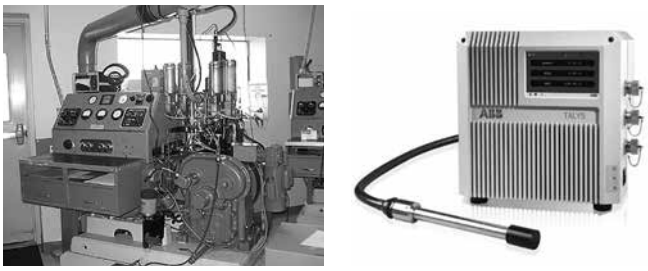
Meandering Through the Oil Industry: Part 2

This technical article is the second in a series characterizing the process that the oil industry follows to bring us one of our favorite commodities, the gasoline that powers our Classics. Might we say - false advertising at the pump?

Gasoline in the Spotlight

By Brian Rohrback

Well, maybe the pump label for octane rating is not quite accurate. It suggests that the Research Octane and the Motor Octane are explicitly measures and averaged (R+M/2) to grade the fuel. What if we could just shine light through the gasoline and look at the spectrum that results – could we then infer the octane rating without ever running the engine? Well, yes. For this, we actually mostly use a portion of the spectrum that is just out of reach of the visible range, known as the near infrared (or NIR for short).



A traditional octane engine on the left and a NIR spectrometer on the right

So, how does this light thingy work? I'm glad you asked. In the first article in this series, I mentioned that gasoline has a lot of different molecules in it, which gives us a whole bunch of (mostly) C-H bonds. When you shine infrared light (think of it as heat) on the molecules they get excited and start to vibrate by absorbing the wavelengths of light that are encouraging them to bend and stretch, kind of like aerobics class. As part of this process, specific frequencies of this energy (those that go towards these wiggles) gets absorbed; frequencies that don't induce motion pass through unchanged. The result is a spectral signature that is a sum of all of the chemical components in the fuel.

The absorbance pattern forms a fingerprint of the particular mixture and we use mathematics (multivariate statistical analysis, also known as chemometrics) to interpret the pattern. The result is that we can do octane analysis at the speed of light, and we get a Green Eggs and Ham moment: we can do it in the pipe, we can do it in a lab, we can do it in the field, we can even do it in your (modern) car, we can measure octane anywhere. This feature gives us a much more comprehensive monitor for gasoline quality than we have had in the past.

Unfortunately, the refineries cannot just purchase any old spectrometer off the shelf and expect it to compute the octane values without doing some work. Each plant needs to introduce a lot of gasoline samples for which they have run their old octane engine to provide a reference value. We need both the engine results and the spectrum from the same samples to train the system to accurately interpret the absorbance signals and come out with an octane rating. This has another layer of complexity as refineries also have to deal with the variation in blend recipes as they work to manage the inventory of input ingredients. They also need to contend with the larger shifts in the gasoline requirements as we move from summer to winter grades of fuel. But that will be a topic for another day.

This whole collection of octane engine results and spectra form a calibration set of samples and we use the aforementioned chemometrics (multivariate mathematics) to process the data and complete the conversion of the plain-old spectrometer into an integrated replacement for the octane engine. The company that pioneered the field of chemometrics and the octane engine replacement happens to be a Pacific Northwest company as well, Infometrix. OK, OK, full disclosure: I am the President of Infometrix.

So, my false advertising claim is really related to the fact that we really do not measure the Research and Motor Octane numbers (which is subtly labeled on every pump); the vast majority of these values are inferred based on the spectroscopy. The octane engine is still in use, but now more as a reference technique, not on the forefront of gasoline quality control. We should not be bothered too much, the accuracy and the precision of the spectroscopic measurements are both higher using light.