



Application Note AN-NIR-074

近外光法液体洗衣液的量控制

Fast determination without using chemicals

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

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.



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

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

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.

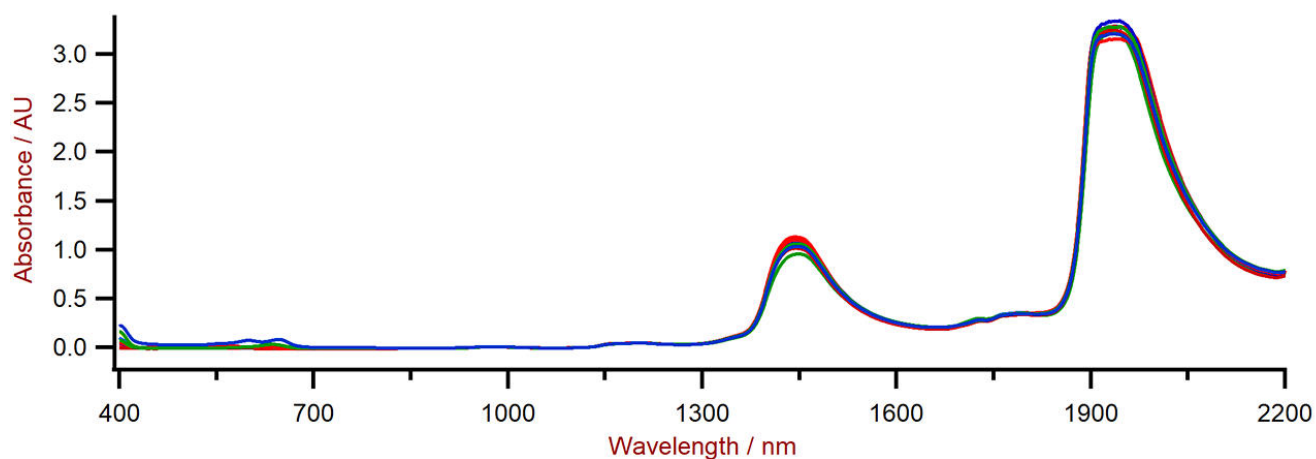


Figure 2 Selection of liquid detergent Vis-NIR spectra obtained using a XDS RapidLiquid Analyzer and a 1 mm quartz cuvette.

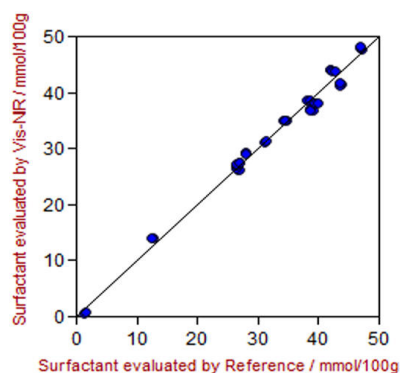


Figure 3 Correlation diagram and the respective figures of merit for the prediction of surfactant in liquid detergent using a XDS RapidLiquid Analyzer. The surfactant lab value was evaluated using HPLC.

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

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)

CONTACT

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NIRS XDS RapidLiquid Analyzer

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- 1 mm
- , 200 nm - 2500 nm 80%
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- NIRS Spacer, 12.5 mm (6.7403.180)
 - DS2500 , 1 mm (6.7492.100)
 - OMNIS NIR,,1 mm (6.07401.010)



Vision Air 2.0 Complete

Vision Air –

Vision Air Complete

Vision Air :

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Vision Air Complete (66072208) :

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Vision Air Complete :

- 66072207 (Vision Air Network Complete)
- 66072209 (Vision Air Pharma Complete)
- 66072210 (Vision Air Pharma Network Complete)