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Application Note

Determination of water content in alcoholic solutions by mobile NIR spectroscopy

with the Liquid Analysis Flow Kit for the trinamiX PAL One spectrometer

Introduction

Mobile NIR spectroscopy has established itself as an invaluable tool for on-site analytics and quality control. The trinamiX PAL One spectrometer is utilized worldwide across various sectors, including plastics identification, textile sorting, and feed ingredient analysis. Recently, trinamiX has expanded the capabilities of this versatile instrument by introducing the Liquid Analysis Flow Kit, which allows for the analysis of liquid materials. This user-friendly attachment opens new possibilities for applications requiring high accuracy, such as compositional analysis and the determination of water content in various liquid products.

Figure 1. trinamiX PAL One NIR spectrometer with the Liquid Analysis Flow Kit to measure liquids. It consists of a transflection cap with reference standard, flow cell, syringe, and tubing.

Residual water in materials is a common concern across various industries, and accurately determining water content is essential for optimizing processes and ensuring material quality. Thanks to its strong NIR absorption characteristics, water content can be effectively analyzed using NIR spectroscopy. This application note demonstrates the determination of water content specifically in alcoholic solutions.

Materials and Methods

Eleven mixtures of ethanol (99.9%) and 2-propanol (98%) with distilled water, ranging from 0% to 5% water content, were prepared for analysis. Each solution was measured three times using the trinamiX PAL One spectrometer equipped with the Liquid Analysis Flow Kit (see Figure 1). For each measurement, the flow cell was refilled with a fresh batch of the solution. A flow cell with a thickness of 0.2 mm was utilized, allowing for measurements in transflection mode, resulting in a total optical path length of 0.4 mm. The sample is injected into the flow cell using an easily connectable syringe. After the analysis, the samples are discarded into a designated container.

Results and Discussion

The averaged spectra from three measurements for different water concentrations are presented in *Figure 2*. A clear increase in the relevant water absorbance bands is observed.

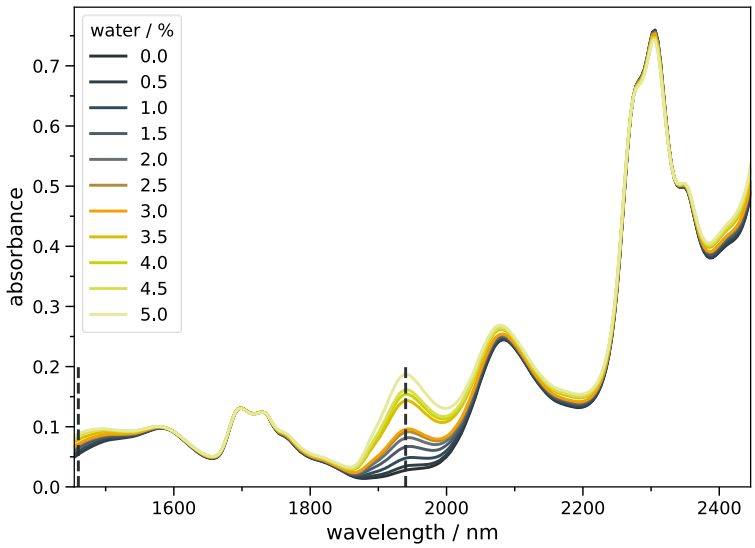

Figure 2. Absorbance spectra of ethanol-water mixtures show that, as water content increases, the intensity of the water combination band at 1940 nm and the OH-stretch overtone at 1450 nm rises. These bands are indicated by dashed lines.

The distinct differences observed in the measured spectra corresponding to varying water content allow for the development of a predictive model for determining the water content of ethanol solutions in the range of 0-5%. In *Figure 3*, each point represents a measured spectrum, with the prepared concentration displayed on the x-axis and the predicted water concentration on the y-axis. The model demonstrates high accuracy, as evidenced by the strong correlation reflected in minimal deviations from the ideal trend line, where the predicted and actual values align perfectly. Based on this analysis, the water content in an

unknown ethanol sample can be determined with an average error of ± 0.28%. Additionally, experiments with mixtures of 2-propanol and water yielded similarly high accuracy, with an average error of ± 0.34%.

Cross-validation results for the modeling of ethanol and 2-propanol

Ethanol:	2-Propanol:
R^2 0.97	R^2 0.95
RMSE 0.28 %	RMSE 0.34 %

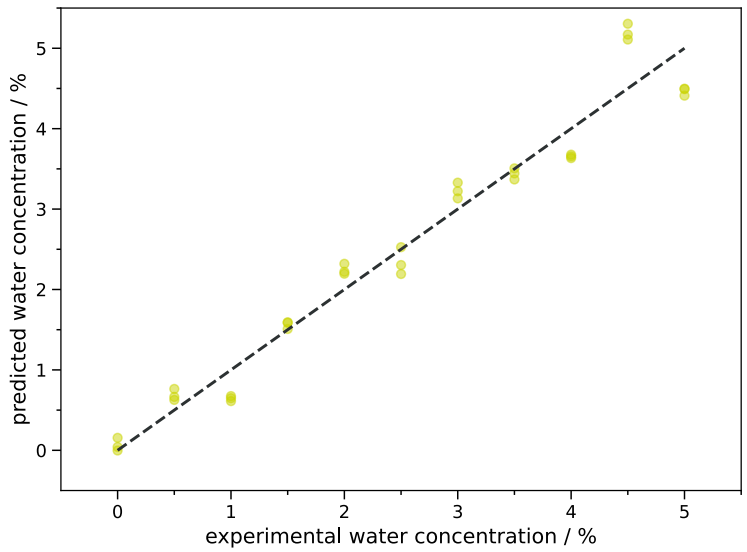

Figure 3. True-vs-predicted plot of cross-validation for ethanol-water mixtures. PLSR is based on two components of the second derivative of the baseline-corrected spectra. Each measurement is depicted as a circle. For reference, a 45° dashed line is added to guide the eye.

Conclusion

The Liquid Analysis Flow Kit enhances the trinamiX PAL One spectrometer, enabling precise determination of the composition of various liquids. This capability has been demonstrated specifically for measuring water content in two different types of alcohol.

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