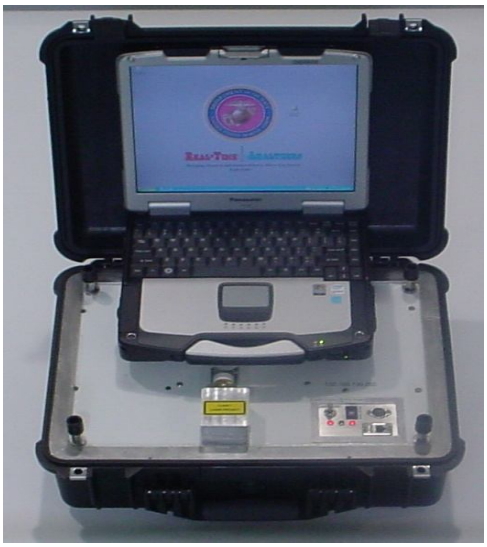
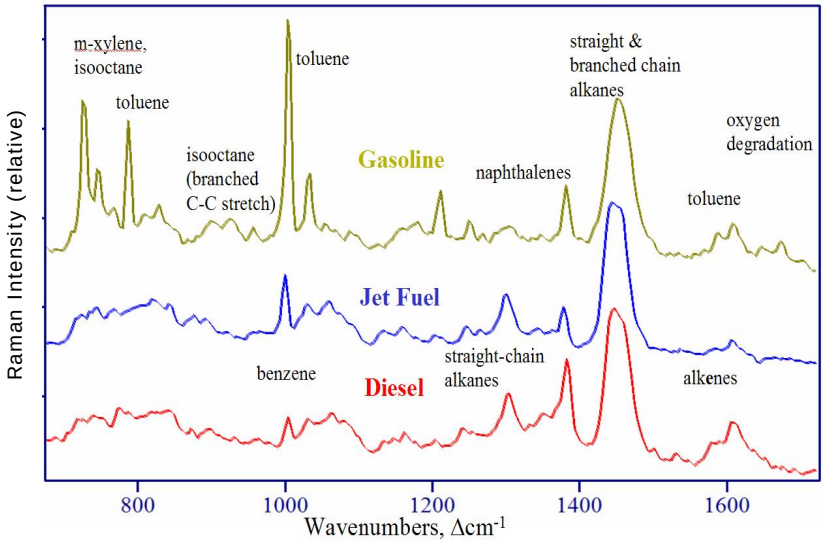
Fuel Applications

RTA Application Note # 04

RTA's **Industrial Raman Analyzer** has been designed specifically for operation in demanding environments, and is suitable for fuel analyses in petrochemical refineries, while a light-weight, battery-operated version, the **Portable Fuel Analyzer**, is suitable for field and tarmac operations.

Fuel Identification and Characterization In simplest terms, the various types of fuels represent crude oil fractions distilled at different temperature. However, the collected fractions are not pure, each consisting of aromatic, heterocyclic, saturated and unsaturated, branched- and straight-chained hydrocarbons that boil at similar temperatures. The rich chemical information provided by the **Portable Fuel Analyzer** can be used to identify the different fuel types relatively easy as shown in the figure to the left. As can be seen, the aromatic content gasoline, added to provide smoother combustion, produces several sharp distinctive peaks.





However, it is more important to characterize fuels in terms of performance properties. For example the gasoline octane number indicates its antiknock performance during combustion, the diesel cetane number indicates its ignition delay and how well an engine will start in cold weather, while the jet fuel viscosity value indicate its atomization and hence combustion properties.

During the past several years, RTA has measured the Raman spectra of more than 700 different fuel samples from around the world. RTA has used this large database to develop correlations between the Raman spectra and the provided fuel properties, such that an unknown fuel can be fully characterized from its Raman spectrum. As stated, however, each sample is composed of hundreds of hydrocarbon components, and performance properties can not be simply correlated to a single chemical component, and certainly not to specific Raman peaks. To meet this challenge, we have used chemometrics to correlate the entire Raman spectrum to the measured fuel properties.

Chemometrics - Principle Component Analysis (PCA), can be used to correlate the Raman spectra to different classes of fuel (e.g. gasoline, diesel or jet fuel). This is useful for determining the type of fuel but it can even predict the fuel grade; in the case of jet fuel it can be used to differentiate JP5, JP8, Jet A, Jet A1, etc. When specific fuel properties need to be known (e.g. density, flash point, freeze point, cloud point, octane number, cetane index, ect.), regression models using Partial Least Squares (PLS), or Principle Component Regression (PCR), can also be used correlate the Raman spectra with the specific fuel property.

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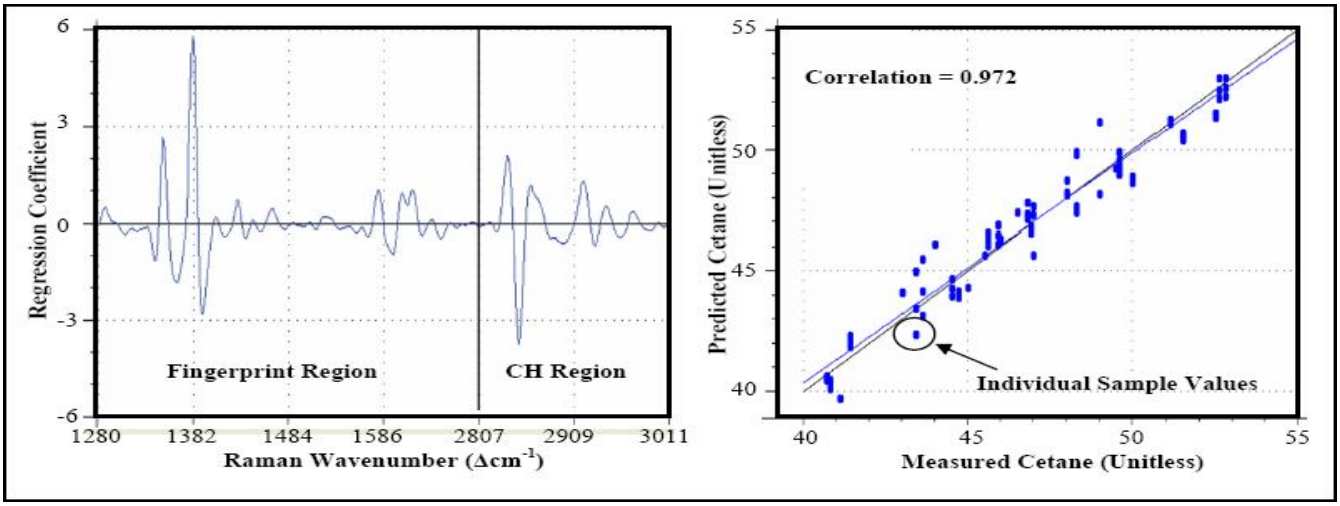
The following figures exhibit PLS calibration models that were built using large data set of Raman spectra. The models were then evaluated using a cross-validation method that utilizes a “leave one out” method and accuracy is reported as RMSEP.

What can we Classify:

Fuel type (Gasoline, Diesel, Jet Fuel)

What properties can we predict with PLS

Gasoline	Diesel	Jet Fuel
Octane (RON, MOM)	Density	Density
Additives:	Cetane Index	Freeze Point
MTBE	Flash Point	Viscosity –20 °C
ETBE	Viscosity +40 °C	Distillation Fxns (IBP, 50%, 90%)
TAME	Distillation Fxns (IBP, 50%, 90%)	Pour Point
	Cloud Point	



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