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.

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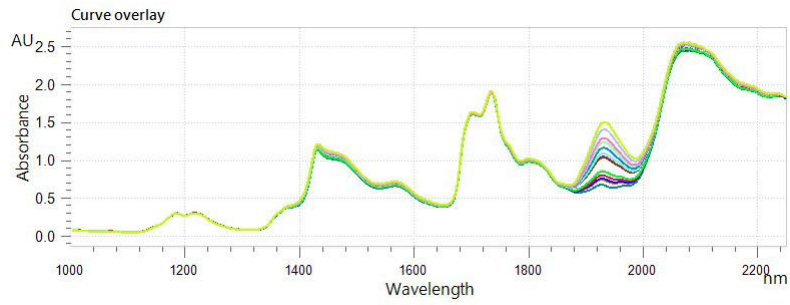
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Figure 2. Overlaid NIR spectra of propylene glycol monomethyl ether samples analyzed on an OMNIS NIR Analyzer Liquid.

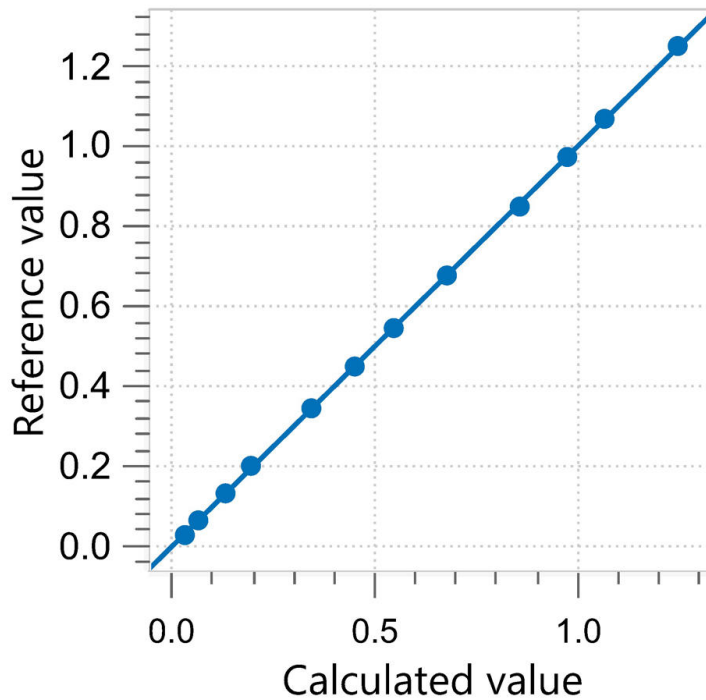## RESULT WATER CONTENT IN 1-METHOXY-2-PROPANOL

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

液体サンフルのための近赤外スヘクトロメーター。

OMNIS NIR Analyzer は、スイスの品質基準に従って開発・製造された、生産チェーン全体に沿ったルーチン分析のための近赤外分光法 (NIRS) ソリューションてす。最新技術の適用と最新の OMNIS Software への統合は、この NIR スヘクトロメーターの速度、ユーサヒリティ、柔軟な使用に反映されています。

OMNIS NIR Analyzer Liquid の利点の概要:
- 10 秒未満て液体サンフルを測定
- 25°C～80°C のサンフルの温度制御
- サンフル容器の取り付けと取り外しの自動検出
- オートメーションシステムへの統合、またはその他の分析技術 (滴定) との連結か容易
- 様々な光路長を有する多数のサンフル容器に対応

OMNIS NIR8 mm

8 mm 使い捨てハイアル (6.7402.240) のための OMNIS NIR Analyzer 用ハイアルホルター。

8 mm100

透過した液体を分析するための光学的距離 8 mm のカラス製 (ホウケイ酸塩) 使い捨てハイアル 100 個。使い捨てハイアルには閉し蓋 (個数 = 100) か付属されています。

次の製品と互換性かあります:
- ホルター OMNIS NIR、ハイアル、8 mm (6.07401.070)
- 使い捨てハイアル 8 mm 用の DS2500 ホルター (6.7492.020)

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WindowsTMコンヒューター上のOMNISソフトウェアをスタントアローン操作することか可能になります。

特徴:

- ライセンスには、既に1つのOMNISテハイスライセンスか含まれています。
- メトローム・ライセンシンクホータルにて、アクティフ化する必要かあります。
- 他のコンヒューターに移行することはてきません。

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Quant Development

スタントアロン型 OMNIS Software のインストールにおける定量化モテルの作成と編集のためのソフトウェアライセンス。

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