Guided Wave
Process Analytical Systems

Application Note:

Octane Number Determination using NIR Spectroscopy

The Octane number rating of a gasoline is an indication of how the gasoline will perform under various engine conditions. Two different ratings are included: Research Octane Number (RON) and Motor Octane Number (MON). Finished gasoline must meet certain Octane number specifications. Thus refineries control this parameter during production and must certify that a gasoline meets specification before it is released. In addition, the Octane number of gasoline blending components (reformate, etc) is an important parameter in unit production. The traditional laboratory method for Octane number determination is the knock engine method in which a gasoline 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. The use of Guided Wave NIR spectrophotometric analyzers allows for easy measurement of Octane number in gasoline and refinery production units using fiber optic-based, Near-Infrared (NIR) spectroscopy. Guided Wave analyzers are designed for process use with built in multiplexing capability.
NIR can be applied in real time directly in process monitoring and proves to be a time and money saving alternative to traditional methods. The use of NIR spectroscopy for Octane determination is well documented in the literature with initial studies bing caried out in 1989. (Kelly)

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. (D. Burns) By measuring the NIR spectra of a series of fuel samples of known Octane number, a quantitative model can be developed allowing the measurement of 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 spectrometer itself.

The Guided Wave system is a multi-channel system, allowing one analyzer to measure multiple parameters on multiple streams (up to 12). The multiplexing capability reduces both cost and complexity of installation for each measurement point.

Experimental

The NIR spectra of a group of different process gasoline samples with known Octane numbers were measured between 1000 and 1600 nm using a Guided Wave NIR Spectrometer. Figure 1 shows the absorbance spectra of some representative gasoline samples collected using an on-line process probe with a 1 cm pathlength. The distribution of Octane numbers for these samples is shown in Figure 2. The RON values range from 89.7 to 101.4 and the MON values range from 80.8 to 89.0. These are standard ranges for blended gasoline. A quantitative calibration model was created using the NIR spectra and laboratory octane data. The calibration is generated using PLS regression in the Unscrambler™ software. For a discussion of PLS and other multivariate calibration techniques please see Martens & Naes (H. Martens)and ASTM E1655 (E1655).

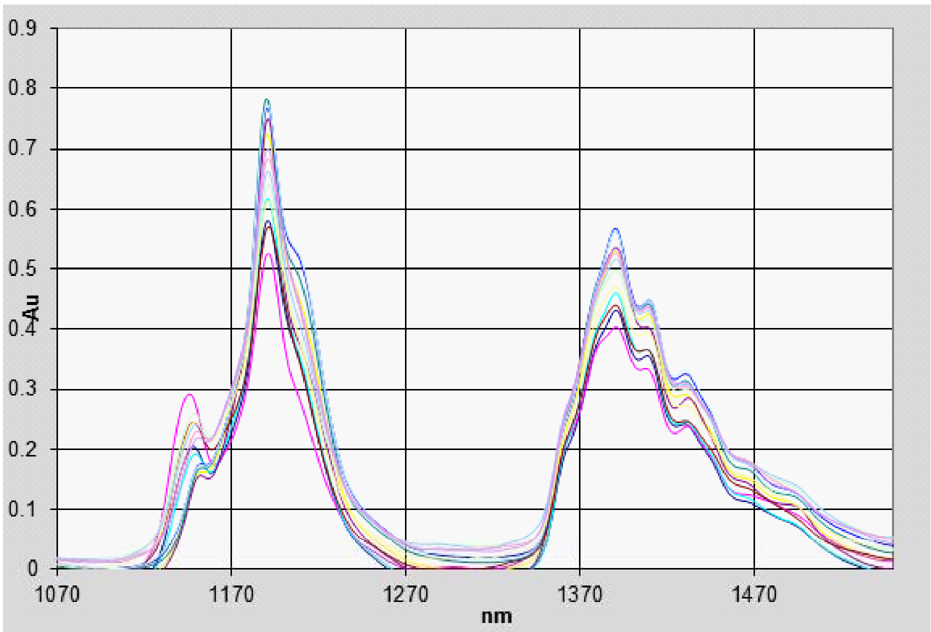

Figure 1: Gasoline Spectra (NIR)

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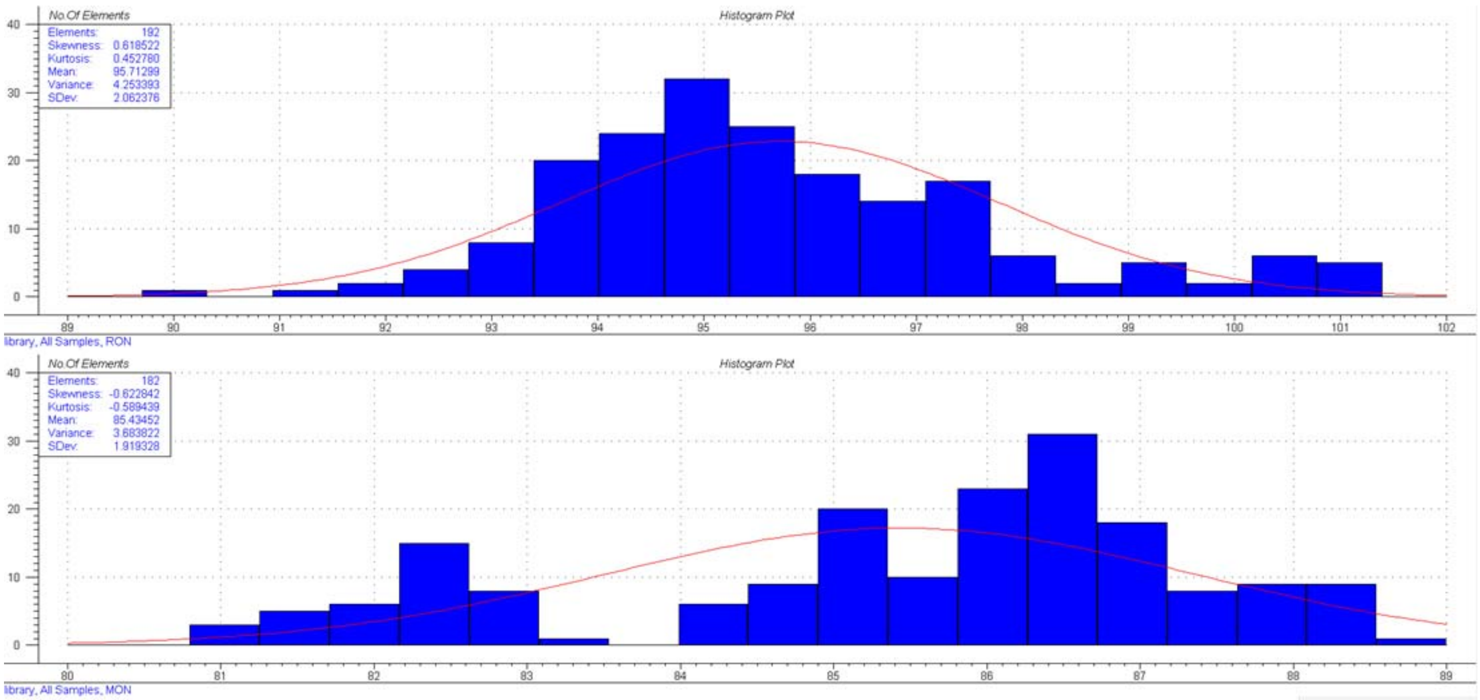

Figure 2: Octane Distribution

Results

The calibration model was used to predict the Octane number of gasoline (RON and MON) using an in-situ probe inserted in a process stream measuring in real time. The results for this are shown in Figure 3 for RON and Figure 4 for MON. Both parameters are in good agreement with the accepted laboratory method. Both models (RON and MON) in this example are set up to operate with multiple grades of blended gasoline. The method easily distinguishes between low, middle, and high Octane samples.

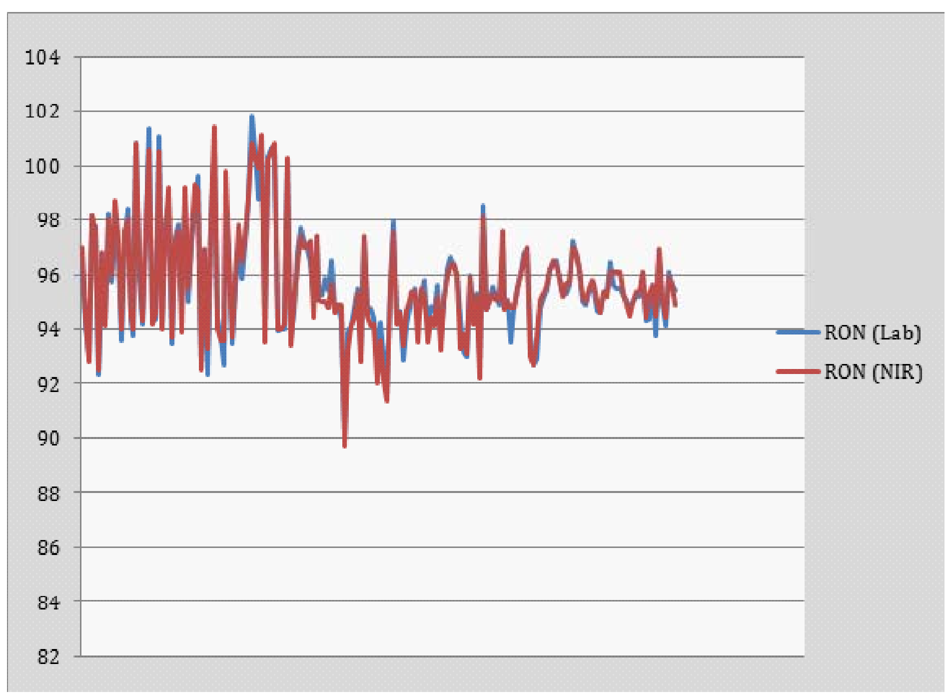

Figure 3: RON Prediction

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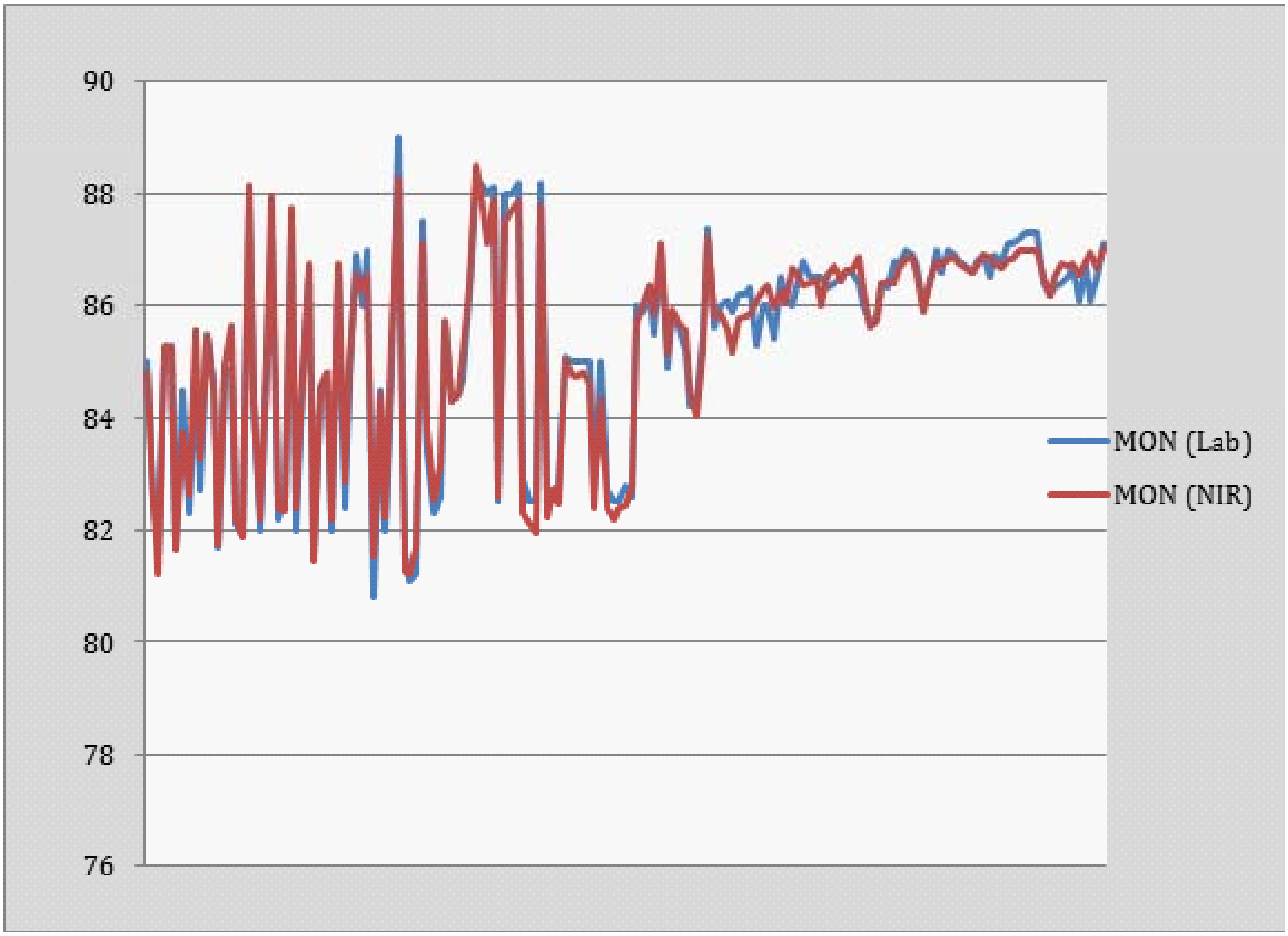

Figure 4: MON Prediction

Conclusion

The measurement of the Octane number of gasoline using NIR spectroscopy is both fast and reliable utilizing Guided Wave NIR analyzers as described here. This method minimizes the need for laboratory sample collection. Results are available in real-time (seconds) for multiple parameters in complex streams. The systems are capable of measuring Octane number and many other parameters such as benzene, density, distillation points, etc for both blended gasoline (all grades) and individual blending components.

D. Burns, E. Ciurczak. Handbook of Near-Infrared Analysis. Marcel Dekker, Inc., 1992.

E1655, ASTM. "Standard Practices for Infrared, Multivariate, Quantitative Analysis." n.d.

H. Martens, T. Naes. Multivariate Calibration. John Wiley & Sons, 1989.

Kelly, Jeffrey J., et al. "Prediction of gasoline octane numbers from near-infrared spectral features in the range 660-1215 nm." Analytical Chemistry (1989): 313-320.

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