



Application Note AN-NIR-121

丙二醇单甲醚(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.

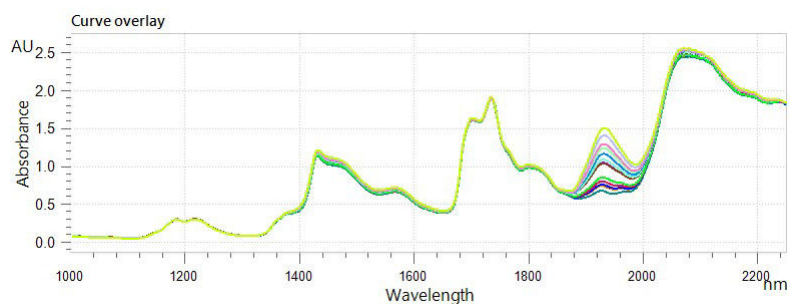


Figure 2. Overlaid NIR spectra of propylene glycol monomethyl ether samples analyzed on an OMNIS NIR Analyzer Liquid.

RESULT WATER CONTENT IN 1-METHOXY-2-PROPANOL

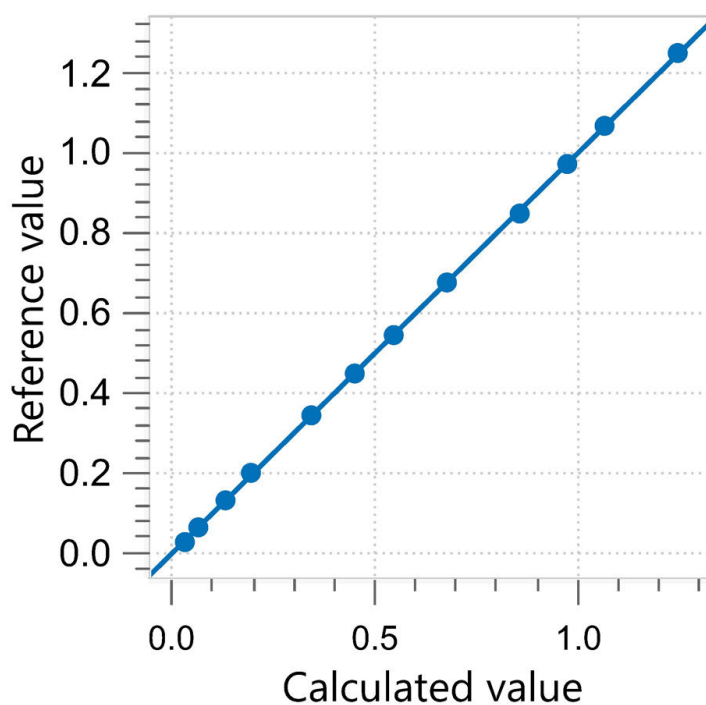


Figure 3. Correlation diagram and the respective figures of merit for the prediction of water content in propylene glycol monomethyl ether using an OMNIS NIR Analyzer Liquid. The lab value was evaluated using KF titration.

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

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

瑞士万通中国
北京市海淀区上地东路1号
院1号楼7层702
100085 北京

marketing@metrohm.com.cn

CONFIGURATION



OMNIS NIR Analyzer Liquid 适合液体样品的近红外光谱仪。

OMNIS NIR Analyzer 是一种按照瑞士质量标准开发和生产的近红外光谱 (NIRS) 解决方案,用于整个生产链的常规分析。使用新技术和嵌入先进 OMNIS Software 反应在该 NIR 光谱仪的速度、可操作性和灵活使用上。

OMNIS NIR Analyzer Liquid 的优点概览:

- 可在 10 秒以内测量液体样品
- 对 25° C – 80° C 的样品进行温度控制
- 自动识别样品容器的插入和取出
- 方便地嵌入自动系统,或者与其它分析技术(滴定)关联
- 支持大量不同路径长度的样品容器



OMNIS NIR8 mm

适合 8 mm 一次性小管的 OMNIS NIR Analyzer 的小管支架 (6.7402.240)。



8 mm 100

100 个玻璃(硼硅)一次性样品瓶,具有 8 mm 的光路长度,适用于分析透射中的液体。一次性样品瓶交付时带有所属的螺旋塞(件数 = 100)。

兼容:

- 支架 OMNIS NIR,小管,8 mm (6.07401.070)
- DS2500 支架适用于 8 mm 一次性样品瓶 (6.7492.020)

OMNIS

A WHOLE NEW LEVEL OF PERFORMANCE

OMNIS

允许单机版 OMNIS 软件在一台 Windows™ 计算机上运行。

特性:

- 该许可证已含有一份 OMNIS 设备许可证。
- 须通过万通许可授权平台进行激活。

OMNIS

A WHOLE NEW LEVEL OF PERFORMANCE

Quant Development

用于在独立 OMNIS Software 安装套件中编写和编辑量化模型的软件许可证。