

APPLICATION NOTE

Cetane Number of Diesel Fuels Using a NIR-O™ Spectrometer

The Cetane number of a diesel fuel is a measure of the ignition properties and is an important specification that must be met during fuel production. The traditional laboratory method for Cetane number determination is the knock engine method in which the fuel is burned and its combustion characteristics compared to known standards. This method is time and labor intensive, and provides no ability for real time control of production. This note discusses the use of our hardware and software tools for the measurement of Cetane number in diesel fuel using fiber optic-based, Near-Infrared (NIR) spectroscopy. NIR is 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 Cetane number, a quantitative model can be developed which will allow the measurement of future samples based only on their NIR spectra. Our GUIDED WAVE™ analyzer systems use fiber optics to allow the sample probe to be located in remote locations away from the spectrometer itself.

Experimental

The NIR spectra of a group of different process diesel fuel samples with known Cetane numbers were measured between 1000 and 1600 nm using our GUIDED WAVE NIR-O™ process analyzer spectrometer. Figure 1 shows the absorbance spectra of representative diesel samples collected using an on-line process probe with a 10 mm 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 a third party software and a calibration model was developed using PLS regression methodology. For a discussion of PLS and other multivariate calibration techniques please see Marten & Naes¹ and ASTM E1655².

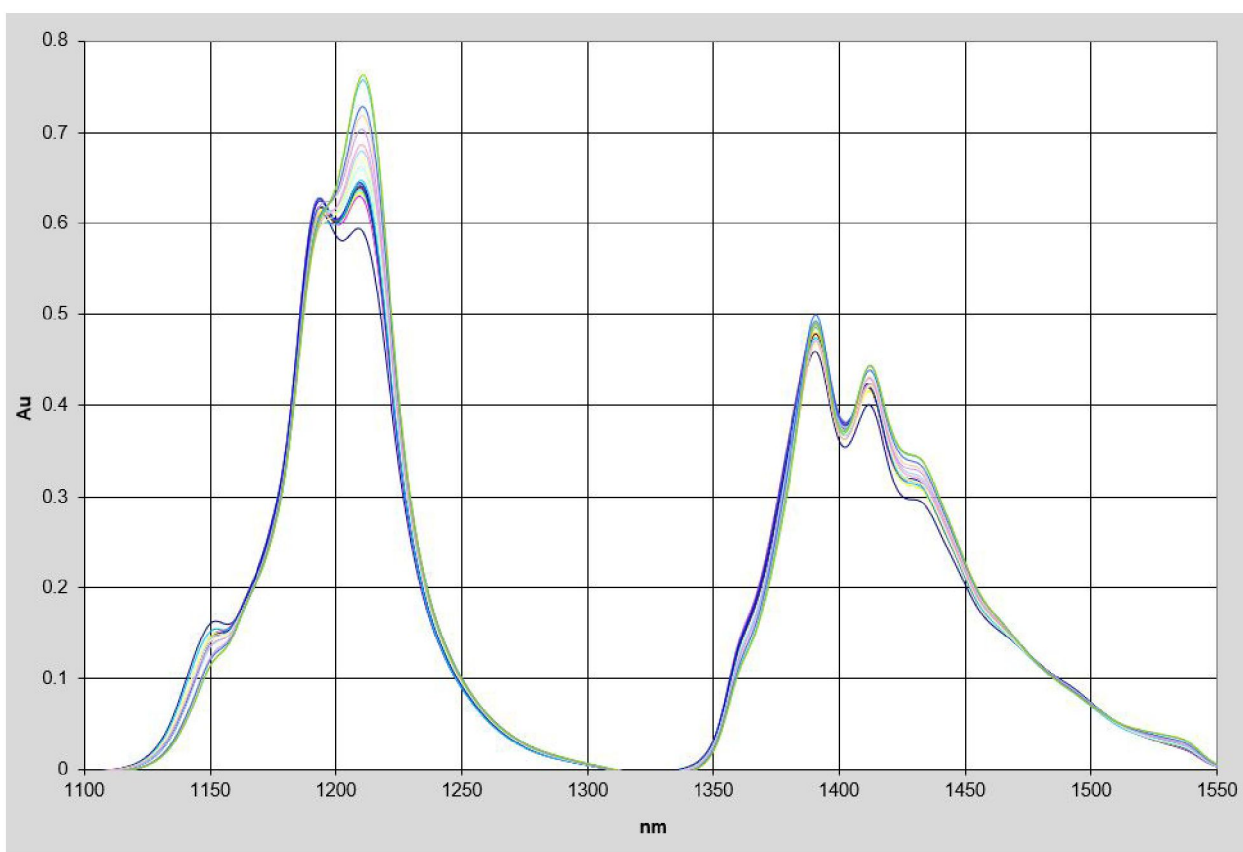


Figure 1: NIR Spectra of Diesel Fuels

Results

The model was used to predict the Cetane number of diesel fuel samples using an insitu probe inserted in a process stream measuring in real-time. The results for this are shown in Figure 2. The RMSEP (Root Mean Square Error of Prediction) is used to measure the model accuracy when compared with the laboratory results. A RMSEP of 0.8 Cetane number was achieved which is in good agreement with the accepted laboratory method.

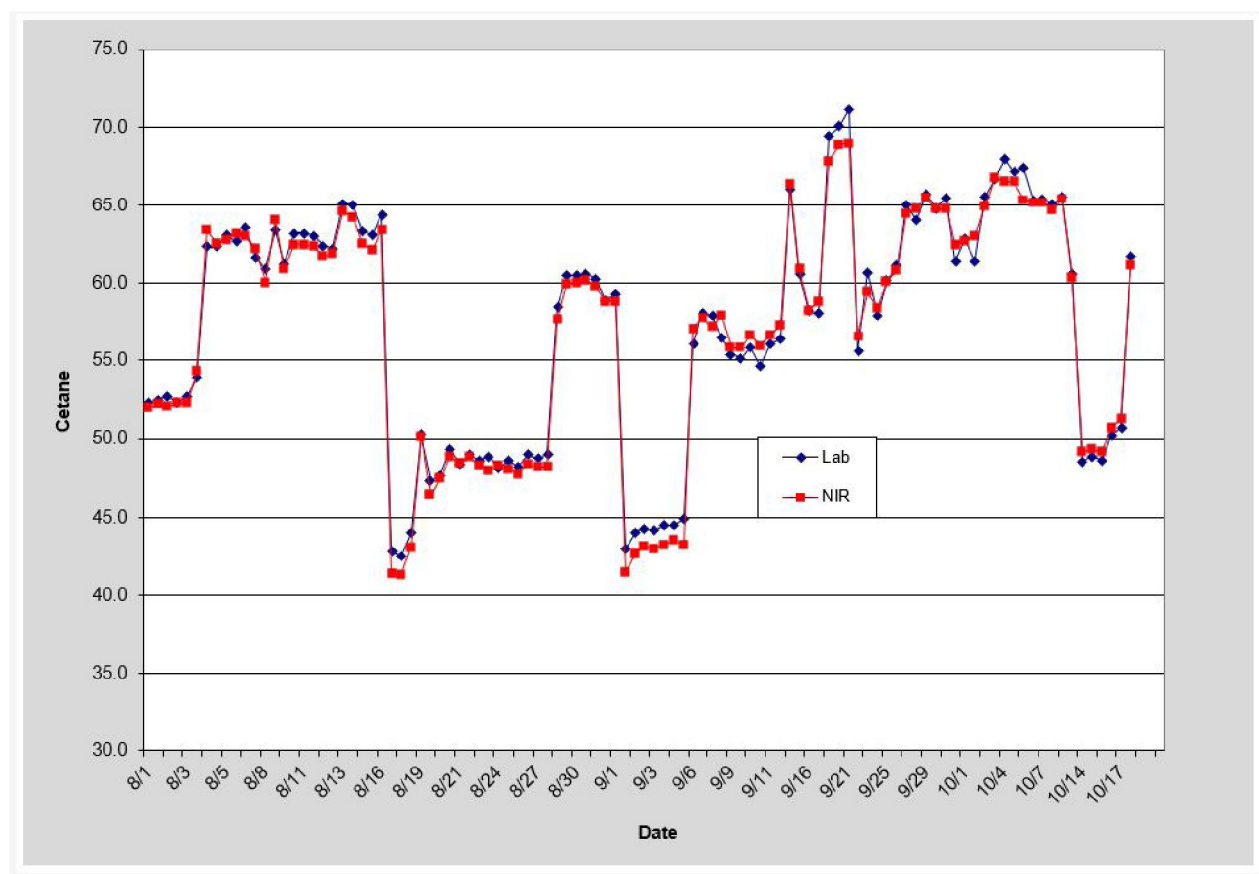


Figure 2: Cetane Number vs. In-Process NIR Analyzer Trend

Conclusion

The measurement of the Cetane number of diesel fuel using NIR spectroscopy is both fast and reliable utilizing the hardware and software tools described here. This method minimizes the need for laboratory sample collection. Results are available in real-time (seconds) for multiple parameters in complex streams. For more detailed information regarding system specifications please contact a Process Insights 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.

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