Application Note AN-NIR-080

Automated quality control of diesel using near-infrared spectroscopy

Fast and straightforward determination of cetane index, cetane number, T95, density, flash point, and viscosity

Key parameters for diesel fuel quality testing include the cetane index (ASTM D613), flash point (ASTM D56), density (ASTM D975), T95 (ISO 3405), and viscosity at 40 °C (ISO 3104). Usually, determining these properties is labor intensive and time consuming, requiring multiple analytical techniques and dedicated instrumentation. The OMNIS NIR Analyzer Liquid provides a fast, reliable, and reagent-free solution to simultaneously determine these diesel fuel properties without sample preparation. The precise temperature control ensures that all samples are measured in compliance with ASTM D8340, ASTM D8321, and ASTM D6122. Combined with the OMNIS Sample Robot M – NIR, the system offers fully automated operation for maximum lab efficiency.

EXPERIMENTAL EQUIPMENT

Diesel samples were measured with an OMNIS NIR Analyzer Liquid (Figure 1) in transmission mode over a wavelength range of 1000–2250 nm. Reproducible spectrum acquisition was achieved using the built-in temperature control at 30 °C. An OMNIS Sample Robot M – NIR was used for fully automated sample measurement with disposable vials (8 mm pathlength). The vials are closed, which reduces the flammability risk for fuel samples to an absolute minimum. OMNIS Software was used for all data acquisition and prediction model development.

Figure 1. OMNIS NIR Analyzer Liquid combined with OMNIS Sample Robot M – NIR.

RESULT

The near-infrared spectra of diesel fuels (Figure 2), along with the corresponding reference values, were used to create prediction models for cetane number, cetane index, density, flash point, T95, and viscosity. The quality of the prediction models was evaluated using the correlation diagrams shown in Figures 3–8 which display a very high correlation between the NIR prediction and the measured values using standard methods. Out of the total, 25% of the samples were selected as the validation set and the other 75% as a calibration set. The respective figures of merit (FOM) display the expected precision of a prediction during routine analysis.

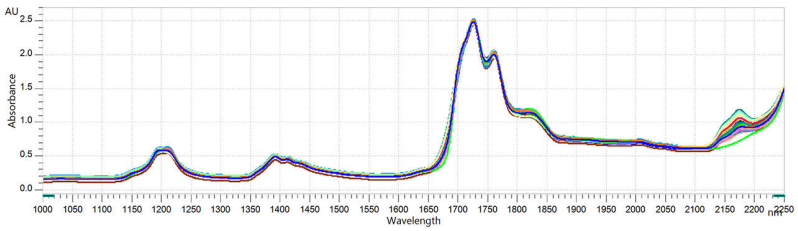


Figure 2. NIR spectra of diesel fuel samples analyzed at 30 °C with the OMNIS NIR Analyzer Liquid.

RESULT CETANE NUMBER IN DIESEL

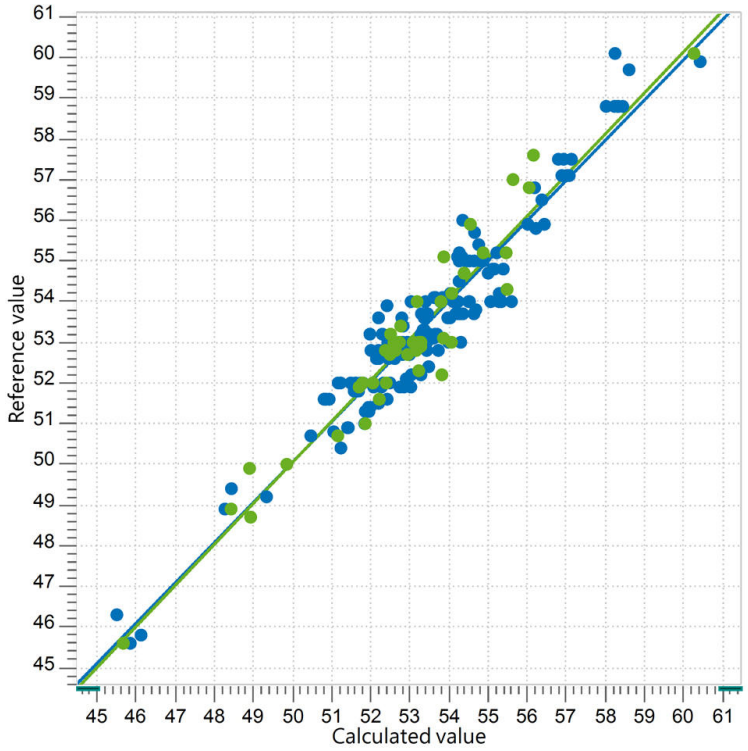


Figure 3. Correlation diagram and the respective FOMs for the prediction of cetane rating in diesel using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2P	SEC	SECV	SEP
0.922	0.61	0.65	0.67

RESULT CETANE INDEX IN DIESEL

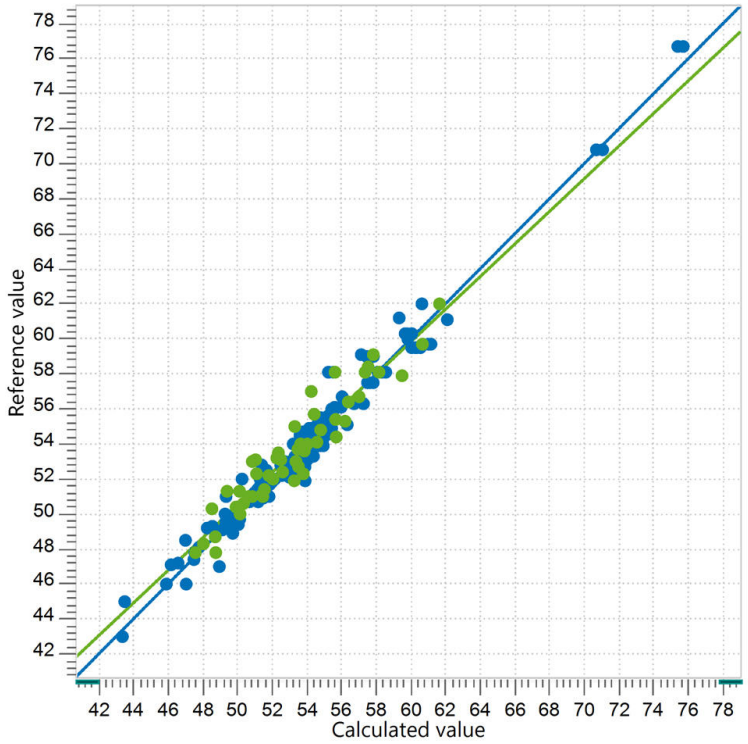


Figure 4. Correlation diagram and the respective FOMs for the prediction of cetane index in diesel using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2P	SEC	SECV	SEP
0.903	0.79	0.80	1.06

RESULT T95 IN DIESEL

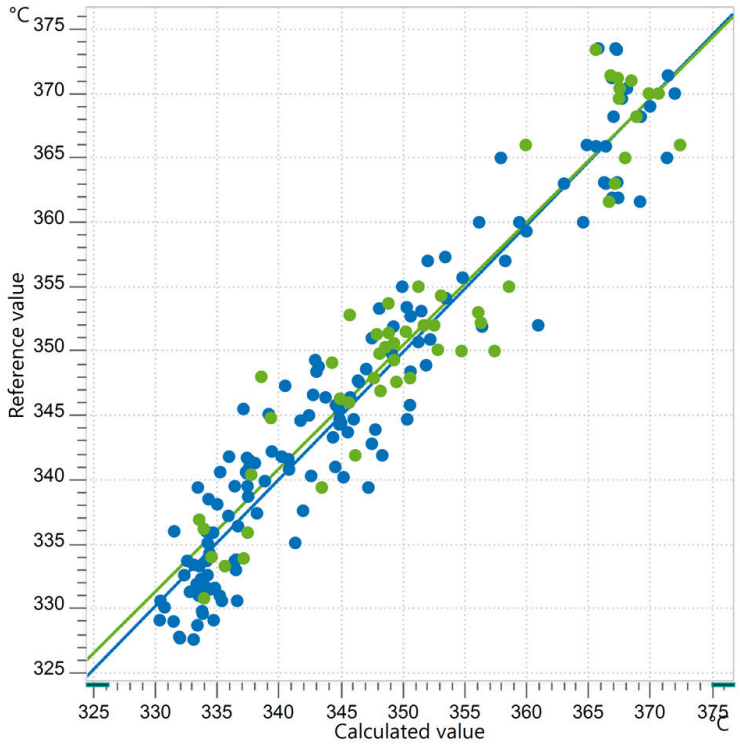


Figure 5. Correlation diagram and the respective FOMs for the prediction of T95 in diesel using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2P	SEC (°C)	SECV (°C)	SEP (°C)
0.895	3.42	3.69	3.75

RESULT VISCOSITY IN DIESEL

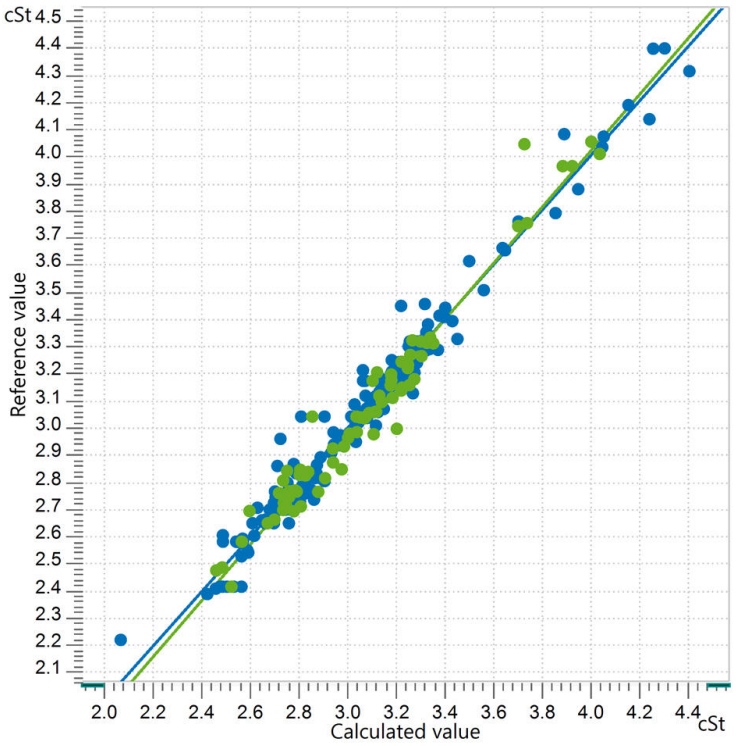


Figure 6. Correlation diagram and the respective FOMs for the prediction of viscosity in diesel using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2P	SEC (cSt)	SECV (cSt)	SEP (cSt)
0.962	0.06	0.06	0.07

RESULT FLASH POINT IN DIESEL

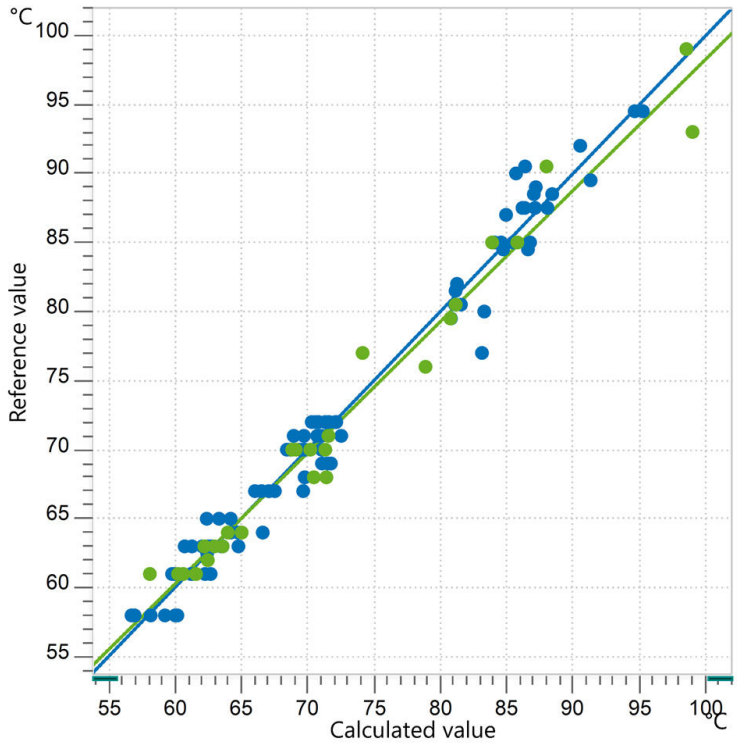


Figure 7. Correlation diagram and the respective FOMs for the prediction of flash point in diesel using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2P	SEC (°C)	SECV (°C)	SEP (°C)
0.973	1.24	1.58	1.90

RESULT DENSITY IN DIESEL

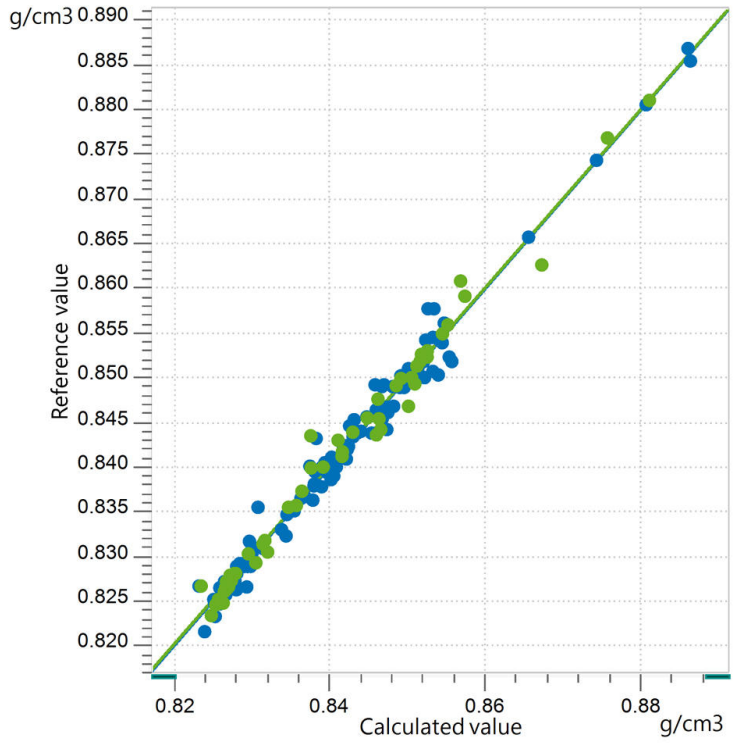


Figure 8. Correlation diagram and the respective FOMs for the prediction of density in diesel using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

R^2P	SEC (g/cm^3)	SECV (g/cm^3)	SEP (g/cm^3)
0.985	0.0012	0.0014	0.0016

CONCLUSION

This Application Note shows the feasibility of using NIR spectroscopy for the quality control of diesel. Determination of cetane index, cetane number, T95, density, flash point, and viscosity in diesel can be done simultaneously in a few seconds by using the OMNIS NIR Analyzer Liquid. The possibility of fully automated analysis in combination with the OMNIS Sample Robot M – NIR increases throughput, maximizing efficiency. With the OMNIS pre-calibration of diesel (6.06008.009), users can measure all the mentioned parameters from day one.

CONTACT

Metrohm Schweiz AG
Industriestrasse 13
4800 Zofingen
info@metrohm.ch

CONFIGURATION

OMNIS NIR Analyzer Liquid

Nahinfrarot-Spektrometer für Flüssigproben.

Der OMNIS NIR Analyzer ist die nach Schweizer Qualitätsstandards entwickelte und produzierte Nahinfrarotspektroskopie(NIRS)-Lösung für die Routineanalytik entlang der gesamten Produktionskette. Die Nutzung neuester Technologien und die Einbindung in die moderne OMNIS Software spiegeln sich in der Geschwindigkeit, der Bedienbarkeit und dem flexiblen Einsatz dieser NIR-Spektrometer wider.

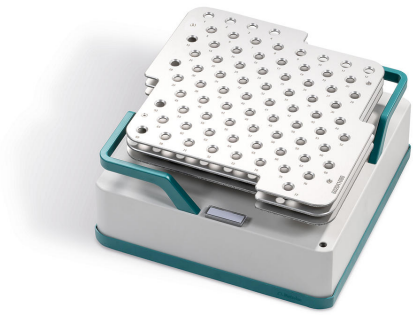
Die Vorteile des OMNIS NIR Analyzer Liquid im Überblick:

- Messungen von Flüssigproben in weniger als 10 Sekunden
- Temperaturregelung an der Probe von 25 °C – 80 °C
- Automatische Erkennung des Einsetzens und der Entnahme des Probengefässes
- Einfache Einbindung in ein Automationssystem oder Verknüpfung mit weiteren Analysentechniken (Titration)
- Unterstützung zahlreicher Probengefässe mit unterschiedlicher Pfadlänge

OMNIS Sample Robot M – NIR

OMNIS Sample Robot M – NIR für den direkten Einstieg in die voll automatisierte Spektroskopie. Das System bietet Platz für drei Probenracks für bis zu 231 Vials mit einem Durchmesser von 8 – 28 mm.

Der OMNIS Sample Robot M – NIR unterstützt die Analysen von sowohl flüssigen als auch festen Proben.



OMNIS Probenrack 77 x 8mm

OMNIS Probenrack zu OMNIS Sample Robot - NIR passend für 77 Einwegvials mit einer optischen Pfadlänge von 8 mm für Messungen in Transmission (6.7402.240).

Halter OMNIS NIR, Vial, 8 mm

Vialhalter für den OMNIS NIR Analyzer für 8 mm Einwegvials (6.7402.240).

Einwegvial, 8 mm, Transmission, Anz. 100

100 Einwegvials aus Glas (Borosilikat) mit einer optischen Pfadlänge von 8 mm für Analysen von Flüssigkeiten in Transmission. Die Einwegvials werden mit den zugehörigen Verschlussstopfen (Stückzahl = 100) geliefert.

Kompatibel mit:

- Halter OMNIS NIR, Vial, 8 mm (6.07401.070)
- DS2500 Halter für 8 mm Einwegvials (6.7492.020)

OMNIS

A WHOLE NEW LEVEL OF PERFORMANCE

OMNIS Stand-Alone Lizenz mit 2 Gerätelizenzen

Ermöglicht den Stand-Alone Betrieb der OMNIS Software auf einem WindowsTM Computer.

Merkmale:

- Die Lizenz enthält bereits zwei OMNIS Geräte Lizenzen
- Muss über das Metrohm Lizenzierungsportal aktiviert werden.

OMNIS

A WHOLE NEW LEVEL OF PERFORMANCE

Softwarelizenz Quant Development

Softwarelizenz für die Erstellung und Bearbeitung von Quantifizierungsmodellen in einer Stand-Alone OMNIS Software Installation.