



Application Note AN-NIR-074

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.

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.

RESULT

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).

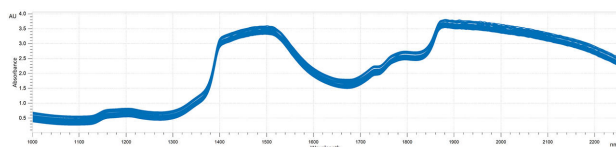


Figure 2. NIR spectra of detergent analyzed on an OMNIS NIR Analyzer Liquid.

Result pH in liquid laundry detergent

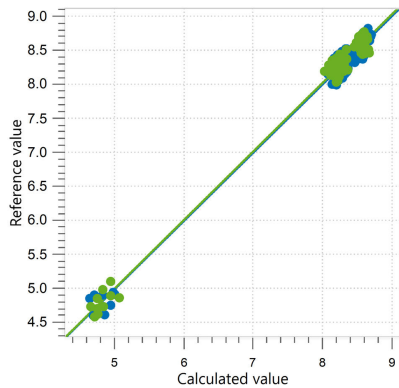


Figure 3. Correlation diagram and the respective FOMs for the prediction of pH value in liquid laundry detergent using an OMNIS NIR Analyzer Liquid. The correlation set is shown in blue, and the external validation set is in green. Reference values were obtained with a pH meter.

R ²	SEC	SECV	SEP
0.990	0.11	0.11	0.12

Result dry matter in liquid laundry detergent

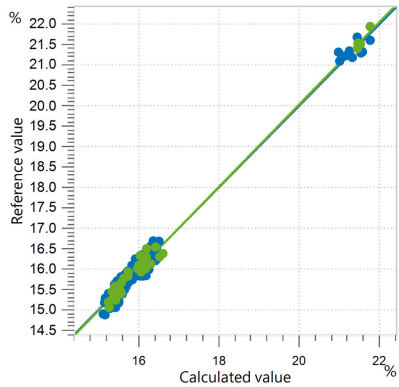


Figure 4. Correlation diagram and the respective FOMs for the prediction of dry matter in liquid laundry detergent using an OMNIS NIR Analyzer Liquid. The correlation set is shown in blue, and the external validation set is in green. Reference values were obtained via loss on drying.

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

Result viscosity in liquid laundry detergent

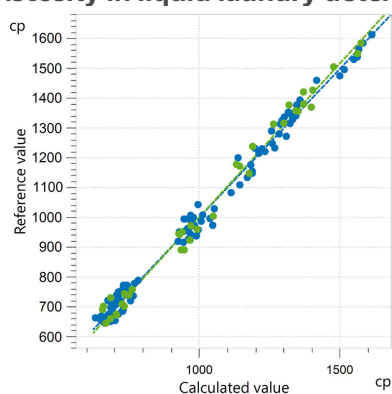


Figure 5. Correlation diagram and the respective FOMs for the prediction of viscosity of laundry detergent using an OMNIS NIR Analyzer Liquid. The correlation set is shown in blue, and the external validation set is in green. Reference values were obtained with a viscometer.

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

Result surfactant in liquid laundry detergent

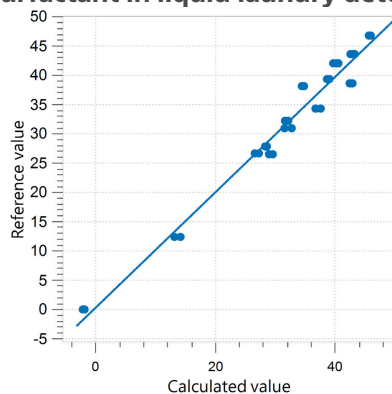


Figure 6. Correlation diagram and the respective FOMs for the prediction of surfactant content in liquid laundry detergent using an OMNIS NIR Analyzer Liquid. No external validation set was used. Reference values were obtained with potentiometric titration.

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

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)

CONTACT

Metrohm Inula
Shuttleworthstraße 25
1210 Wien

office@metrohm.at

CONFIGURATION



OMNIS NIR Analyzer Liquid

Nahinfrarot-Spektrometer für Flüssigproben.

Der OMNIS NIR Analyzer ist die nach Schweizer Qualitätsstandards entwickelte und produzierte Nahinfrarot-Spektroskopie (NIRS) Lösung für die Routineanalytik entlang der gesamten Produktionskette. Die Nutzung neuester Technologien und die Einbindung in die moderne OMNIS Software spiegeln sich in der Geschwindigkeit, der Bedienbarkeit und dem flexiblen Einsatz dieser NIR-Spektrometer wider.

Die Vorteile des OMNIS NIR Analyzer Liquid im Überblick:

- Messungen von Flüssigproben in weniger als 10 Sekunden
- Temperaturkontrolle an der Probe von 25°C – 80°C
- Automatische Erkennung des Einsetzen und der Entnahme des Probengefäßes
- Einfache Einbindung in ein Automationssystem oder Verknüpfung mit weiteren Analysetechnologien (Titration)
- Unterstützung zahlreicher Probengefäße mit unterschiedlicher Pfadlänge



Halter OMNIS NIR, Vial, 8 mm

Vialhalter für den OMNIS NIR Analyzer für 8 mm Einwegvials (6.7402.240).



OMNIS
A WHOLE NEW LEVEL OF PERFORMANCE

OMNIS
A WHOLE NEW LEVEL OF PERFORMANCE

Einwegvial, 8 mm, Transmission, Anz. 100

100 Einwegvials aus Glas (Borosilikat) mit einer optischen Pfadlänge von 8 mm für Analysen von Flüssigkeiten in Transmission. Die Einwegvials werden mit den zugehörigen Verschlussstopfen (Stückzahl = 100) geliefert.

Kompatibel mit:

- Halter OMNIS NIR, Vial, 8 mm (6.07401.070)
- DS2500 Halter für 8 mm Einwegvials (6.7492.020)

OMNIS Stand-Alone Lizenz

Ermöglicht den Stand-Alone Betrieb der OMNIS Software auf einem Windows™ Computer.

Merkmale:

- Die Lizenz enthält bereits eine OMNIS Geräte Lizenz.
- Muss über das Metrohm Lizenzierungsportal aktiviert werden.

Softwarelizenz Quant Development

Softwarelizenz für die Erstellung und Bearbeitung von Quantifizierungsmodellen in einer Stand-Alone OMNIS Software Installation.