Center for Process Analytical Chemistry (CPAC)

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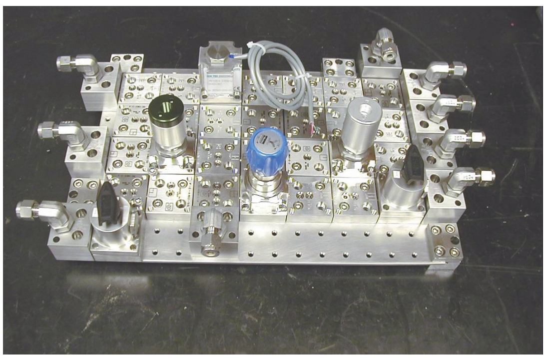
New Sampling and Sensor Initiative (NeSSI™)



Although process analyzers have undergone significant technological advances recently, the systems that deliver samples to them have hardly changed in the last fifty years. An initiative, launched in 2000 by the Center for Process Analytical Chemistry (CPAC), is primarily concerned with the treatment and continuous analysis of samples extracted from process equipment. NeSSI™ provides specifications, guidelines and a forum for the on-going development of a Lego®-style building block platform for analytical systems. It was widely recognized that CPAC's leadership had developed NeSSI™ into a valuable global ad hoc initiative comprised of end users and suppliers and is resulting in permanent changes within the process analysis field. It has now been commercialized by several hardware manufactures and is being specified on major new-build projects. Several engineering companies now provide networked connectivity for all components of the NeSSI™ platform, opening the door to smart diagnostics and improved remote technical support. NeSSI™ is now used to enable improved process analytical measurements in the petrochemical, chemical and oil refining industries and is being studied for applications in the pharmaceutical and bio-technology industries.

Economic Impact: These new NeSSI™ platforms are showing reduced costs (both in the cost to build and the cost to own) with increasing reliability, and hence the value delivered by process analyzers. The combined benefits to industry are growing and will soon be measured in tens of millions of dollars per year.

Non-Destructive Spectroscopic Measurement: Inline Octane Sensor

The Center for Process Analytical Chemistry (CPAC) pioneered a revolutionary approach to octane determination in oil refineries. This ground-breaking new octane sensing method uses a non-destructive spectroscopic measurement followed by multivariate calibration techniques to predict diverse physical, chemical, and consumer properties of fuel. This industry-changing advance was possible because the spectrum of the material clearly reveals the number and types of functional groups (e.g., methyls, methylenes, olefins, aromatics). In combination these determine gasoline's physical, chemical, and consumer properties. 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 non-destructively on one cc of sample. Results are available instantaneously. The approach has proven an invaluable adjunct to process analytical chemistry.

Economic Impact: This octane determination method represents a vast improvement over previous octane determination methodologies because gasoline octane levels were determined by rather antiquated ASTM-CFR test engines, wherein 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. The now commercially available, in-line, real time, "octane sensor" is now universally used worldwide by oil refining companies because it quickly, accurately and in real time predicts octane levels from the near-infrared vibrational spectrum of the inline sample. Worldwide, This in-line octane sensor saves the oil gasoline refinement industry many millions of dollars per day; an estimated 1.5 billion dollars per year.

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Robust Vapochromic Sensors for O_2 Sensors

Vapochromic materials are metallo-organic compounds whose absorption or emission spectrum changes in the presence of analytes (chemicals) of interest. This vapochromic sensor methodology allows selective and fast spectroscopic detection of a broad range of analytes (permanent gasses, common solvents, moisture, small molecular weight organics and halo-organics). To illustrate the breakthrough, measurement of oxygen in gases or as dissolved oxygen in water can be done with such sensors. With suitable fiber optic connections, these sensors can be used for remote process or environmental measurements, many in hostile environments. The technology for this oxygen sensor has now been demonstrated in a variety of applications and it has unique advantages over existing approaches. Sensor uses range from process measurements for production plant operations to medical and environmental sensing applications.

> **Economic Impact:** A variety of other potential vapochromic sensors are being studied that could have wide applications and economic impacts for variety of industries.

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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 of the process of chemometrics 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. 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. Chemometric 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.

Several new companies have been established to help chemical and material companies learn to use chemometric tools developed at CPAC. Most chemical, material, pharmaceutical, food, and fuel companies depend on internal chemometric groups who do exploratory and routine analysis of process and product data. As well, many analytical instruments have now incorporated chemometrics in their operating systems. Recent efforts at CPAC to enhance the treatment of data, development of alignment algorithms for GC data and data fusion methods for multisensory analysis, will further add value to the field of chemometrics.

> **Economic Impact:** The impact of utilizing chemometrics is in the many millions of dollars relative to its effect on process control for optimizing processes across many industries.

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