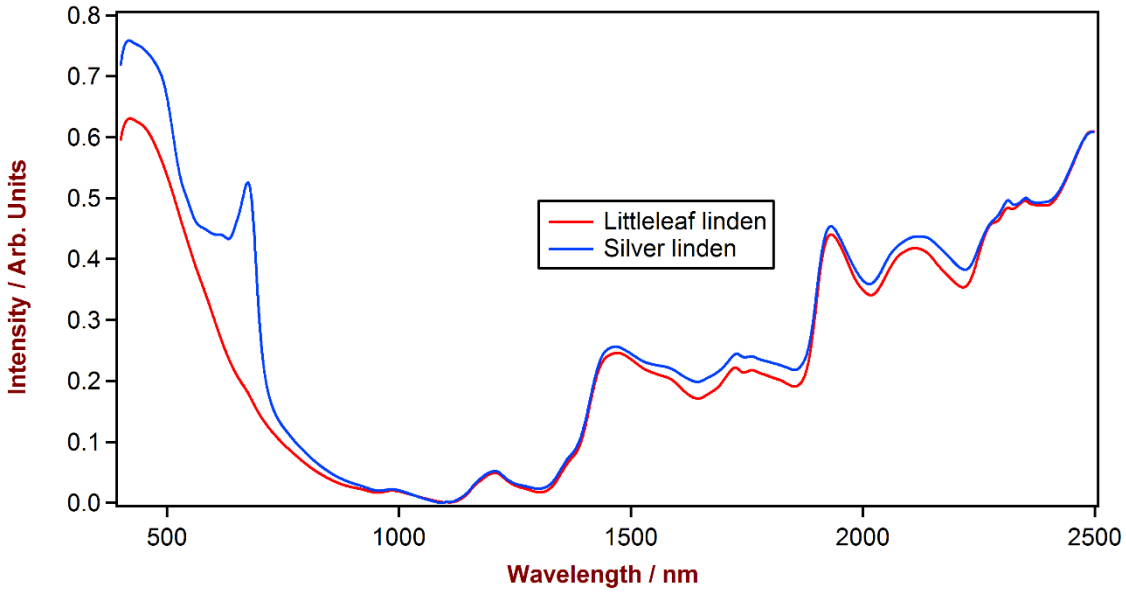
NIR Application Note NIR-28

Data and method transfer from System II analyzer to Metrohm NIRS XDS or DS 2500 analyzers



This Application Note shows the analytical method transfer for near-infrared spectroscopy (NIRS) from FOSS NIRSystems System II (5000/6500) Analyzers to Metrohm NIRS XDS and DS2500 Analyzers. It also demonstrates the advantages of new NIRS XDS and DS2500 Analyzers with extended spectral range and improved resolution compared to FOSS NIRSystems System II Analyzers.

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Method description

Introduction

After more than 20 years in the market the support for the near-infrared analyzer System II ends on May 31, 2017 and it is recommended to replace the old instruments with new Metrohm XDS or DS2500 instruments. These devices have many advantages compared to the System II Analyzers, which are mainly:

- Improved resolution (0.5 nm instead of 2 nm)
- Extended spectral range (400-2500 nm)
- Reduced integration time (two times faster compared to System II)
- Improved wavelength precision
- Networking possibility
- Easy-to-replace lamp with enhanced lamp life
- Modular design
- More flexibility

The qualitative and quantitative models developed on System II instruments cannot be directly transferred to new analyzers like XDS or DS2500 due to differences in spectral range and spectral resolution. However, the spectra used for the development of models on System II can easily be transferred to new analyzers and can be used for the redevelopment of analog models.

The advantage of such a data transfer process is, that users can immediately use the Vis-NIR XDS instrument with no need for a complete new data collection and development of new models. Finally, new data sets, collected on the new instrument with improved resolution and extended spectral range, can be used to update the existing model or to replace it by a new model with enhanced analytical figures of merit. However there are different effects, which one has to take into account due to the data and model transfer depending on the type of application (qualitative or quantitative).

One of the main effects, which influence the data transfer is, that different instruments can have slight differences in photometric sensitivity and wavelength precision. The influence of photometric sensitivity can be reduced by the photometric correction. Additionally, the development of a robust calibration models, which needs an expertise in chemometrics and can be supported by local Metrohm agency, can enhance analytical figures of merit and reduce the influence of differences in wavelength precision between master and slave instruments.

The current application note describes the transfer of the data from System II to XDS or DS2500 Analyzers for several types of applications and demonstrates the simplicity of this process and advantages of the use of XDS and DS2500 Analyzers. This transfer can be easily supported by local Metrohm agencies.

Methods

For the data transfer, simple additional measurements should be acquired on the old System II instrument. All of the final steps can be done in Vision software version 4.1 (Tab. 1).

Tab. 1: Used equipment

Equipment	Metrohm code
Vision 4.1	6.6069.412

Experimental

System II data are quite often non-reference standardized. This can be checked by right clicking on the product and selecting “Properties”. If the data is not reference standardized, a reference standardization has to be performed for the use on the new instruments.

Because modern XDS and DS2500 Analyzers have improved spectral resolution, the data has to be converted by the function convert in the menu File/Project. Additionally if the data has been collected on System II 5000 analyzers, which has a reduced spectral range of 1100-2500 nm, all spectra has to be expanded to full range of 400-2500 nm since all Metrohm instruments cover this spectral range.

Finally one can proceed to go through Sample Selection and Regression functions in Vision software to develop a new calibration equation using the standardized, converted and expanded data. Frequently the same math treatments and regression techniques can be used. A new Operations Method should be created using the Reference Standardized DCM and the new Calibration Equation.

Regarding quantitative models, it is recommended to perform a validation with an independent sample set, which should cover the whole concentration range of the used model. In case of constant deviations in concentrations during validation, the model can be corrected by the bias/slope adjustment.

Results and discussion

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Method description

Extended spectral range and improved resolution of XDS and DS2500 Analyzers can improve the analytical method compared to System II. This improvements differ for different types of applications (qualitative or quantitative). The advantages of the Metrohm NIRS XDS or DS2500 Analyzers compared to System II for qualitative analysis can be demonstrated by the examples of raw material identification of pharmaceuticals or herbal products, shown in the section Qualitative analysis below. The benefits of an extended spectral range for quantitative applications are shown in the section Quantitative analysis by the example of the determination of density of polyethylene.

Qualitative analysis

One of the benefits of the Metrohm NIRS XDS and DS2500 Analyzers is the improved resolution, which is four times higher compared to System II. Therefore, the details of the absorption peaks of overlapping bands become much clearer as demonstrated in **Fig. 1** on the example of propafenone.

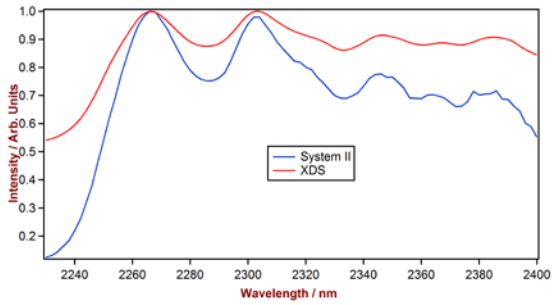

Fig. 1: Spectra of propafenone measured on System II und Metrohm NIRS XDS SmartProbe Analyzer, normalized to maximum after baseline correction. Only spectral region between 2220 and 2400 nm is shown.

Additionaly, the extended spectral range provides more information about the sample analyzed as shown in **Fig. 2** on the example of littleleaf and silver linden. It is evident, that the spectra of both herbal producs are similar in the spectral range between 1100 and 2500 nm, which is used in System II 5000 Analyzers. On the other hand, the use of the Vis-NIR systems provides additional spectral information, which uncover significant difference within both products. This spectral information can be used to improve qualitative models and to reduce complexity.

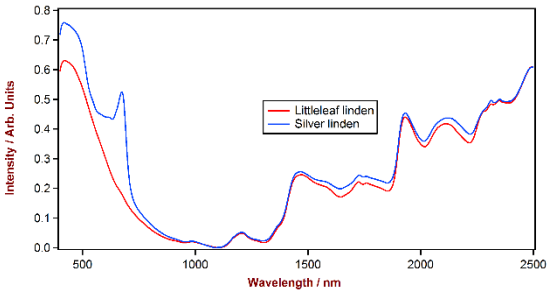

Fig. 2: Spectra of littleleaf and silver linden measured on Metrohm NIRS XDS Analyzer.

Quantitative analysis

Regarding quantitative models, the extended spectral range can improve the analytical figures of merit when additional spectral information is available. The benefits of the spectral range below 1100 nm can be demonstrated e.g. by the quantification of density of polyethylene. The analytical figures of merit for the quantification with the whole spectral range and reduced spectral range are shown in **Tab. 2**. It's evident that the extended spectral range increases the linearity of the model as shown by the correlation coefficient (R^2). Furthermore, standard error of calibration (SEC) and standard error of cross validation (SECV) are significantly lower, when the extended spectral range is used. Additional information is available in the Application Note NIR-34.

Tab. 2: Analytical figures of merit for the determination of density in polyethylene for different spectral ranges.

Equipment	System II 5000, 1100-2500 nm	Metrohm XDS Analyzer, 400-2500 nm
R^2	0.942	0.965
SEC / g/cm³	0.0038	0.0029
SECV / g/cm³	0.0041	0.0032

Conclusions

The current application note demonstrates, that the replacement of the System II (5000/6500) with the Metrohm NIR XDS and DS2500 Analyzers can enhance the analytical figures of merit of the NIR application because of the improved resolution and extended spectral range. The data transfer, which is associated with the replacement of old analyzers is supported by Metrohm application specialists worldwide.

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