



Application Note AN-NIR-121

## 丙二醇甲(PGME)中的水分含量

### 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.

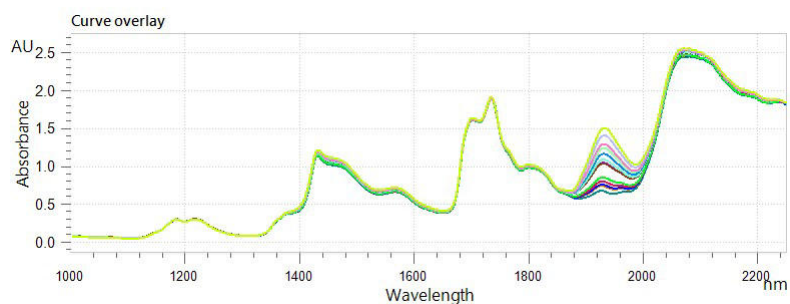
**Table 1.** Hardware and software equipment overview.

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

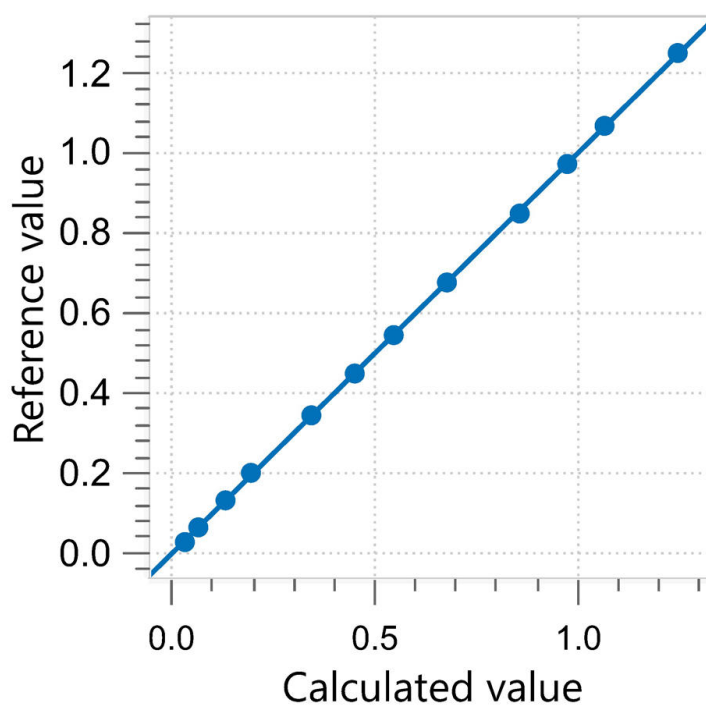
The obtained NIR spectra (**Figure 2**) were used to create a prediction model for quantification of the water in 1-methoxy-2-propanol. The quality of the prediction model was evaluated using the correlation diagram in **Figure 3** which displays a very high

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

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

Metrohm AG  
Ionenstrasse  
9100 Herisau

[info@metrohm.com](mailto:info@metrohm.com)

## CONFIGURATION



### OMNIS NIR Analyzer Liquid

#### 合液体品的近外光。

OMNIS NIR Analyzer 是一按照瑞士量准和生的近外光 (NIRS) 解决方案,用于整个生的常分析。使用新技和嵌入先 OMNIS Software 反在 NIR 光的速度、可操作性 and 活使用上。

OMNIS NIR Analyzer Liquid 的点概:

- 可在 10 秒以内量液体品
- 25° C – 80° C 的品行温度控制
- 自品容器的插入和取出
- 方便地嵌入自系,或者与其它分析技(滴定)
- 支持大量不同路径度的品容器



OMNIS NIR8 mm

8 mm OMNIS NIR Analyzer (6.7402.240)



8 mm 100

100 (), 8 mm ,( = 100)

:

- OMNIS NIR,,8 mm (6.07401.070)
- DS2500 8 mm (6.7492.020)

OMNIS  
A WHOLE NEW LEVEL OF PERFORMANCE

OMNIS

OMNIS Windows™

:

- OMNIS
- 
- 

OMNIS  
A WHOLE NEW LEVEL OF PERFORMANCE

Quant Development

OMNIS Software