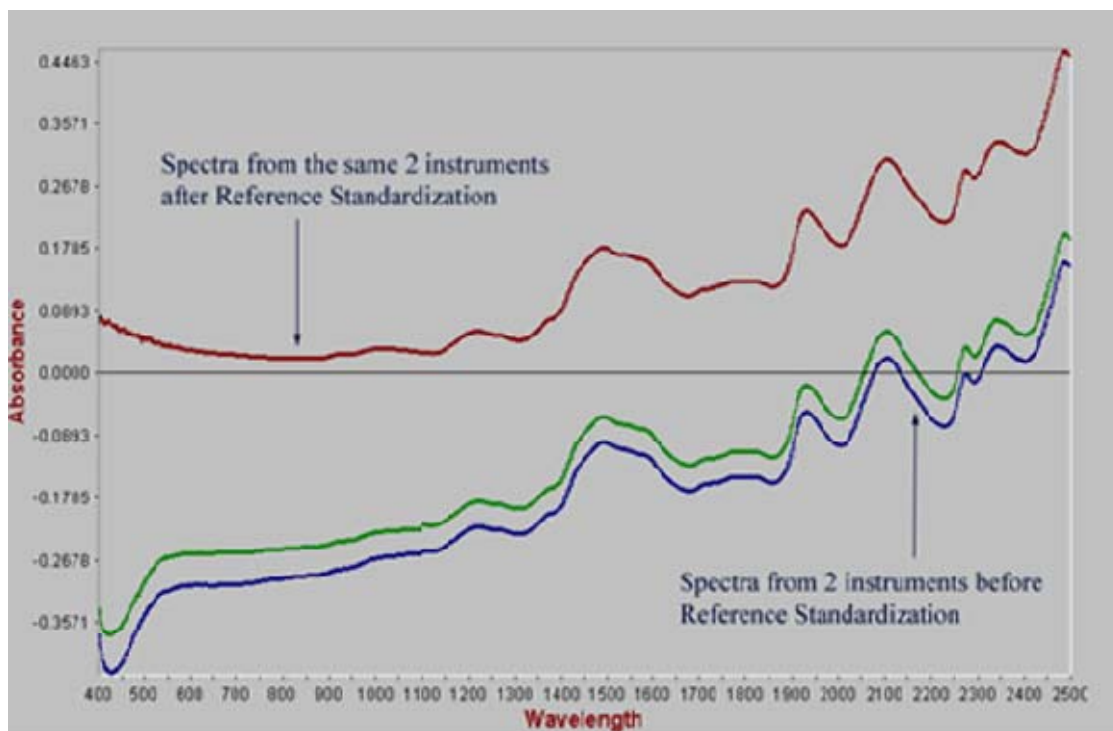


Increase the accuracy of your NIR measurements with reference standardization



This Application Note describes how the accuracy of your NIR measurements can be increased by using reference standardization.

Method description

Introduction

Metrohm NIRSystems XDS instruments increase the accuracy of your NIR measurements and allow the seamless transfer of data, methods, and equations, in part, through the use of a calibrated external standard and a Vision exclusive Reference Standardization program. Reference Standardization is used on most NIRS XDS instruments (laboratory and process) performing reflectance, immersion, and transmission measurements.

Experimental

In reflectance and immersion measurements the NIRS Reference Standardization program provides an accurate measurement of the spectroscopic reference by removing the influence of the physical attributes of that reference. For XDS process transmission measurements, the response of the transmission pair fibers is measured and the signal is "normalized" to provide a 100% background reference scan. This is required on XDS process transmission instruments, which use an internal fiber for the background reference. It is not required for XDS OptiProbe Transmission instruments, which take the background reference using the transmission pair.

In laboratory instruments using a ceramic reference, Reference Standardization removes spectral features attributable to the individual ceramic reference. Each ceramic reference has its own NIR "fingerprint". In process instruments, Reference Standardization removes spectroscopic differences between the reference channel and the sample channel. In both cases an external photometric standard of known reflectivity, as measured on an absolute reflectance scale, is scanned on the instrument. The differences between the instrument internal reference reflectivity and the external standard reflectivity are mapped and a photometric correction is calculated at each data point. The correction is then applied to every subsequent spectrum collected on the instrument to make each spectrum appear as if taken with a 100% reflectance reference.

In Process instruments performing transmission measurements, air is used as the reference. The optical response to a controlled pathlength of air is measured and stored. A correction is applied to bring the sample channel to "0 Absorbance", corresponding to the ideal response of an air measurement in transmission. This accounts for differences between the reference fiber path and the sample fiber path. XDS Liquid Analyzers and transmission pair OptiProbes do not require this correction, because the reference is collected through the sample fiber path and therefore no difference in response is created.

Results and discussion

A graphic comparison between spectra collected on 2 separate instruments Reference Standardized (spectra overlay) and non-Reference Standardized spectra can be seen below.

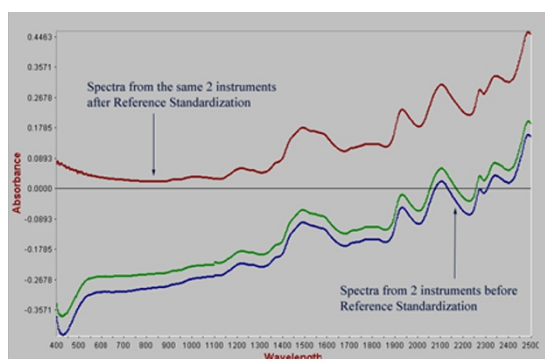


Fig. 1. Graphic comparison between spectra collected on 2 separate instruments

When a Reference Standardization file is created for an instrument, the photometric correction is stored on the motherboard of the instrument. The motherboard can store up to nine different photometric corrections. In XDS Laboratory instruments the sampling module serial number is linked to the photometric correction of that particular sampling module. In XDS Process instruments it is the sample channel number that is linked to this information.

In addition to the increased accuracy of the spectroscopic measurement, Reference Standardization is crucial to the successful transfer of data, Library methods and calibration equations from instrument to instrument without the necessity of additional sample spectra collection or bias adjustments.