Accurate Determination of Moisture Content of Soft Contact Lenses by Near-Infrared (NIR) Spectroscopy

Dr. Hari Narayanan, Dr. Keith Freel[1]

NIR

Summary

Near infrared (NIR) spectroscopy is a rapid, non-destructive method for analysis of routinely measured products. NIR can eliminate lost time and lost product while improving real time quality control. The delicate properties of soft contact lenses require a minimal-contact method for analysis to avoid damage to the lens itself. NIR spectroscopy provides a quick and damage-free solution. Four sets of soft contact lenses with known moisture levels were analyzed by NIR spectroscopy. The spectra were analyzed for quantitative model development. Difficulties arose due to moisture loss by evaporation. However, with careful attention to testing procedures, a model was successfully developed and used to determine the embedded moisture levels in soft contact lenses with an error less than 1 %. Several methods were tested and evaluated based on accuracy, precision, experimental simplicity, and potential for lens damage

Sample Presentation

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. Successful NIR method development starts with the proper sample presentation. To measure good NIR spectra, the proper sample presentation is of utmost importance for the delicate soft contact lenses. In this work we studied the influence of three different sample presentations, Reflectance, Trans-reflectance and Transmission. Calibration was built using all the sampling methods and the results were compared for prediction accuracy, precision, ease of use and damage to the product.

Experiment

Four sets of lenses with varying embedded water quantities were available for analysis. The known embedded water content for these four sets were 24%, 38%, 48%, and 58%. 20+ spectra were used to build a spectral library for method development – using five to six samples from each of the four lots. Each spectrum consisted of 32 co-added scans of sample and reference in the scan range of 400-2500 nm. The lens was first patted dry with a Kim wipe, then centered on the respective lens mount and the NIR spectrum was acquired. The time duration from the beginning of the pat dry to spectrum acquisition was closely monitored and ranged from 45-70 seconds. Consistent timing was required in order to reduce the effect from air drying. Each sample spectrum was collected in 16 seconds.

Figure 1 shows the reflectance measurement using NIRS XDS SmartProbe Analyzer using an 80% reflectance standard as the background. Transmission sample presentation was tested using NIRS XDS Transmission OptiProbe Analyzer and NIRS XDS RapidLiquid Analyzer (RLA), which are shown in Figures 2 and 3, respectively. A special lens holder was designed for mounting lenses in RLA. Samples were measured in Trans-reflectance mode using NIRS XDS RapidContent Analyzer (Figure 4). The contact lens was placed on a gold-plated reflector and into a quartz cup for analysis. The reflector provides an optical pathlength of 2 mm.

Instrumentation and Sample Presentation

Fig.1: Reflectance : NIRS XDS SmartProbe Analyzer

Fig.2: Transmission: NIRS XDS Transmission OptiProbe Analyzer

Fig.3: Transmission: NIRS XDS RapidLiquid Analyzer

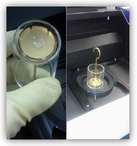

Fig.4:Trans-Reflectance: NIRS XDS RapidContent Analyzer

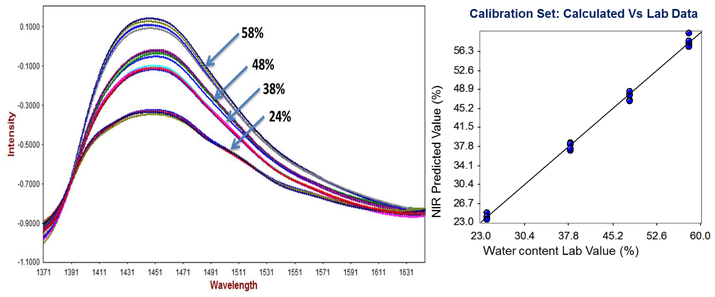

Fig.5: shows the water absorption region of the NIR absorption spectra of the contact lenses with various percentages of embedded water collected using RCA in trans-reflectance mode. The standard error of calibration using only two factors was 0.82 % with an R^2 value of 0.9964.

Results and Discussion

A quantitative model was developed in the Vision® chemometric software using spectra within the region above. A partial least squares regression model was developed from 1272-1648 nm to correlate the spectra profile with embedded moisture percentage. The trends for the various concentrations are clearly distinguishable. The standard normal variate math treatment was applied to the spectra shown in Figure 5 to reduce effects from scattering. There was another water absorption band near 1900 nm, however this was not included in the model since it appeared to overlap with absorption features specific to the lens material. Note that absorption features in other regions of the spectrum could easily distinguish the differences in the lens material itself – with far better accuracy than the embedded water content.

The correlation value, standard error of calibration and prediction for each type of sample presentation is summarized in the table below. The models were validated with NIR spectra of lenses with the same concentrations but separate from those spectra used to build the model. The various known concentrations are compared to the values obtained from the experiment. Values obtained using trans-reflectance mode was in very good agreement compared to the other sample presentation methods.

Sample Presentation	Correlation	Number of Factors	Standard Error of Calibration	Cross Validation Error	Precision	Simplicity	Sample Damage
Transmission - Optiprobe	0.9882	2	1.48%	1.50%	Good	Good	NO
Trans-reflectance - RCA with Liquid Kit	0.9964	2	0.82%	0.92%	Very Good	Very Good	NO
Transmission - RLA sample mount	0.9931	3	1.14%	1.30%	Very Good	Very Good	NO
Reflectance - SmartProbe	0.9186	3	0.92%	0.96%	Good	Good	YES

Conclusion

The results indicate that NIR can be successfully used to monitor the percentage of embedded water in soft contact lenses. NIR measurements take approximately 15 seconds and offer a number of unique advantages over traditional methods of analysis including; no sample preparation, rapid analysis times, and recovery of the intact sample. The reference values submitted were rounded numbers. More accurate and precise lab values will result in more accurate NIR predictions. The submitted values were assumed to be label claim or estimates used for feasibility. The trans-reflectance offered easy sample presentation with good prediction, accuracy and intact sample recovery.

[1]Metrohm USA,Laurel, MD 20723, kfreel@metrohmusa.com