Gasoline BTEX and Oxygenate Analysis by NIR Spectroscopy

The Portable Fuel Property Analyzer (PFPA) provides rapid fuel quality assessment using Near-Infrared Spectroscopy combined with advanced Chemometric methods. Key fuel properties that dictate engine performance are obtained in seconds with only a 2-mL sample of fuel. To meet engine specification requirements and EPA regulation limits, the chemical composition of specific constituents must be known. The following chemicals need to be quantified: aromatics, benzene, toluene, ethylbenzene, and the xylenes (BTEX). Gasoline also contains oxygenates that are added to the fuel to limit emissions byproducts from combustion; these additives include ethanol, MTBE, TAME, and ETBE.

Near-Infrared Spectroscopy (NIR) measures the molecular bonds of organic chemicals, and those chemicals can be quantified using chemometric methods such as partial least squares (PLS) analysis. The PFPA is calibrated at the factory per ASTM D6277 and D5845 using a diverse matrix of pseudo-gasoline mixtures. Multivariate correlation models that conform to ASTM E1655 are built and used to predict the chemical properties from a validation set of real gasoline samples.

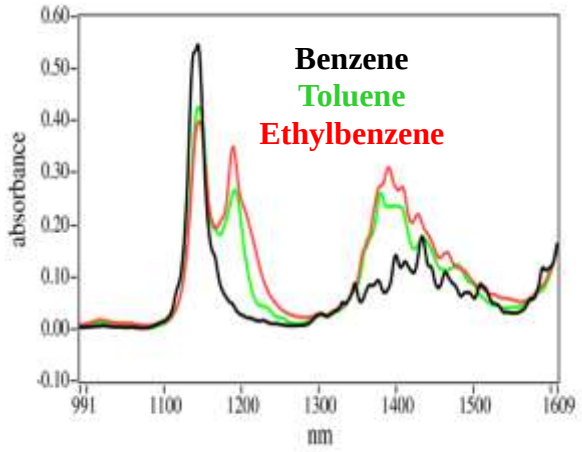

Figure 1. BTEX components in Gasoline

Gasolines Containing Ethanol

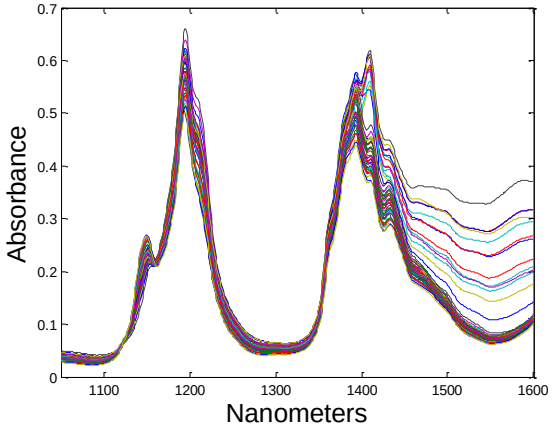

Figure 2. Calibration set of Gasoline samples

Some of the individual BTEX components in gasoline are shown in Figure 1, and the NIR spectra of hundreds of real gasolines are shown in Figure 2. Because of the diverse matrix of chemicals and the lack of isolated spectroscopic peaks, multivariate chemometric correlations using PLS are required.

Benzene in Gasoline Calibration

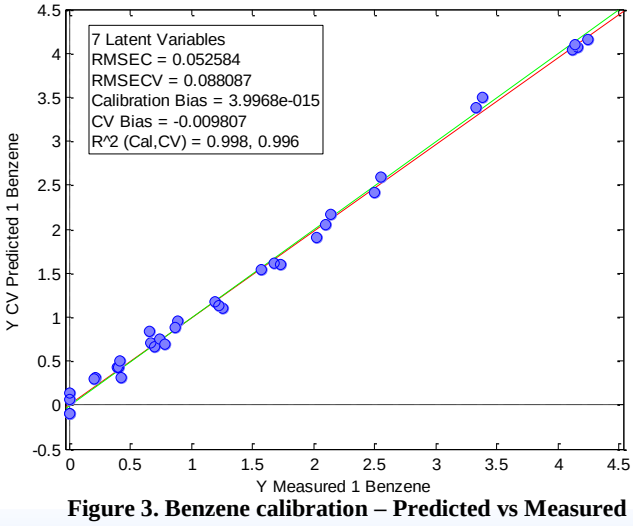

Figure 3. Benzene calibration – Predicted vs Measured

Ethanol in Gasoline Calibration

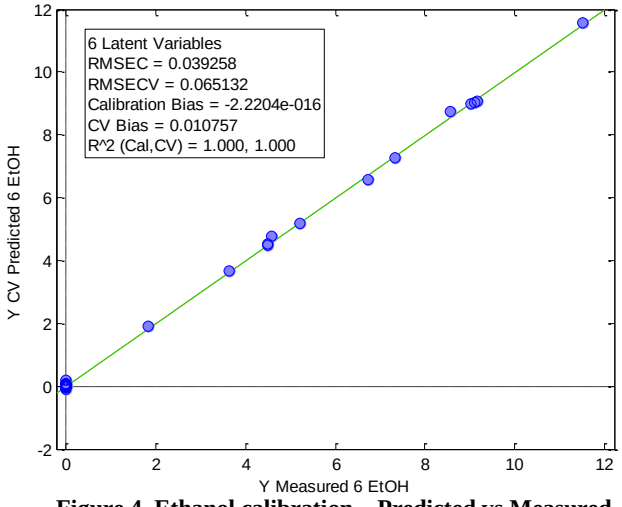

Figure 4. Ethanol calibration – Predicted vs Measured

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The calibration models for benzene and ethanol in gasoline are shown in Figures 3 and 4. Both calibrations exhibit excellent correlations, with R^2 values >0.99 and an error of prediction better than 0.1% by volume.

The use of NIR to predict physical and chemical properties in the petroleum industry has successfully been used for many years. Because the size and cost of spectrometers have come down in recent years, the ability to measure fuel properties now extends to places outside the laboratory. Figure 5 shows benchtop and field-portable versions of gasoline analyzers used to determine BTEX and oxygenates in gasoline. Figure 6 shows the graphical user interface of the easy-to-use software.

Figure 5. Benchtop and Portable versions of the Fuel Property Analyzer

Advantages

- ***Only 2 mL of Fuel Required***
- ***No Sample Preparation Required***
- ***Analyzer Warm-Up takes <1 Minute***
- ***Complete Analysis in 10 Seconds***
- ***Permanently Aligned and Calibrated***
- ***Easy To Use***
- ***Rugged Design, No Moving Parts***
- ***Analysis Based on ASTM Data, Developed and Validated According to ASTM E1655 using Eigenvector PLS Toolbox***
- ***Economically Priced!***

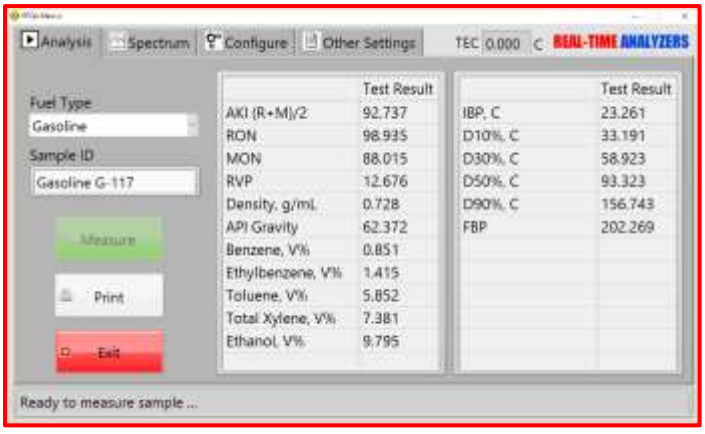

Figure 6. User Interface of Software showing predicted results

The Portable Fuel Analyzer is used as follows:

1) The unit is turned *On* (warm-up takes 1 minute).
2) A Reference Vial is placed in the analyzer for background scan (measurements take 10 seconds).
3) The Sample is placed in a disposable 2-mL vial and placed in the analyzer.
4) The Results are displayed in 10 seconds, and can be printed.

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