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.

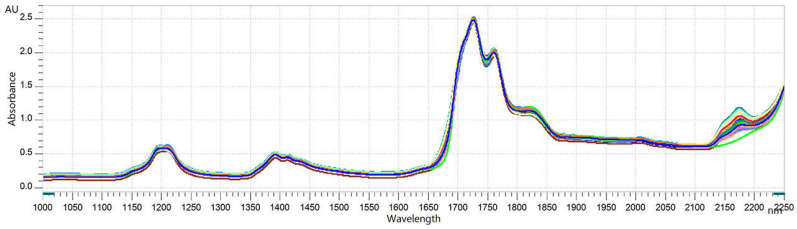



**Figure 2.** NIR spectra of diesel fuel samples analyzed at 30 °C with the OMNIS NIR Analyzer Liquid.

## RESULT CETANE NUMBER IN DIESEL

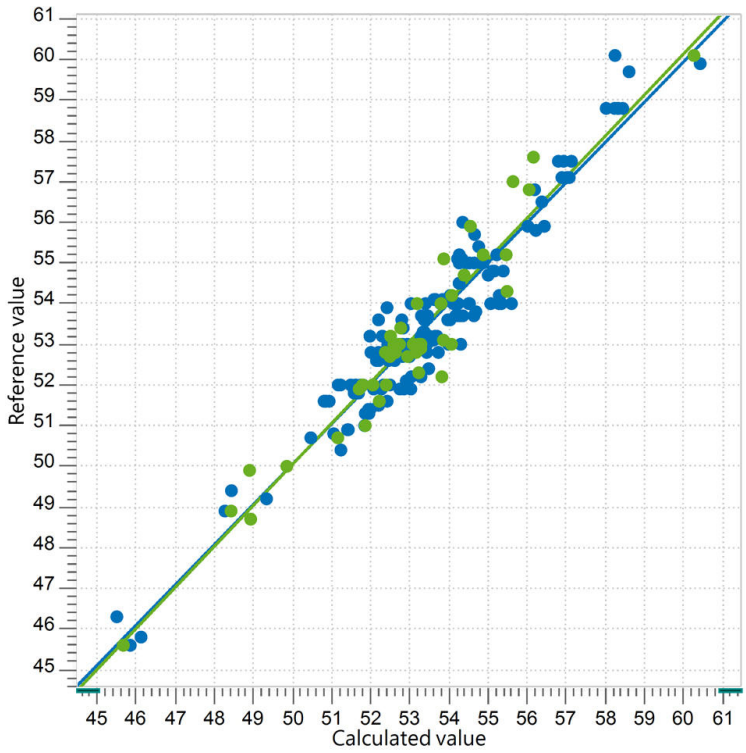



**Figure 3.** Correlation diagram and the respective FOMs for the prediction of cetane rating in diesel using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

| $R^2P$ | SEC | SECV | SEP |
|---|---|---|---|
| 0.922 | 0.61 | 0.65 | 0.67 |

## RESULT CETANE INDEX IN DIESEL

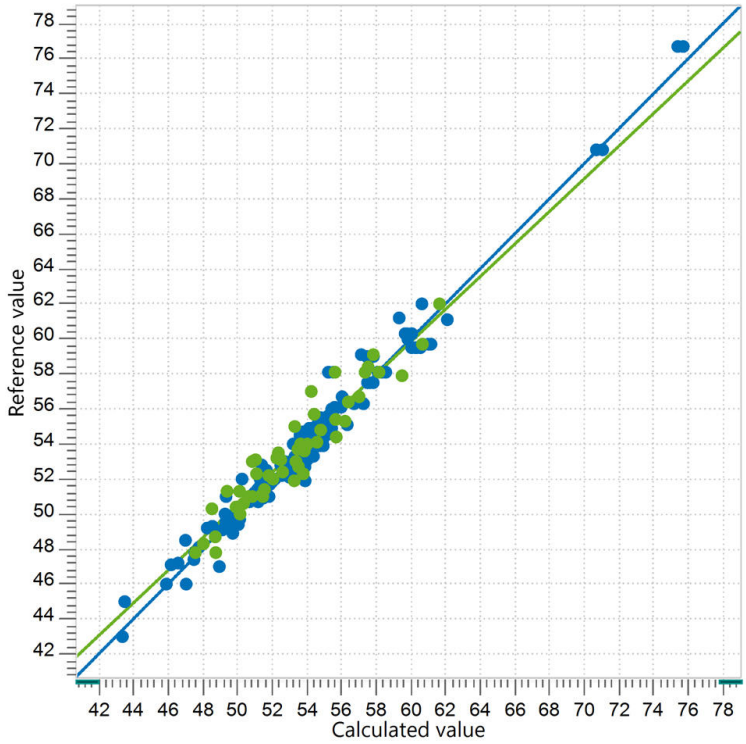



**Figure 4.** Correlation diagram and the respective FOMs for the prediction of cetane index in diesel using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

| $R^2P$ | SEC | SECV | SEP |
|---|---|---|---|
| 0.903 | 0.79 | 0.80 | 1.06 |

## RESULT T95 IN DIESEL

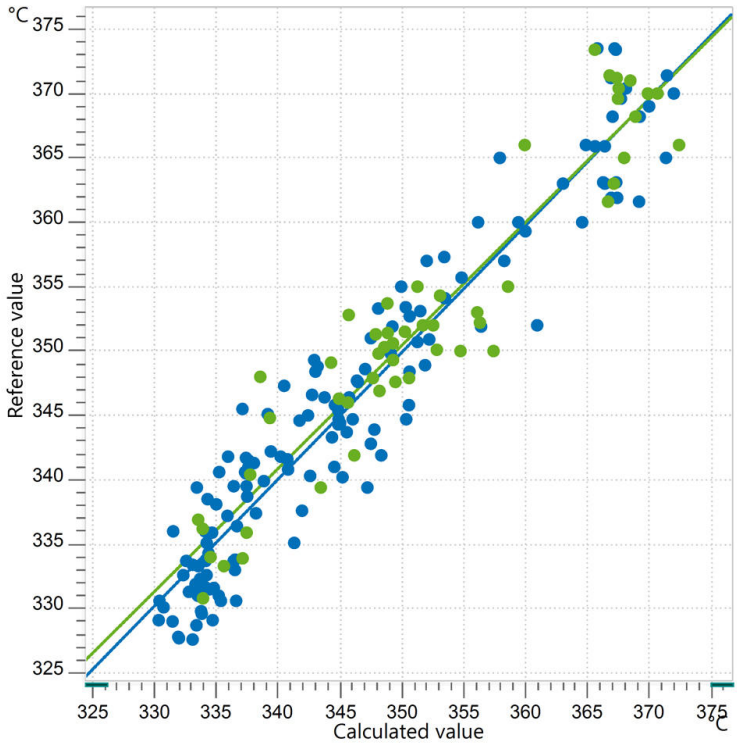



**Figure 5.** Correlation diagram and the respective FOMs for the prediction of T95 in diesel using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

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

## RESULT VISCOSITY IN DIESEL

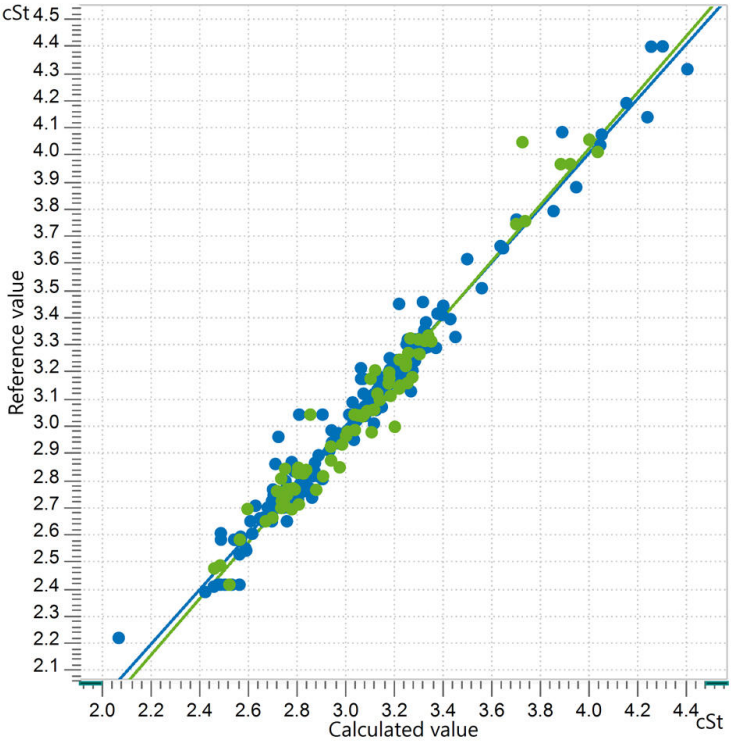



**Figure 6.** Correlation diagram and the respective FOMs for the prediction of viscosity in diesel using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

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

## RESULT FLASH POINT IN DIESEL

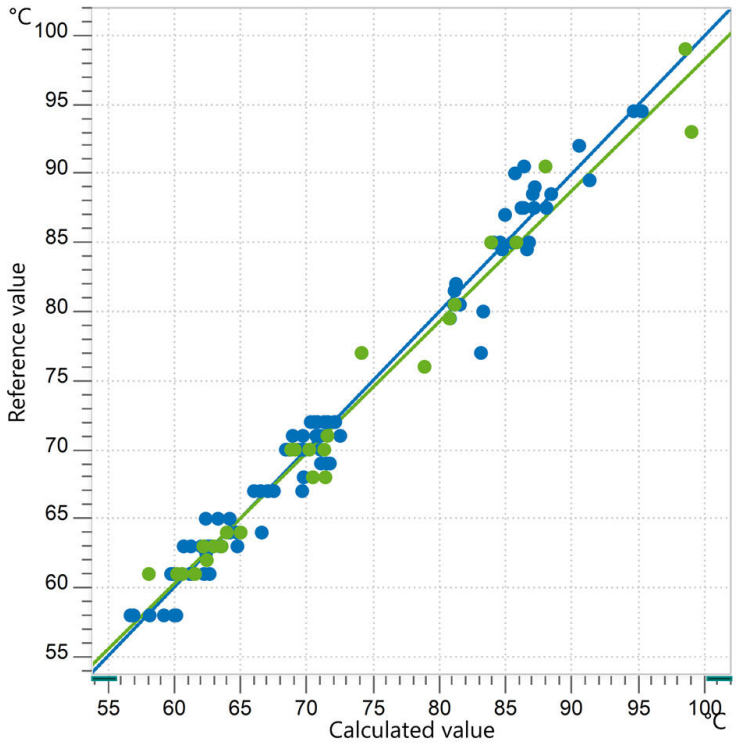



**Figure 7.** Correlation diagram and the respective FOMs for the prediction of flash point in diesel using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

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

## RESULT DENSITY IN DIESEL

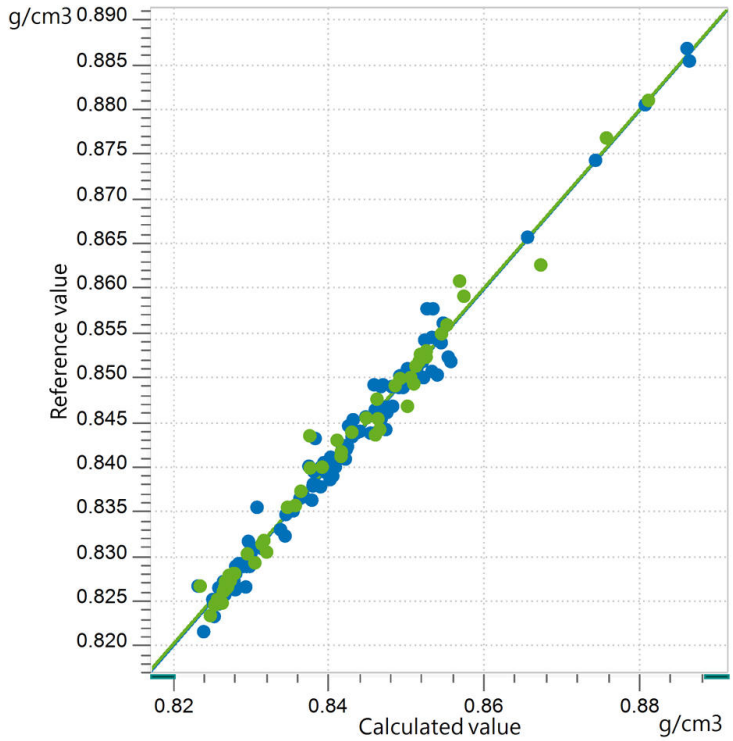



**Figure 8.** Correlation diagram and the respective FOMs for the prediction of density in diesel using an OMNIS NIR Analyzer Liquid. The calibration dataset is shown in blue, and the external validation dataset is in green.

| $R^2P$ | 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 Polska
ul. Centralna 27
05-816 Opacz-Kolonia
info@metrohm.pl

## CONFIGURATION

OMNIS NIR Analyzer Liquid

Near-infrared spectrometer for liquid samples.

Developed and produced in accordance with Swiss quality standards, the OMNIS NIR Analyzer is the near-infrared spectroscopy (NIRS) solution for routine analysis along the entire production chain. Its application of the latest technologies and its integration in the modern OMNIS Software are reflected in its speed, operability, and flexible utilization of this NIR spectrometer.

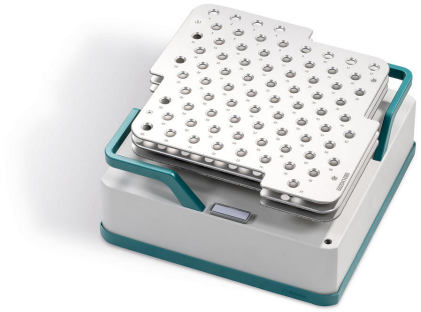
Overview of the advantages of the OMNIS NIR Analyzer Liquid:

- Measurements of liquid samples in less than 10 seconds
- Temperature control on the sample from 25–80 °C
- Automatic detection of the insertion and removal of the sample vessel
- Simple integration in an automation system or link with additional analysis technologies (titration)
- Supports numerous sample vessels with different path lengths

OMNIS Sample Robot M – NIR

OMNIS Sample Robot M – NIR for the direct transition to fully automated spectroscopy. The system provides space for 3 sample racks for up to 231 vials with diameters of 8–28 mm.

The OMNIS Sample Robot M – NIR supports the analyses of both liquid and solid samples.



### OMNIS sample rack 77 x 8 mm

OMNIS sample rack for OMNIS Sample Robot – NIR suitable for 77 disposable vials with an optical path length of 8 mm for measurements in transmission (6.7402.240).

### Holder OMNIS NIR, vial, 8 mm

Vial Holder for the OMNIS NIR Analyzer for 8 mm disposable vials (6.7402.240).

### Disposable vial, 8 mm, transmission, qty. 100

100 disposable glass vials (borosilicate) with an optical path length of 8 mm for analyses of liquids in transmission. The disposable vials are supplied with the associated stoppers (number of pieces = 100).

Compatible with:

- Holder OMNIS NIR, vial, 8 mm (6.07401.070)
- DS2500 holder for 8 mm disposable vials (6.7492.020)

OMNIS

A WHOLE NEW LEVEL OF PERFORMANCE

### OMNIS stand-alone license with 2 instrument licenses

Enables stand-alone operation of the OMNIS Software on a WindowsTM computer.

Features:

- The license already includes two OMNIS instrument licenses.
- Must be activated via the Metrohm licensing portal.

OMNIS

A WHOLE NEW LEVEL OF PERFORMANCE

### Software license Quant Development

Software license for the creation and editing of quantification models in a stand-alone OMNIS Software installation.