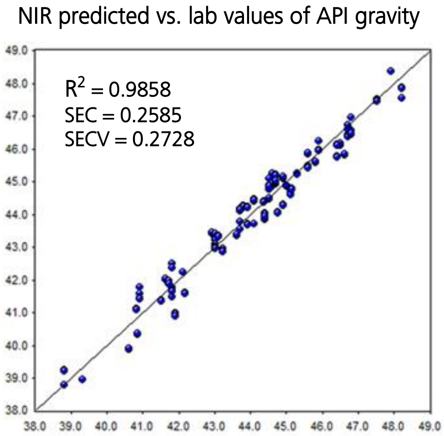
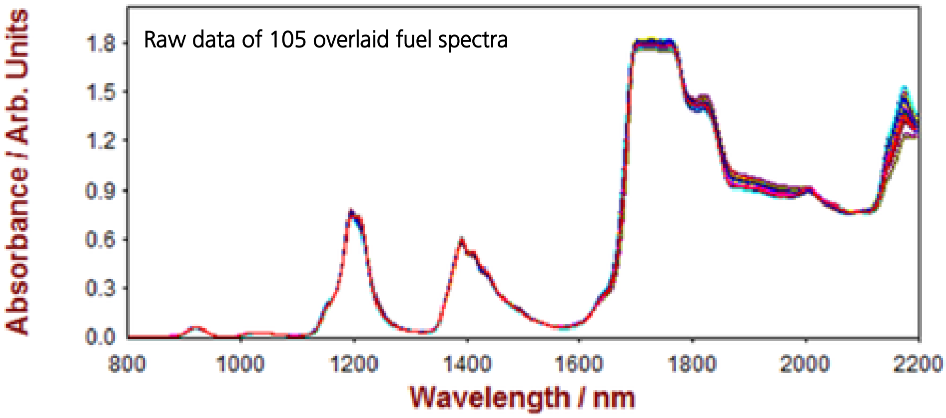
Real-time inline predictions of jet fuel properties by NIRS



NIRS XDS Process Analyzer



This Application Note describes the determination of different important parameters (API gravity, density, aromatic content, cetane index, boiling profiles at 10, 20, 50, and 90% distillation recovery, flash point, freezing point, hydrogen content, and viscosity) for the characterization of jet fuel (also aviation turbine fuel, AFT) using a NIRS XDS Process Analyzer. In contrast to the wet chemical determinations – which are time-consuming and demanding –, the presented NIR spectroscopy method is extremely fast and can be performed by unskilled operators.

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Method description

Introduction

The quality and grade of jet fuel is characterized by a variety of physical and chemical properties that affect the performance and use of fuel. These properties are quantified and reported by a variety of time consuming and sometimes elaborate and expensive lab methods. Most often the methods are based on standardized methods published by the ASTM or ISO. Variations in the characteristic physical properties of jet fuel (freezing point, viscosity, etc.) are known to change based on differences in the chemical composition of the fuel. This link between chemical composition and physical properties permits accurate predictions of these physical properties by correlation with results from direct chemical analysis. Near-infrared (NIR) spectroscopy can do this. This technique uses NIR light to record a spectrum of many chemical characteristics such as the presence and abundance of different types of chemical components or chemical bonds. The chemical measurements taken with NIR spectroscopy can be correlated to the defining physical properties of jet fuel. Scattering effects correlate directly to physical properties.

Experimental

105 samples were analyzed using a NIRS XDS Process Analyzer (**Table 1**) equipped with a stainless steel immersion probe (gap size of 6 mm, 12 mm total path length) placed in a sample container. Each sample was measured three times with stirring in-between. The collection range was 800–2200 nm with 32 scans per spectrum.

Table 1: Used equipment

Instrumentation	Article number
NIRS XDS Process Analyzer – Microbundle 4 Channels	29280120
NIRS Immersion Probe SS	67440010

The samples were supplied from different manufacturers and locations. The samples include a variety of jet fuel grades. Samples were analyzed by NIR and the corresponding standard ASTM method. The parameters of interest were:

- API gravity
- Density at 15 °C
- Aromatic content
- Cetane index
- Boiling profiles at 10%, 20%, 50% and 90% recovery
- Flash Point
- Freeze point
- Hydrogen content
- Viscosity at – 20 °C

A quantitative model for each parameter was developed using Vision (Metrohm`s chemometric software) with the acquired spectral data and corresponding ASTM values. Thus, not all 12 parameters were represented in all samples; a minimum of at least 62 samples were used for model development. The 2nd derivative pre-math treatment was used to produce the best correlation, which corrected for baseline and multiplicative shifts. A leave-one-out cross validation was used to ensure the stability of the developed regression model. Further the method robustness was confirmed with an independent validation set.

Results:

The measured NIR spectra of the jet fuel samples are displayed in **Figure 2**, where absorption bands correspond to vibrational overtones and combinations of different types of chemical bonds.

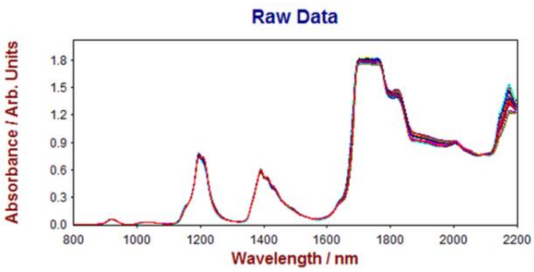

Figure 1: Raw spectrum of the overlay of 105 jet fuel samples measured over a collection range from 800 to 2200 nm

All the samples shared similar absorption features because overall the chemical makeup of each sample is similar. Small chemical differences produce small changes in the NIR spectra. These spectral changes can then be correlated to the changes in physical properties. These small differences are highlighted by pretreating the measured spectra with a second derivative (**see Figure 3**).

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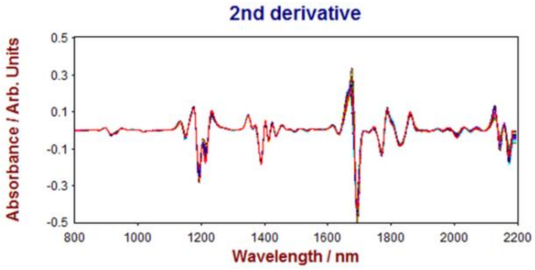

Figure 2: Overlay of the 2nd derivative spectra of 105 jet fuel samples.

The NIR predictions for each parameter are compared to the ASTM values for each sample. The standard error of calibration (SEC), the standard error of cross-validation (SECV), and the standard error of prediction (SEP) are compared to the ASTM precision for each parameter.

Results for API gravity, density at 15 °C, aromatics and cetane index:

	API gravity	Density [kg/L]	Aromatics [V %]	Cetane Index
Sample numbers	104	104	99	101
Max. conc. value	48.2	0.8353	24.4	49.0
Min. conc. value	37.8	0.7874	10.8	33.0
ASTM precision	0.3	0.0012	2.63	< 2.0
NIR SEC	0.26	0.0013	0.5	0.85
NIR SECV	0.27	0.0013	0.51	0.89
NIR SEP	0.29	0.0016	0.72	0.84
R^2	0.986	0.984	0.962	0.934

Results for Flash Point, freeze point, hydrogen content, viscosity at 20 °C:

	Flash Point [°C]	Freeze Point [°C]	Hydrogen content [wt %]	Viscosity at – 20°C [cSt]
Sample numbers	105	104	98	95
Max. conc. value	78.3	– 40.6	14.20	12.440
Min. conc. value	38.0	– 65.5	13.28	1.7
ASTM precision	4.3	0.8	0.16	0.0694
NIR SEC	1.9	1.9	0.05	0.2139
NIR SECV	2.1	2.1	0.05	0.2172
NIR SEP	2.3	2.0	0.05	0.2331
R^2	0.925	NA	0.939	0.905

Results for Temperature (T) at 10%, 20%, 50% and 90% recovery:

	at 10% recovery [°C]	at 20% recovery [°C]	at 50% recovery [°C]	at 90% recovery [°C]
Sample numbers	104	73	104	104
Max. conc. value	210.3	203.9	228.5	273.5
Min. conc. value	153.9	166.0	185.0	157.8
ASTM precision	3.6	-	2.97	3.6
NIR SEC	3.2	1.9	2.2	3.6
NIR SECV	3.3	1.9	2.2	3.6
NIR SEP	3.6	2.0	2.4	3.6
R^2	0.879	0.952	0.927	0.839

Conclusions

The API gravity, density, aromatic content, cetane index, boiling profiles at 10%, 20%, 50% and 90% distillation recovery, flash point, freezing point, hydrogen content, and viscosity were investigated using NIR methods. All parameters gave a good correlation between the changes in the parameters and the spectral variation. NIR spectroscopy can be used to obtain accurate predictions of important parameters for fuel characterization from a single 30-second measurement. The accuracy matched well with the precision of the ASTM method for all of the parameters. The real-time data can be used to monitor and achieve consistent product quality.

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