Surfactant in laundry detergent by Vis-NIR spectroscopy

Fast determination without using chemicals

Summary

Liquid laundry detergents contain fabric softeners, bleaching agents, surfactants, as well as enzymes. Out of these, the surfactant is the most important factor for the cleaning effect, as it breaks down the interface between polar and nonpolar compounds. This allows the detergent to be effective against greases as well as stains from soil or drinks.

Quantification of surfactant content is most commonly performed by primary analyses (e.g., two-phase potentiometric titration). Disadvantages include manual sample preparation steps such as dilution and pH adjustment, and the method itself is time-consuming. In contrast, Vis-NIR spectroscopy has a time-to-result of less than 1 minute and does not require any sample preparation or chemicals for high quality data.

Experimental

Figure 1. The NIRS XDS RapidLiquid Analyzer with a 1 mm quartz cuvette, used to collect the spectra of surfactant samples.

A total of 37 samples with varying surfactant content were provided by a customer. The Vis-NIR spectra (**Figure 2**) were acquired on a Metrohm NIRS XDS RapidLiquid Analyzer equipped with 1 mm quartz cuvette (**Figure 1**). The samples were measured as-is, without any sample preparation steps. Data collection and model development was carried out with the Vision Air complete software package.

Table 1. Hardware and software equipment overview.

Equipment	Metrohm number
XDS RapidLiquid Analyzer	2.921.1410
NIRS 1mm quartz cuvette	6.7401.200
Vision Air 2.0 Complete	6.6072.208

2.921.1410 - NIRS XDS RapidLiquid Analyzer

Rapid, precise analyses of liquids and suspensions of all types.The NIRS XDS RapidLiquid Analyzer enables rapid, precise analyses of liquid formulations and substances. Precise measurement results at the push of a button make the NIRS XDS RapidLiquid Analyzer an equally reliable and simple solution for quality monitoring in laboratories and processes. The samples are transferred to quartz cuvettes designed for multiple use or disposable glass vials; a tempered sample compartment ensures reproducible analysis conditions and thus accurate measurement results.

6.7401.200 - NIRS 12.5 mm quartz cuvette 1 mm

Quartz glass cuvette with a window made of quartz glass of maximum purity and homogeneity. The cuvettes have a transmission of more than 80% in the wavelength range of 200 nm - 2,500 nm.A number of different pathlengths are available:1 mm pathlength and a volume = 350 L (order number: 67401200); 2 mm pathlength and a volume = 700 L (order number: 67401210); 5 mm pathlength and a volume = 1,750 L (order number: 67401220); 10 mm pathlength and a volume = 3,500 L (order number: 67401230); The NIRS Spacer for 12.5 mm cuvette set (order number: 67403180) ensures spacers for an optimum position of the cuvette in the sample holder.

6.6072.208 - Vision Air 2.0 Complete

Vision Air - Universal spectroscopy software. Vision Air Complete is a modern and simple-to-operate software solution for use in a regulated environment.Overview of the advantages of Vision Air: Individual software applications with adapted user interfaces ensure intuitive and simple operation; Simple creation and maintenance of operating procedures; SQL database for secure and simple data management; The Vision Air Complete version (66072208) includes all applications for quality assurance using Vis-NIR spectroscopy: Application for instrument and data management; Application for method development; Application for routine analysis; Additional Vision Air Complete solutions: 66072207 (Vision Air Network Complete); 66072209 (Vision Air Pharma Complete); 66072210 (Vision Air Pharma Network Complete);

Result

The obtained graph (**Figure 3**) displays a high correlation (R^2 = 0.97) between the values predicted by NIRS and the reference method. The nearly perfect ratio of the SEC and SECV illustrates the validity of the model.

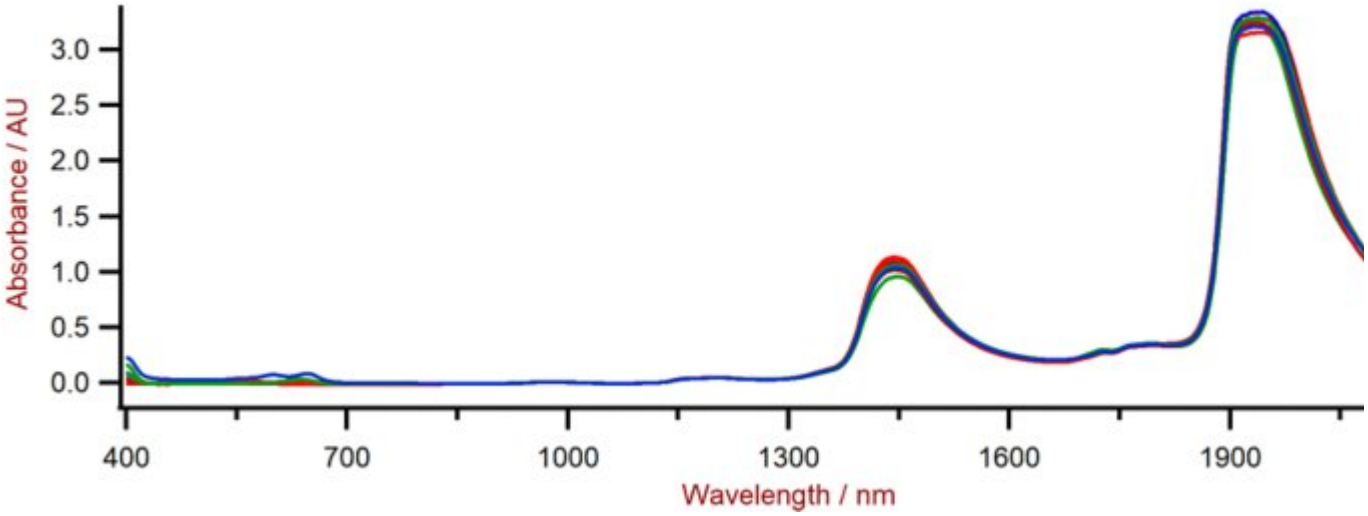

Figure 2 Selection of liquid detergent Vis-NIR spectra obtained using a XDS RapidLiquid Analyzer and a 1 mm quartz cuvette.

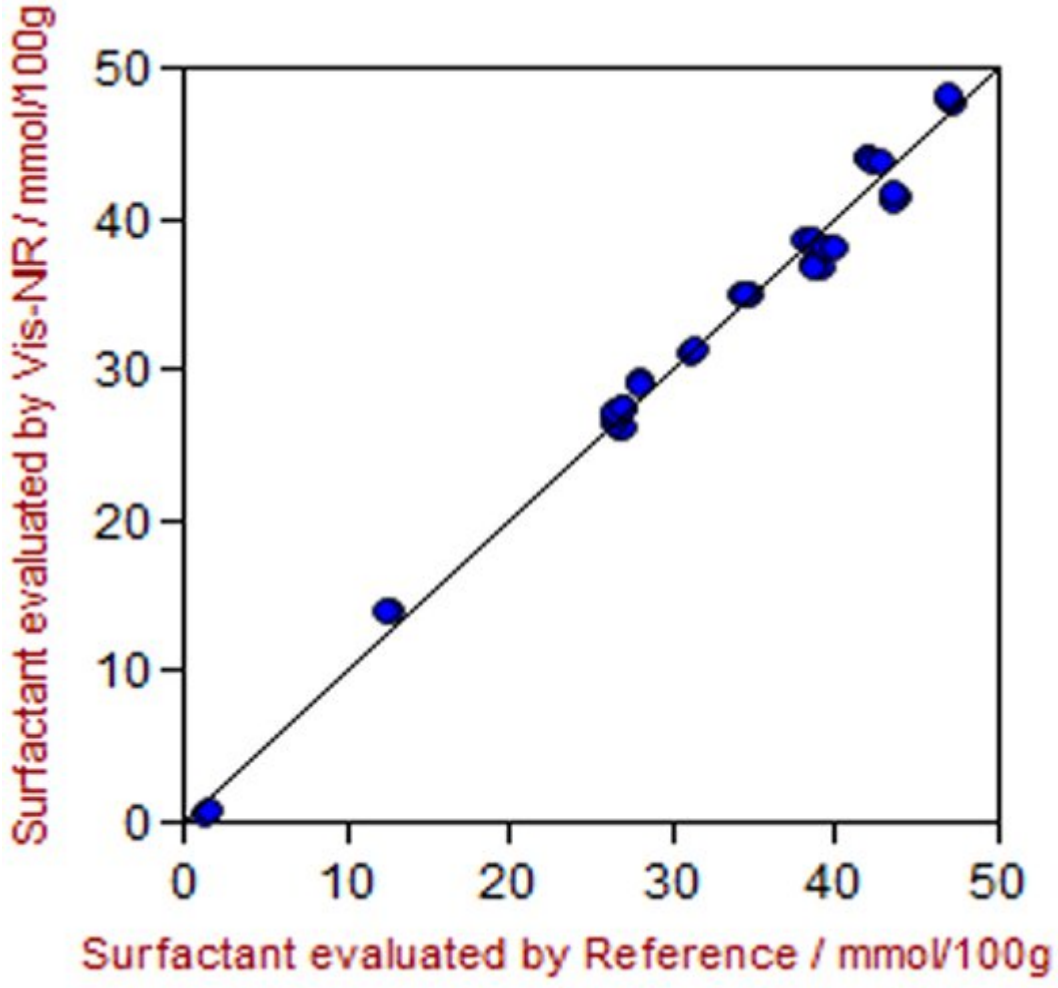

Figure 3 Correlation diagram and the respective figures of merit for the prediction of surfactant in liquid detergent using a XDS RapidLiquid Analyzer. The surfactant lab value was evaluated using HPLC.

Table 2. Figures of merit for the prediction of the surfactant content in liquid detergent using a XDS RapidLiquid Analyzer.

Figures of merit	Value
R^2	0.97
Standard error of calibration	2.20 mmol/100 g
Standard error of cross-validation	2.38 mmol/100 g

Conclusion

The results presented herein show that the Vis-NIR method is excellently suited for the fast quantification of surfactant concentration in detergents. Using Vis-NIR for this application saves 10 minutes per sample compared to other methods (**Table 3**).

Table 3. Time to result overview for the different parameters

Parameter	Method	Time to result
Surfactant (anionic)	Potentiometric titration	10 min (adding solutions, stirring, pH-adjustments, determination)

Metrohm AG
Ionenstrasse
9100 Herisau
mailto:info@metrohm.com