Center for Process Analytical Chemistry (CPAC)

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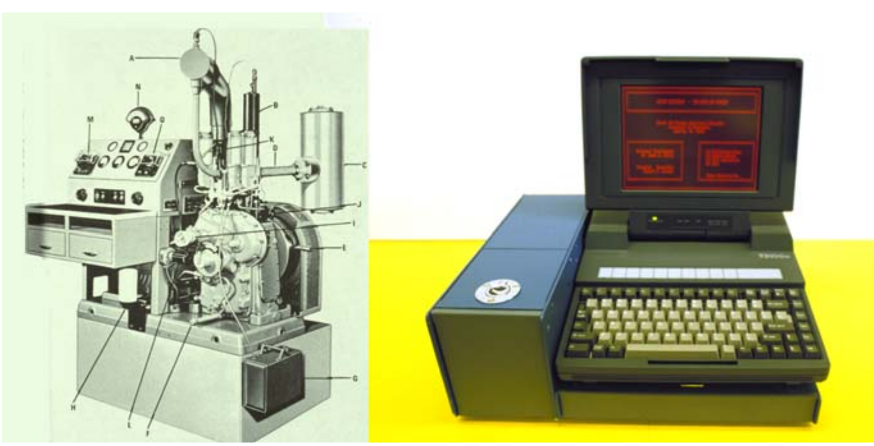
Non-Destructive Spectroscopic Measurement: Inline Octane Sensor

The Center for Process Analytical Chemistry (CPAC) pioneered a revolutionary approach to octane determination in oil refineries. The new method uses a non-destructive spectroscopic measurement followed by multivariate calibration techniques to predict diverse physical, chemical, and consumer properties of fuel. The now commercially available "octane sensor" is now used by oil companies worldwide because it quickly, accurately and in real time predicts octane levels from the near-infrared vibrational spectrum of the inline sample. This is possible because the spectrum of the material clearly reveals the number and types of functional groups (e.g., methyls, methylenes, olefins, aromatics). These together determine gasoline's physical, chemical, and consumer properties. This octane determination method represents a vast improvement over previous octane determination methodologies because octane levels were determined by a specially designed, ASTM-CFR test engine, where the sample's performance was compared to reference fuel blends.

The instrumentation required for the measurement was very expensive (over $100,000), required constant maintenance, needed frequent standardization, consumed approximately one pint of gasoline per test and, most importantly, required 20 minutes to produce results. As a bonus, the octane sensor can simultaneously predict a number of important properties of gasoline such as density, vapor pressure, and percent aromatics. All of these measurements are made nondestructively on one cc of sample. Results are available instantaneously. The approach has proven an invaluable adjunct to process analytical chemistry. It literally saves the oil gasoline refinement industry many millions of dollars per day. For more information, contact James Callis, 206-543-1208; e-mail: callis@u.washington.edu.



Above: Before and after images of the equipment.

Process Chemometrics

Through the efforts of the Center for Process Analytical Chemistry (CPAC), the tools of chemometrics were introduced to the chemical industry, allowing important process and product performance quantities to be obtained from indirect chemical measurements. An important example is the calculation of the fuel performance standard, such as the octane number of gasoline, from infrared and near infrared spectroscopic data obtained on-line during the blending process. Another is the estimation of product performance at an early state in the manufacturing process such as elongation strength of finished polymer fibers. And, for the first time, Multivariate Statistical Process Control (MSPC) allowed manufacturing processes to be controlled using all of the process measurements together as opposed to the old methods of Statistical Process Control (SPC) which demanded the analysis of control charts for each process variable. Chemometrics methods have allowed industrial chemists and engineers to extract all of available information from data acquired during the manufacturing process. Additionally, it has provided tools to determine the actual value of process measurements and/or control parameters leading to a major cost savings by discontinuing the acquisition of useless information.

Today, a number of new companies are available to help chemical and material companies learn to use chemometrics tools developed at CPAC. Many of the mathematical methods are so useful that industry has developed protocols for their use that are approved ASTM standards. Finally, most medium to large chemical, material, pharmaceutical, food, and fuel companies employ at least one chemometrician and several have chemometric groups who do exploratory and routine analysis of process and product data as well as train others to use chemometrics tools to, in general, improve manufacturing processes. For more information, contact Bruce Kowalski, e-mail: bskowalski@mydurango.net or Mel Koch, 206-616-4869; e-mail: mel@cpac.washington.edu.