中的量。

DS2500 Liquid Analyzer 是一成熟且活的解决方案,其用于在整个生中行液体常分析。其固耐用的使 DS2500 Liquid Analyzer 不受灰、潮湿、振的影,因此非常用于在劣的生境中使用。

DS2500 Liquid Analyzer 覆盖 400 至 2500 nm 的整个光范,将品加至 80° C 高温,并与各不同的一次性小瓶和石英比色皿兼容。因此,DS2500 Liquid Analyzer 可的个性化品要求,助在一分内得精和具有可重性的果。借助集成的品架装置和自的 Vision Air 件,保了用能松和安全地行操作。

如果是大的品量,可通将流通池与一个 Metrohm 机器人自器搭配使用的方法著提高生率。



### DS2500 8 mm 直径 8 mm 且更加智能的一次性玻璃小瓶支架



## Vision Air 2.0 Complete

### Vision Air – 通用的光分析件。

Vision Air Complete 是用于管范境的先易用的件解决方案。

Vision Air 点一:

- 独特的件用和配的用界面保了直的操作方式
- 操作程的建与方式
- SQL 数据,可安全且地管理数据

Vision Air Complete (66072208) 版本包含所有用于可近外光分析量保程的用:

- 器和数据管理用
- 方法用
- 常分析用

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)