Application Note:

Percent Aromatics in Gasoline

The aromatic content of gasoline determines many of its combustion properties. Since it also impacts the environmental characteristics of the fuel it is desirable to have accurate measurements of this parameter. The traditional analytical method for measuring aromatics is either gas chromatography (GC) or an older method entitled fluorescent indicator adsorption (FIA), both of which are time and labor intensive. This note will discuss the use of Guided Wave hardware and software tools for the measurement of % aromatics in fuel products 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.

Measurement Background

The NIR region of the electromagnetic spectrum allows the use of the overtone and combination bands of the C-H, O-H, and N-H fundamentals. By measuring the NIR spectra of a series of fuel samples of known aromatic concentration, a quantitative model can be developed which will allow the measurement of % aromatics in future samples based only on their NIR spectrum. Guided Wave 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 a large number of different process gasoline samples with known aromatics concentration ranging between 2.0 to 62.0% aromatics were measured between 1000 and 1600 nm using a Guided Wave NIR-O™ process anlyzer spectrophotometer. Figure 1 shows the absorbance spectra of some representative gasoline samples collected using an on-line process probe with a 1 cm pathlength. For this application, data preprocessing consisted of a simple 2-point baseline correction to remove any offset. 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 & Naes[1] and ASTM E1655 [2.]
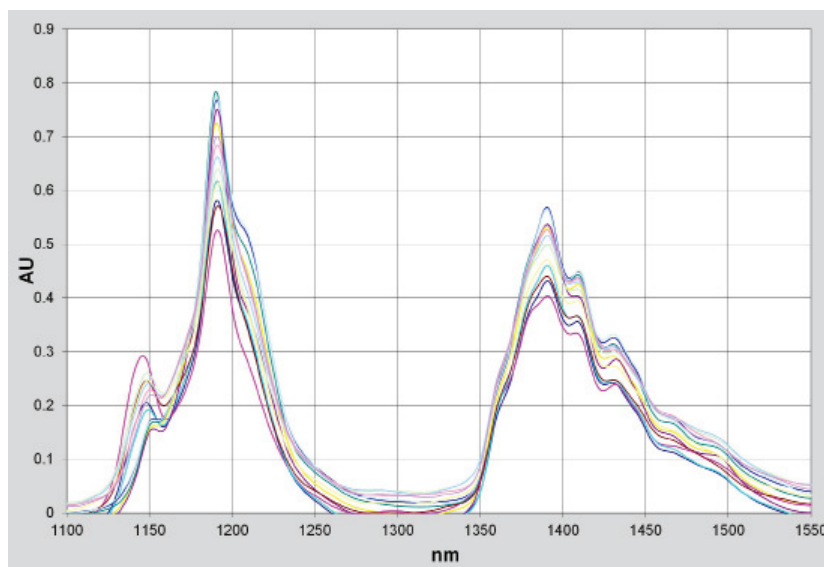

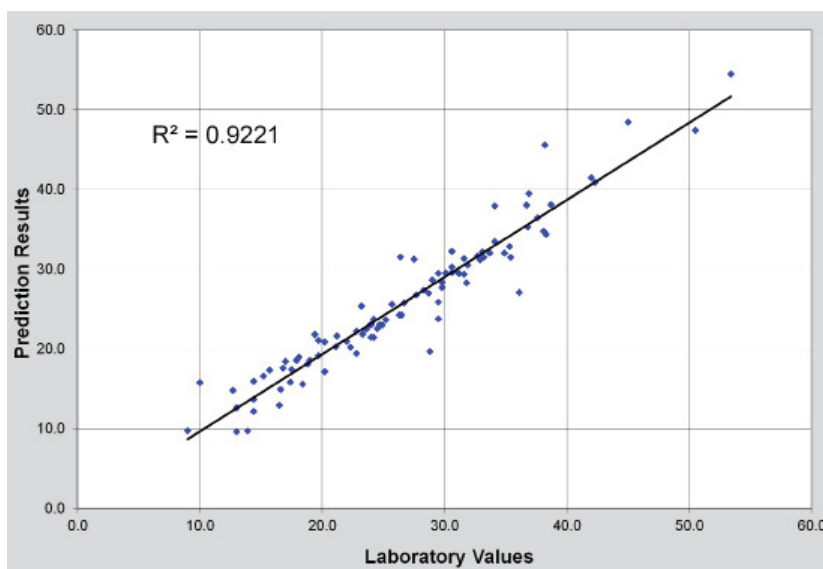Figure 1: NIR Spectra of Gasoline Samples

Figure 2 - Laboratory vs NIR %Aromatics (scatter plot)
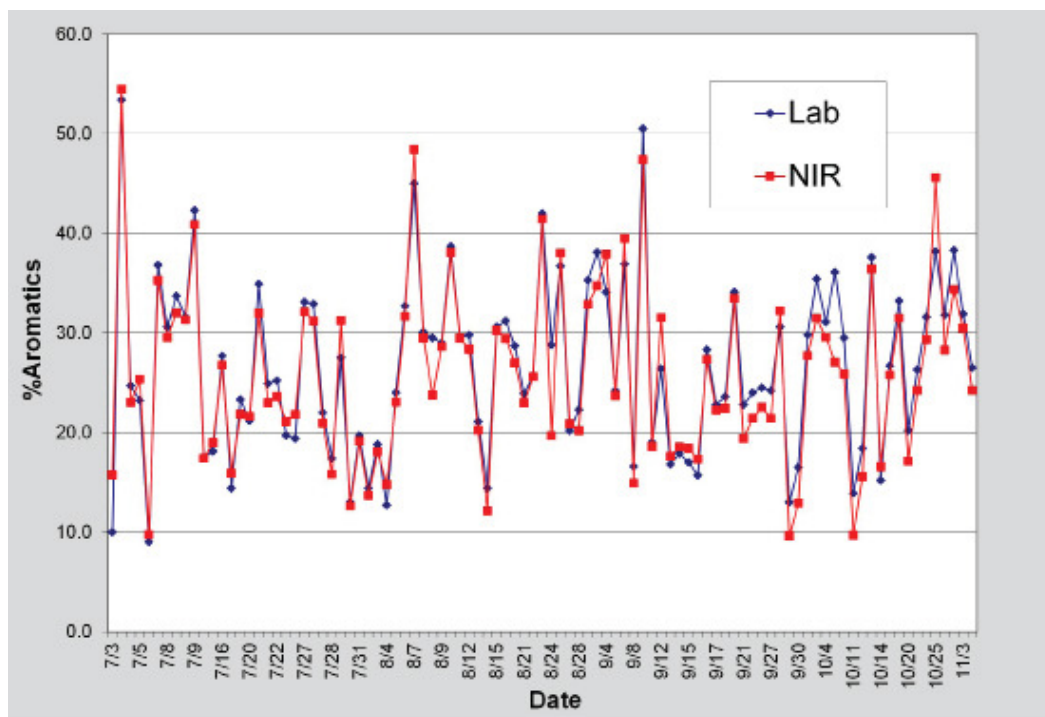
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Figure 3 - Laboratory vs NIR % Aromatics (trend plot)

Results

The model was used to predict aromatic concentrations over a 3 month time period using an in-situ probe inserted in a gasoline process stream measuring in real time. The results for this are shown in Figure 2 as a scatter plot and in Figure 3 as a trend plot. The model produced a prediction RMSEP (root mean square error of prediction) of 2.5% aromatics. This is in good agreement with the accuracy of the standard laboratory method.

Conclusion

The measurement of aromatics in gasoline 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 laboratory sample collection. Results are available in real-time (seconds) for aromatics content and multiple other parameters in other complex hydrocarbon streams. For more detailed information regarding system specifications and capabilities 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.