Quality control of liquid laundry detergents by NIR spectroscopy

Multiparameter determination of surfactants, dry matter, pH, and viscosity in a few seconds

Liquid laundry detergents contain fabric softeners, bleaching agents, surfactants, and enzymes. Of these, the surfactant is the most important contributor for the cleaning effect, as it breaks down the interface between polar and nonpolar compounds. This allows detergents to be effective cleaning agents against grease and stains. Surfactant content together with viscosity, pH value, and dry matter are important quality control parameters in detergent formulations. Measurement of these parameters is usually performed by time-consuming primary analysis methods (e.g., two-phase potentiometric titration for surfactants), often requiring different techniques. Near-infrared spectroscopy (NIRS) is a fast, chemical-free alternative for use atline or in a quality control lab.

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EXPERIMENTAL EQUIPMENT

Samples of liquid laundry detergent were measured at 30 °C in an OMNIS NIR Analyzer Liquid (**Figure 1**) in transmission mode (1000–2250 nm) using 8 mm disposable vials. Vessel temperature control was selected.
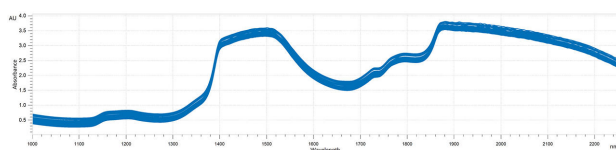
Reference values of dry matter were measured by loss on drying. The pH value and viscosity were measured with a pH meter and viscometer, respectively. Surfactant content in detergent was measured with potentiometric titration.

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

**Figure 1.** OMNIS NIR Analyzer Liquid/Solid with 8 mm vials.

The obtained NIR spectra (**Figure 2**) were used to create prediction models for the quantification of dry matter, pH, viscosity, and surfactants in laundry detergent. The quality of the prediction models was evaluated using correlation diagrams which display the relation 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**).
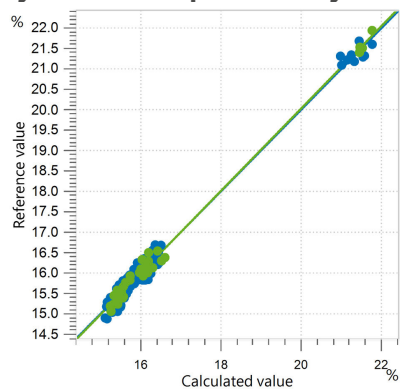

Figure 2. NIR spectra of detergent analyzed on an OMNIS NIR Analyzer Liquid.

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Result pH in liquid laundry detergent
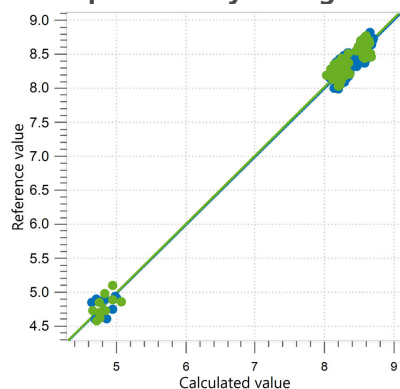
Figure 3. Correlation diagram and the respective FOMs for the prediction of pH value in liquid laundry detergent using an OMNIS NIR Analyzer Liquid. The correlation set is shown in blue, and the external validation set is in green. Reference values were obtained with a pH meter.

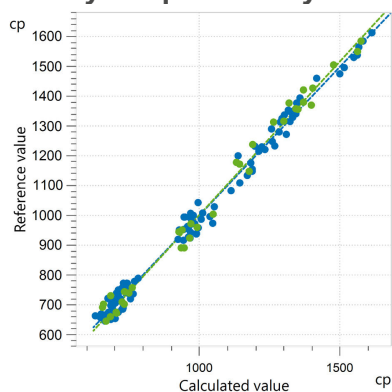| R^2	SEC	SECV	SEP
0.990	0.11	0.11	0.12

Result dry matter in liquid laundry detergent

Figure 4. Correlation diagram and the respective FOMs for the prediction of dry matter in liquid laundry detergent using an OMNIS NIR Analyzer Liquid. The correlation set is shown in blue, and the external validation set is in green. Reference values were obtained via loss on drying.

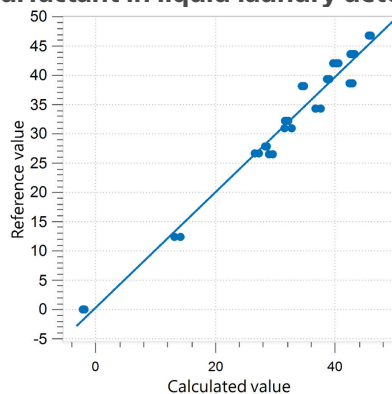| R^2	SEC (%)	SECV (%)	SEP (%)
0.994	0.15	0.16	0.14

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Result viscosity in liquid laundry detergent

Figure 5. Correlation diagram and the respective FOMs for the prediction of viscosity of laundry detergent using an OMNIS NIR Analyzer Liquid. The correlation set is shown in blue, and the external validation set is in green. Reference values were obtained with a viscometer.

R^2	SEC (cp)	SECV (cp)	SEP (cp)
0.990	27.26	28.75	32.42

Result surfactant in liquid laundry detergent

Figure 6. Correlation diagram and the respective FOMs for the prediction of surfactant content in liquid laundry detergent using an OMNIS NIR Analyzer Liquid. No external validation set was used. Reference values were obtained with potentiometric titration.

R^2	SEC (mmol/100g)	SECV (mmol/100g)	SEP (mmol/100g)
0.970	1.73	2.00	N/A

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CONCLUSION

This Application Note shows the feasibility of using near-infrared spectroscopy for the analysis of dry matter, pH value, viscosity, and surfactant content in liquid detergent. These quality control parameters can be measured simultaneously in seconds without any chemicals or sample preparation.

NIRS saves laundry detergent manufacturers time and money as it can be used in several steps of the production chain or during quality control of the final product. Additionally, only one technology is required with NIRS, compared to the other standard analytical techniques often used for these determinations (Table 1).

Table 1. Overview of standard methods used for the determination of different reference values in liquid laundry detergents.

Parameter	Method	Time to result
Dry matter	Loss on drying	30 min
pH	pH meter	5 min
Viscosity	Viscometer	15 min (sample preparation + measurement)
Surfactant (anionic)	Potentiometric titration	10 min (adding solutions, stirring, pH adjustments, determination)

Internal reference: AW NIR CN-0015-102018

CONTACT

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CONFIGURATION

OMNIS NIR Analyzer Liquid
Near-infrared spectrometer for liquid samples.

Developed and produced in accordance with Swiss quality standards, the OMNIS NIR Analyzer is the near-infrared spectroscopy (NIRS) solution for routine analysis along the entire production chain. Its application of the latest technologies and its integration in the modern OMNIS Software are reflected in its speed, operability, and flexible utilization of this NIR spectrometer.

Overview of the advantages of the OMNIS NIR Analyzer Liquid:

- Measurements of liquid samples in less than 10 seconds
- Temperature control on the sample from 25–80 °C
- Automatic detection of the insertion and removal of the sample vessel
- Simple integration in an automation system or link with additional analysis technologies (titration)
- Supports numerous sample vessels with different path lengths

Holder OMNIS NIR, vial, 8 mm

Vial Holder for the OMNIS NIR Analyzer for 8 mm disposable vials (6.7402.240).

Disposable vial, 8 mm, transmission, qty. 100

100 disposable glass vials (borosilicate) with an optical path length of 8 mm for analyses of liquids in transmission. The disposable vials are supplied with the associated stoppers (number of pieces = 100).

Compatible with:

- Holder OMNIS NIR, vial, 8 mm (**6.07401.070**)
- DS2500 holder for 8 mm disposable vials (**6.7492.020**)

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OMNIS Stand-Alone license

Enables stand-alone operation of the OMNIS software on a WindowsTM computer.

Features:

- The license already includes one OMNIS instrument license.
- Must be activated via the Metrohm licensing portal.
- Not transferable to another computer.

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Software license Quant Development

Software license for the creation and editing of quantification models in a stand-alone OMNIS Software installation.

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