

Application Note:

Iodine Value of Oils

An important characteristic of a fatty oil product is its iodine value (IV). This is a measure of the unsaturated fatty acid content and indicates the ease of oxidation or the drying capacity of the product. Empirically, the IV is expressed in terms of the number of centigrams of iodine per gram of sample. The laboratory analysis for IV determination is both time consuming and involves the use of hazardous materials. This note will discuss the use of Guided Wave hardware and software tools for the measurement of the iodine value of fatty oils using fiber optic based, Near-Infrared (NIR) spectroscopy. NIR can be applied in real time directly in process monitoring or as a laboratory procedure. In either case NIR is a time and money saving alternative to traditional methods. NIR also offers the benefit of increased safety over traditional methods.

Measurement Background: The NIR region of the electromagnetic spectrum contains information from the overtone and combination bands of the C-H, O-H, and NH fundamentals. This information is related to the chemical composition and can be used for both quantitative and qualitative analysis. By measuring the NIR spectra of a series of fatty oil samples of known iodine value, a quantitative model can be developed which will allow the measurement of iodine value in future samples based only on their NIR spectrum. Guided Wave NIR analyzer systems use fiber optics to allow the sample probe to be located in remote locations away from the spectrophotometer itself.

Experimental: The NIR spectra of a group of different fatty oil samples were measured between 1100 and 1600 nm using a Guided Wave spectrophotometer. Figure 1 shows the absorbance spectra of some representative samples using an online process probe with a 1 cm pathlength. The probe is connected to the spectrophotometer using 100 meters of fiber optic cable. The iodine value for these samples ranges from 34 to 74. For this application, the spectra and concentration data were submitted to the Unscrambler™ software and a calibration model was developed using PLS regression methodology. For a discussion of PLS and other multivariate calibration techniques please see Martens & Naes¹ and ASTM E1655².

Results: The model was used to predict iodine values in a laboratory setting. The results for this are shown in Figure 2 as a scatter plot. The model produced a prediction RMSEP (root mean square error of prediction) of 0.93. This is in good agreement with the accuracy of the standard laboratory method.

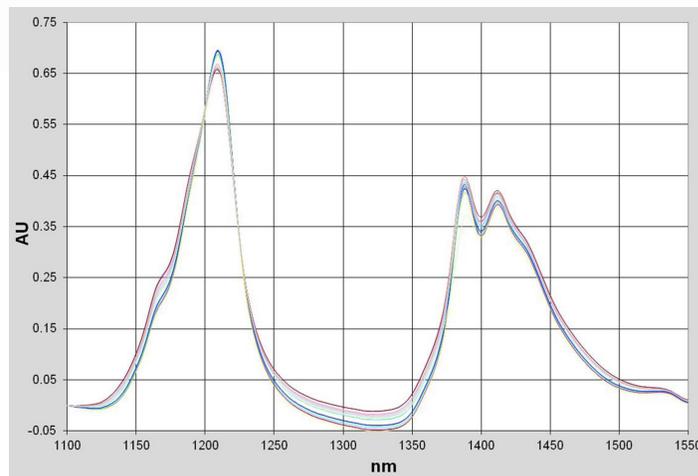


Figure 1: NIR Spectra of Fatty Oil Samples

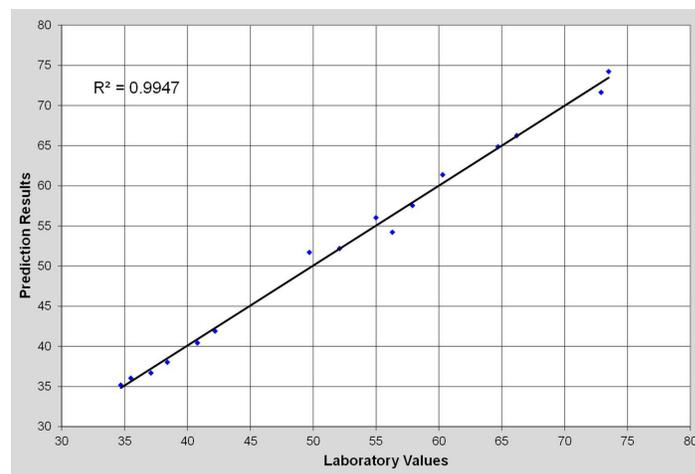


Figure 2 - Iodine Value Laboratory vs. NIR

Conclusion: The measurement of the iodine value of fatty oils using NIR spectroscopy is both fast and reliable utilizing the Guided Wave hardware and software tools as described here. This method minimizes the need for performing the previous laboratory method and hence the results are available in real-time (seconds). This method can be applied in either a laboratory or a process environment. For more detailed information regarding system specifications please contact a Guided Wave sales or technical specialist.

References

1. H. Martens, T. Naes, Multivariate Calibration, John Wiley & Sons, 1989.
2. ASTM E1655 Standard Practices for Infrared, Multivariate, Quantitative Analysis.