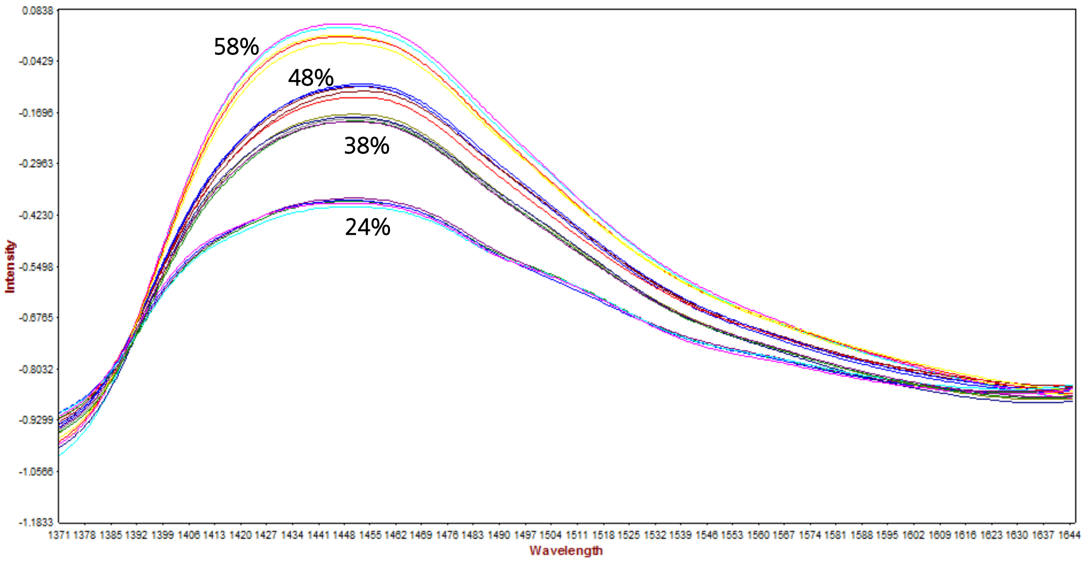
Near-Infrared Spectroscopy Application Note NIR–20

Quantification of embedded H_2O in soft contact lenses by NIR spectroscopy



This application note describes the determination of water content in soft contact lenses by NIRS. Using a liquid sample kit with a gold diffuse reflector, the soft contact lenses were analyzed in transflection mode. A PLS model for regression was built to predict the water content.

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Method description

Introduction

Because of their delicate nature, soft contact lenses require a minimal-contact analysis method to avoid damage. NIR spectroscopy provides a quick and damage-free solution. Four sets of soft contact lenses with varying, known moisture levels were analyzed by NIR spectroscopy and a quantitative model was developed. Difficulties that arose due to moisture loss by evaporation were overcome by paying careful attention to testing procedures. A model was developed and successfully used to predict the embedded moisture levels of H_2O in soft contact lenses with a standard error of prediction near 1%.

Experimental

Four sets of lenses with varying amounts of embedded water were available for analysis, each set consisting of 3 samples. Laboratory values for the calibration were provided by the customer and are listed in **Table1**.

Table 1: Samples and provided reference values

Product (% H_2O)	Number of lenses per product	Spectra per Product
24 %	3	5
38 %	3	5
48 %	3	5
58 %	3	5

The lens was first patted dry by gently pressing between two dry wipes four times. It was then quickly centered on a diffuse gold reflector and placed in a transflection vessel as shown in **Figure 1**.

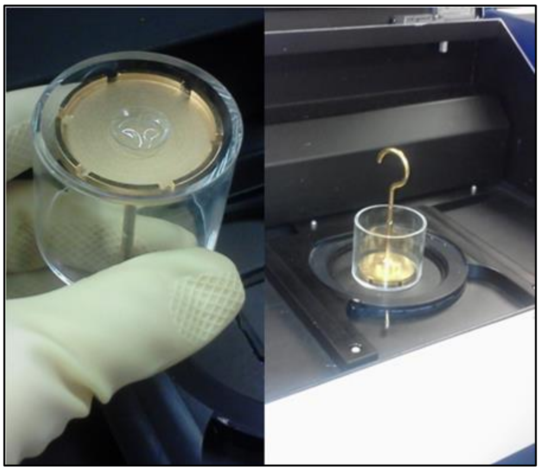

Figure 1: The lens is centered on a diffuse gold reflector in a transflection vessel

The transflection vessel was placed centrally on the sample window of a NIRS XDS RapidContent Analyzer using an iris adapter (**Table 2**). The NIR spectrum was acquired by transflection through the bottom of the vessel. Each sample spectrum was collected in 16 seconds. The duration of pat drying, sample placement, and scanning was consistently 1 min ± 10 sec.

Table 2: Used equipment for Data Acquisition

NIRS XDS RapidContent Analyzer	2.9211.110
Iris Adapter	6.7425.000
Liquid Sample Kit for RCA	6.7400.010

Method development:

A quantitative model was developed in the Vision software using 12 spectra – 3 of each product (1 of each lens). The partial least squares (PLS) regression model was developed to correlate the spectra profile with the embedded moisture percentage. The method development parameters are listed in **Table 3.**

Table 3: Parameter for the PLS Regression Method

Method	Partial Least Squares
Regions	1372 - 1648 nm
Factors	3
Math Pretreatments	Standard Normal Variate (SNV, 1120 - 2500nm)
Std. Error of Calibration	1.69 %
Std. Error of Prediction	1.36 %
R^2	0.9879

An external validation was not feasible due to the small number of samples. However, two samples per product were measured twice, and these spectra were used as a self-validation.
An additional experiment was carried out to examine the dependence of the predicted value on air-drying time. Air-drying time is defined here as the time that the lens is exposed to air after being patted dry but before data acquisition.

Results

Figure 2 shows the water absorption region of the NIR absorption spectra of the different contact lenses. The trends for the different concentrations are clearly distinguishable. The standard normal variate (SNV) math treatment was applied to the spectra to reduce effects from scattering and path length variations.

Method description

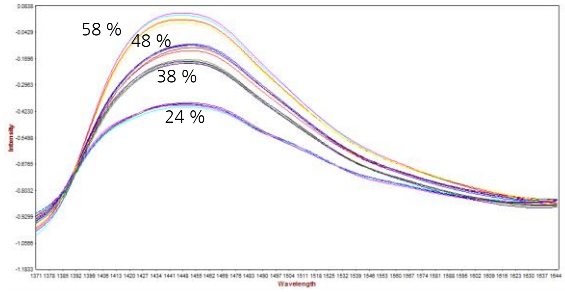

Figure 2: NIR spectra (with SNV) of the water absorption in soft contact lenses with 24%, 38%, 48%, and 58% embedded water.

PLS calibration furnished a quantitative model. The standard error of calibration (SEC) using three factors was 1.69% with an R^2 value of 0.9879. The standard error of prediction (SEP) for the self-validation was 1.36%. The scatter-plots of calculated vs. lab-reported values for the calibration and validation are shown **Figure 3** and **Figure 4**, respectively. There is very good agreement.

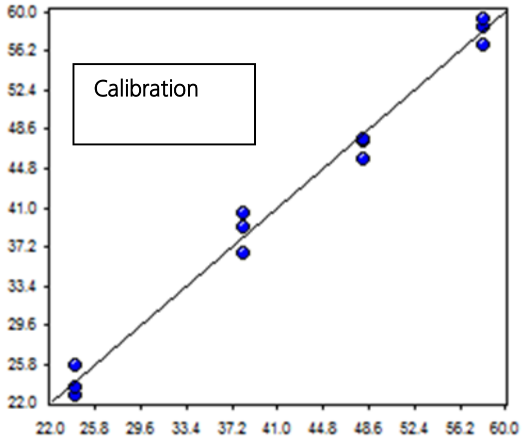

Figure 3: Values calculated from NIRS data using a PLS model vs. lab values for the percentage of embedded water measurement in soft contact lenses.

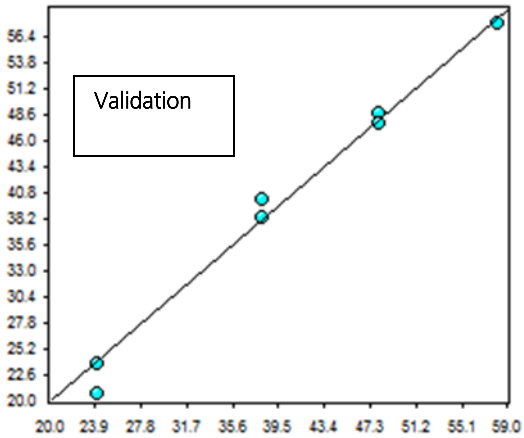

Figure 4: Values calculated from the validation NIR spectra vs. lab values for the percentage of embedded water measurement in soft contact lenses.

Table 4 shows the effect of air drying on the accuracy of the measurement. The sample column lists the time that the lens was exposed to additional air drying. The NIR prediction is listed next to the respective time. The results show that the NIR prediction underestimates the moisture level as exposure time is increased. It is thus crucial that the time allowed for data collection after patting dry each sample is equal in each measurement. Deviations from the set procedures could result in error.

Table 4: Effect of air drying on the accuracy of the measurement

Sample	NIR Prediction	Units
48%, 1 min	48	%
48%, 3 min	47	%
48%, 5 min	46	%
48%, 7 min	44	%
48%, 9 min	43	%
48%, 11 min	41	%

Conclusions

Method description

The results indicate that NIR can be successfully used to monitor the percentage of embedded water in soft contact lenses. Water content is a good application for near-infrared spectroscopy, as spectra can be collected quickly and with ease. A near-infrared solution for analysis offers a number of unique advantages over traditional methods of analysis including; no sample preparation, rapid analysis times, and recovery of the intact sample. In addition, as the near-infrared method does not use solvents or destroy samples, it generates no waste. One cause of error was due to the lens folding over on itself while taking the spectra. This error can be removed by using a reflector with a longer gap length (~ 1 mm) that would not deform the lens. A 1 mm gap reflector was not available for this study.

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