近外光法在除臭量控制中的用

Determination of pH, density, viscosity, and aluminum content in a few seconds

Personal care products like deodorants are tested using various time-consuming analytical methods during production as well as after the final product is made. This Application Note demonstrates how quality parameters such as viscosity, pH, density, and aluminum content in deodorant can be measured with near-infrared spectroscopy (NIRS) simultaneously and without any sample preparation. NIRS is a fast, chemical-free technology that is very user-friendly. NIR spectroscopy can be used either atline during the production process or offline in a quality control laboratory.

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EXPERIMENTAL EQUIPMENT

Sixty samples of deodorant were measured in an OMNIS NIR Analyzer Solid (**Figure 1**). All measurements were performed in transflection mode (1000–2250 nm) using a 1 mm gap size large reflector and a transflection vessel.

Reference values of aluminum content were measured with titration (AN-T-228), pH values with a pH meter, and viscosity and density with a viscometer and density meter, respectively.

OMNIS Software was used for all data acquisition and prediction model development.

Figure 1. OMNIS NIR Analyzer Solid with transflection vessel and large reflector.

Table 1. Hardware and software equipment overview.

Equipment	Article number
OMNIS NIR Analyzer solid	2.1071.0010
Large reflector OMNIS NIR, 1mm	6.07402.940
Transflection vessel OMNIS NIR, 60mm	6.07402.260
OMNIS Stand-Alone license	6.06003.010
Software license Quant Development	6.06008.002

RESULT

The obtained NIR spectra of deodorant samples (**Figure 2**) were used to create prediction models for pH, viscosity, density, and aluminum content. The quality of the prediction models was evaluated using correlation diagrams which display 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 (**Figures 3–6**).
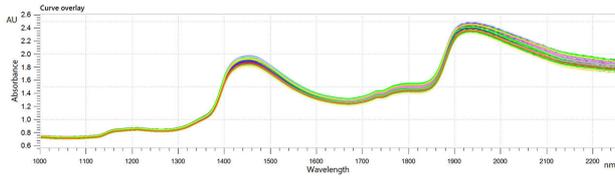
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Figure 2. NIR spectra of various deodorant samples analyzed on an OMNIS NIR Analyzer Solid.
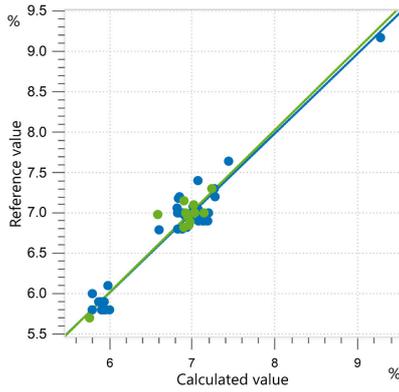
Result aluminum content

Figure 3. Correlation diagram and the respective figures of merit for the prediction of aluminum content in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. Titration was used as a reference method for the determination of aluminum in deodorant.

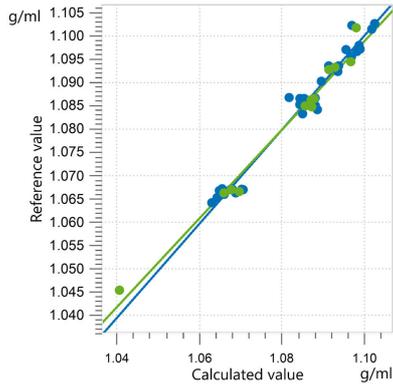| R^2	SEC (%)	SECV (%)	SEP (%)
0.908	0.12	0.16	0.14

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Result density

Figure 4. Correlation diagram and the respective figures of merit for the prediction of density in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. A density meter was used as the reference method.

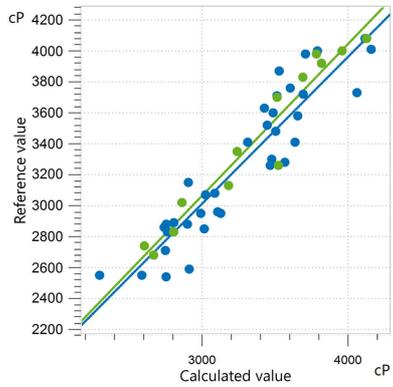| R^2	SEC (g/mL)	SECV (g/mL)	SEP (g/mL)
0.979	0.0017	0.0020	0.0023

Result viscosity

Figure 5. Correlation diagram and the respective figures of merit for the prediction of viscosity in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. Reference values were obtained with a viscometer.

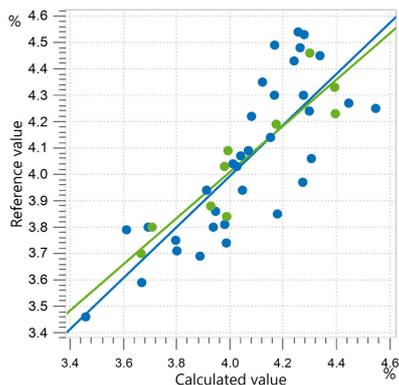| R^2	SEC (cP)	SECV (cP)	SEP (cP)
0.941	147.05	176.05	133.74

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Result pH

Figure 6. Correlation diagram and the respective figures of merit for the prediction of pH value in deodorant using an OMNIS NIR Analyzer Solid. The calibration dataset is shown in blue, and the external validation dataset is in green. A pH meter was used as the reference method for the pH measurement of deodorant.

R^2	SEC	SECV	SEP
0.832	0.13	0.18	0.10

CONCLUSION

This Application Note shows the feasibility of using NIR spectroscopy for the analysis of aluminum content, pH, viscosity, and density in deodorants. With NIRS, the measurement can be conducted within seconds and requires no chemicals. This solution is easier, much faster than other conventional techniques, and can be used atline in several steps of the production chain or during quality control of the final product, saving manufacturers time and money.

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CONFIGURATION

OMNIS NIR Analyzer Solid
合固体和粘性品的近外光。

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、可操作性和活使用上。

OMNIS NIR Analyzer Solid 的点概:

- 在 10 秒以内量固体和粘性品
- 自化多位置量,即使在品不均匀,也能得可重的果
- 方便地嵌入自系,或者与其它分析技(滴定)
- 支持大量品容器

OMNIS NIR1 mm

液体行透射反射量的隙量 1 mm(光路度 2 mm)的反射器。

用于透射容器(**6.07402.260** 和 **6.7401.000**)。

OMNIS NIR60 mm

液体行光量的光学平面透射反射器皿。

OMNIS

允机版 OMNIS 件在一台 WindowsTM 算机上行。

特性:

- 可已含有一 OMNIS 可。
- 通万通可授平台行激活。
- 不可再外算机上使用。

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A WHOLE NEW LEVEL OF PERFORMANCE

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