Measurement of Benzoic Acid Concentration in Toluene

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## APPLICATION NOTES

Analyte: Benzoic Acid $C_7H_6O_2$

Detector: Reveal XNIR (Extended Near Infrared 1100–2100 nm)
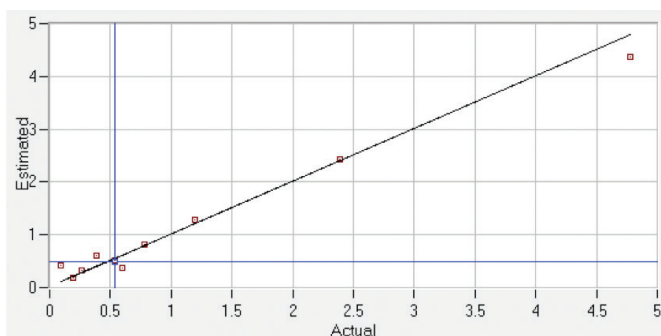
HIGHLIGHTS

- Millisecond measurement times
- Internal referencing, wavelength and linearity validation for stable, continuous operation
- WiFi, Ethernet, OPC, ModBus, Ethernet/IP communications standard
- Hazardous area enclosure options
- Various sampling options
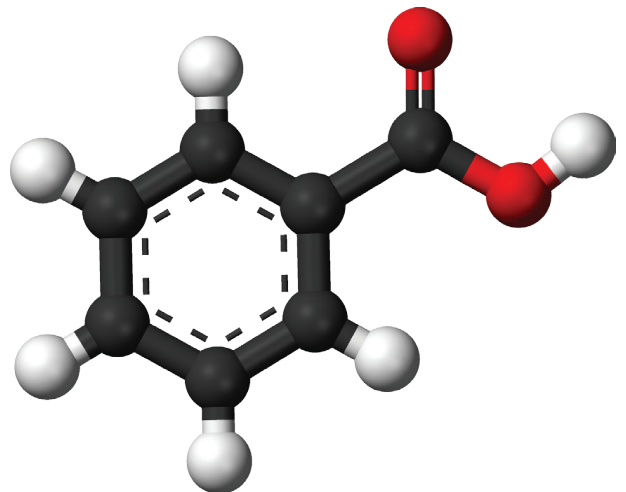
REGRESSION ANALYSIS

Summary

Benzoic acid is a ubiquitous building block for many different organic chemistry synthesis reactions. For example, different end products of reactions containing benzoic acid result in varied products such as plasticizers or food preservatives like sodium benzoate. Benzoic acid is formulated from liquid phase air oxidations of toluene, so knowing the concentration of newly formed benzoic acid in toluene enables researchers to understand the efficiency of their industrial reaction, and thereby the purity grade of the benzoic acid preparation, based off of how much unreacted toluene may be present.

Benzoic Acid Analysis

The Prozess XNIR Analyzer was employed to evaluate how well the concentration of a commercial benzoic acid preparation could be quantified in toluene. Various concentrations of benzoic acid in 99% toluene were generated, and measured with the XNIR system.

Figure 1 illustrates the NIR spectral data of three different concentrations of benzoic acid in toluene, and reveals spectral regions containing linearity with alterations in benzoic acid concentration, indicating that direct quantitation of benzoic acid was feasible from the spectral data alone. Regression models were also developed to take into consideration the entire spectrum, as exemplified in *Figure 2*.
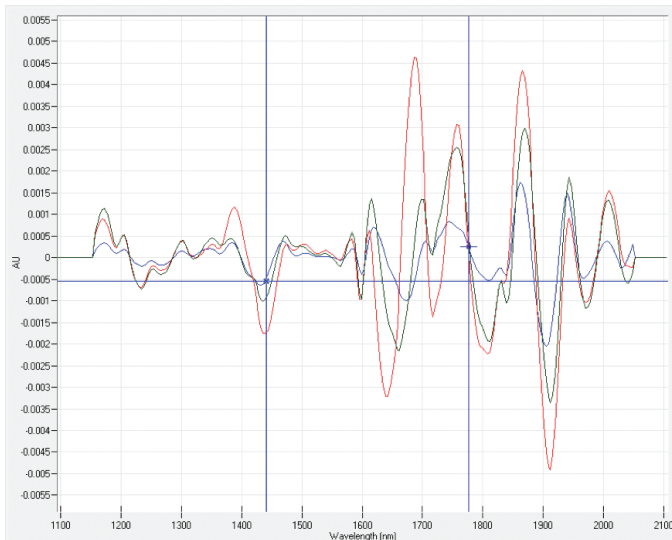

Figure 1: Reveal XNIR: benzoic acid referenced to toluene (blue 0.78% benzoic acid, green 2.15% benzoic acid, and red 4.78% benzoic acid) after second derivative spectral processing.
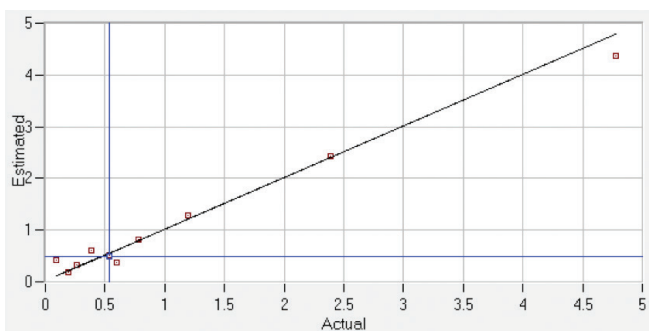

Figure 2: Partial least squares regression demonstrates standard predictive error of ±0.2% relative to titration over the 5% tested range.

Reveal

The Prozess Technologie Reveal XNIR instrument provides millisecond measurements, a variety of sample interfaces, and rugged system designs for the manufacturing environment, enabling users to acquire data in real-time, and make modifications during their process to ensure proper quality control and efficiency.

The Reveal contains integrated light sources and dispersive spectrometers utilizing linear diode array detectors, with no moving parts for high throughput and maximum stability. The Reveal contains automated internal hardware for lamp referencing and for wavelength and photometric linearity validation, all of which can be performed at user-defined intervals. Standard communications in the system include WiFi, Ethernet, OPC, ModBus and Ethernet/IP for upstream and downstream interface with distributed control systems, computers, or tablets. Sampling options range from flow cells with selectable path lengths, to measuring heads that mate to sight glasses in vessels, to fiber probes for contact or non-contact measurement in various insertion points.

Prozess provides a myriad of engineering solutions to integrate into customers' process streams. Hazardous area enclosures, additional analog and digital inputs and outputs, and sample head integration are just a few of Prozess' competencies to ensure a turnkey and trouble-free implementation. With high stability and genuine real-time measurement, the Reveal is a dependable device for monitoring moisture content in both continuous and batch processes.

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