Water content in propylene glycol monomethyl ether (PGME)

Water determination possible within seconds using NIRS

SUMMARY

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.

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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.

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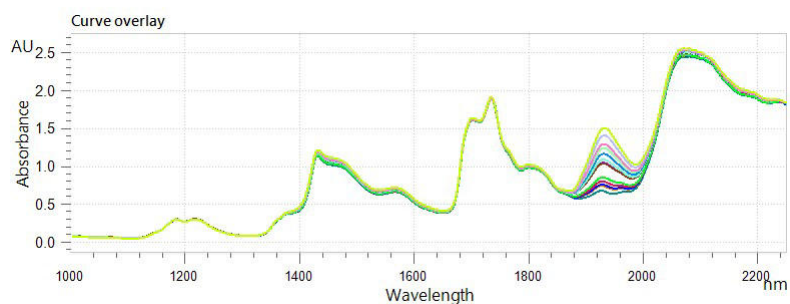
Figure 2. Overlaid NIR spectra of propylene glycol monomethyl ether samples analyzed on an OMNIS NIR Analyzer Liquid.

RESULT WATER CONTENT IN 1-METHOXY-2-PROPANOL
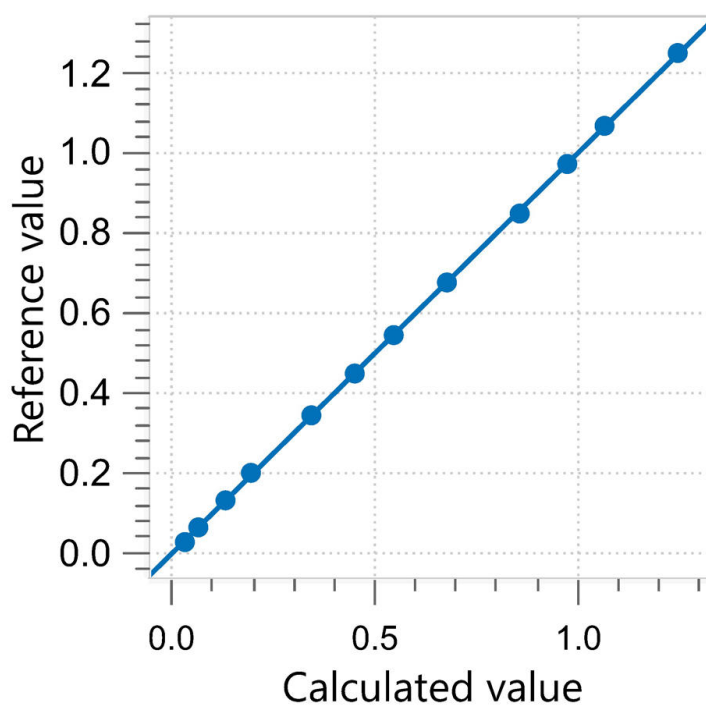
Figure 3. Correlation diagram and the respective figures of merit for the prediction of water content in propylene glycol monomethyl ether using an OMNIS NIR Analyzer Liquid. The lab value was evaluated using KF titration.

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

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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

OMNIS NIR Analyzer (NIRS) OMNIS Software NIR
OMNIS NIR Analyzer Liquid :
- 10
- 25°C ~ 80°C
-
- ()
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OMNIS NIR8 mm

8 mm (6.7402.240) OMNIS NIR Analyzer

8 mm100

 8 mm () 100 (= 100)

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- OMNIS NIR8 mm (**6.07401.070**)
- 8 mm DS2500 (**6.7492.020**)

OMNIS

WindowsTMOMNIS

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Quant Development

 OMNIS Software

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