

Application Note AN-NIR-121

Water content in propylene glycol monomethyl ether (PGME)

Water determination possible within seconds using NIRS

Propylene glycol monomethyl ether (1-methoxy-2-propanol, or PGME) is one of many glycol ether solvents with a wide variety of applications. It is used as an intermediate and in formulations for industrial, professional, or consumer applications, mainly in surface coatings, inks for printing, cleaning solutions, deicing/anti-icing formulations, and agrochemical purposes. It is also used as an extractant and as a coalescing agent and flow improver in water-based paints.

Water in propylene glycol methyl ether is usually measured by Karl Fischer (KF) titration which requires chemicals and takes about five minutes per determination. This Application Note describes how near-infrared spectroscopy (NIRS) can be used as a faster and more cost-efficient alternative for water determination in PGME.

EXPERIMENTAL EQUIPMENT

Samples of 1-methoxy-2-propanol with varying water content (from 0.03% to 2%) 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 at 30 °C. For convenience, disposable vials with a pathlength of 8 mm were used which made it unnecessary to clean the sample vessels. 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 obtained NIR spectra (Figure 2) were used to create a prediction model for quantification of the water in 1-methoxy-2-propanol. The quality of the prediction model was evaluated using the correlation diagram in Figure 3 which displays a very high correlation between the NIR prediction and the reference values. The respective figures of merit (FOM) display the expected precision of a prediction during routine analysis.

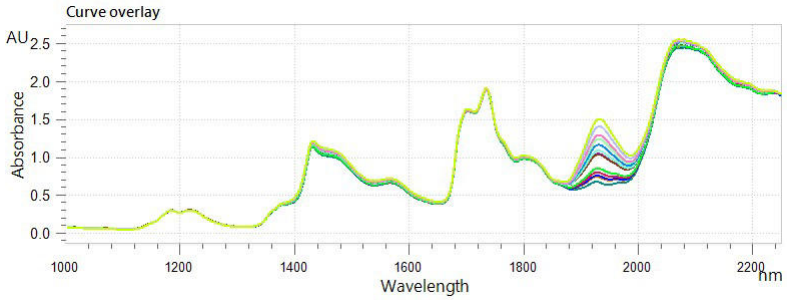


Figure 2. Overlaid NIR spectra of propylene glycol monomethyl ether samples analyzed on an OMNIS NIR Analyzer Liquid.

RESULT WATER CONTENT IN 1-METHOXY-2-PROPANOL

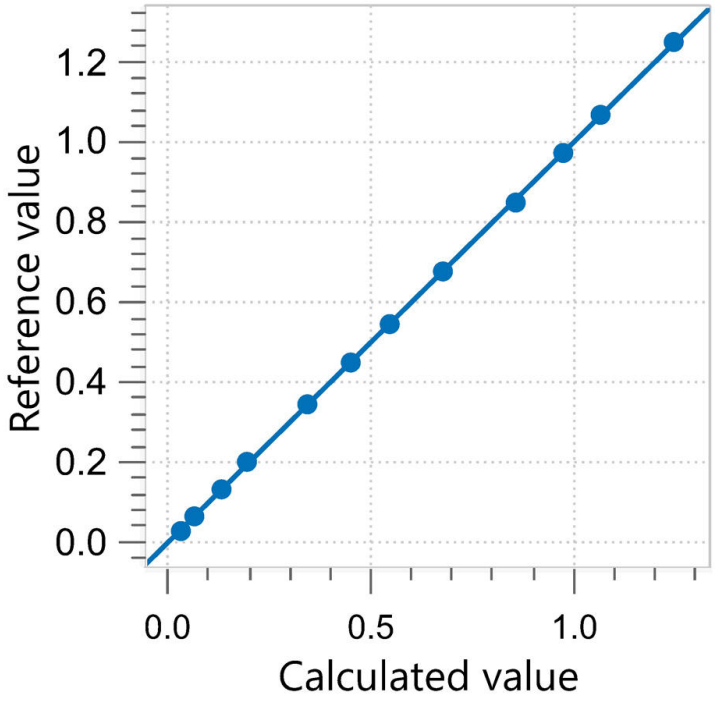


Figure 3. Correlation diagram and the respective figures of merit for the prediction of water content in propylene glycol monomethyl ether using an OMNIS NIR Analyzer Liquid. The lab value was evaluated using KF titration.

R^2	SEC (%)	SECV (%)
1.000	0.0042	0.0048

CONCLUSION

This Application Note demonstrates the feasibility to determine a key parameter for the quality control of propylene glycol monomethyl ether (water content) with NIR spectroscopy. The main advantages of 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 water content determination via KF titration.

Parameter	Method	Time to result
Water	Karl Fischer titration	5 minutes

CONTACT

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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



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)

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A WHOLE NEW LEVEL OF PERFORMANCE

OMNIS Stand-Alone license

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

Features:

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

OMNIS
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Software license Quant Development

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