Process Insights
Premium Insights Into Process

GuidedWave

Application Note:

Online Process Monitoring of Styrene / Acrylonitrile / Methyl-ethyl-ketone (MEK)

The Problem

Getting the correct blend of copolymers to achieve the desired physical properties can be a challenging task for process engineers in the polymer industry. Near-infrared (NIR) spectroscopy is a convenient and cost effective tool for monitoring reaction processes in situ to ensure that the correct chemical ratios, average molecular weight, and physical properties are within specifications.

When transparency is a concern, the process engineer has several options. If polystyrene's mechanical properties are insufficient, the process engineer can tailor a specific formulation of Styrene–acrylonitrile copolymers or SANs (Figure 1a). These copolymers typically contain between 20–30% acrylonitrile. Due to the polar structure of acrylonitrile, SANs copolymers have better resistance to breakdown in hydrocarbon streams than polystyrene. SAN copolymers also have a higher softening point, rigidity, impact and strength, yet maintain their transparency.

As the acrylonitrile content of the SAN copolymer is increased, there is an improvement in the toughness and chemical resistance. The trade-off is a greater difficulty in molding and potential yellowness of the resin.

SANs copolymers are also used in polyols processing to strengthen other polymer types. Monitoring stream composition during processing allows manufacturers to maintain product quality.

The Solution

By incorporating a Near-infrared (NIR) spectrometer and in situ process probe, a process engineer can quickly identify when the mixture of component concentrations are out of specification. The NIR region of the electromagnetic spectrum measures the overtone and combination bands of the C-H, O-H, and N-H fundamentals absorption bands. These spectra are unique to the molecule thus permitting the process engineer to make real-time corrections and ensure that product quality is maintained. In the case of SANs, NIR spectroscopy can be used to monitor the concentration of Styrene, Acrylonitrile, and MEK molecules shown in Figure 1b.

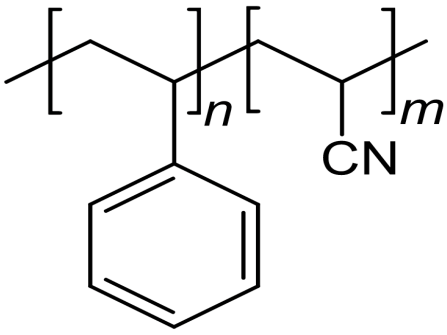

Figure 1a. Molecular Structure of SANs

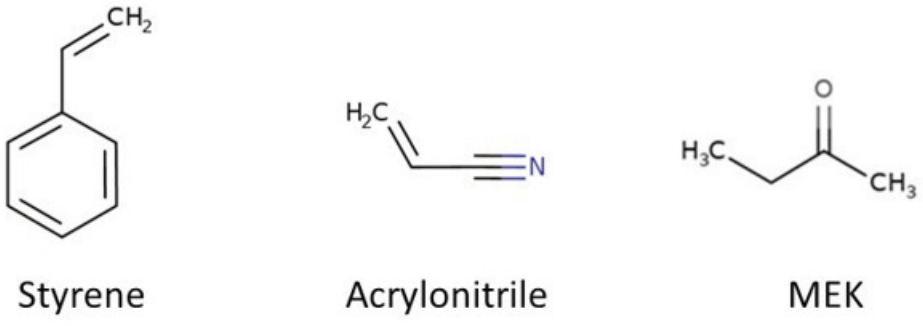

Figure 1b. Molecular Structure of Styrene, Acrylonitrile, and MEK.

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The Experimental Setup

A proof of concept study was conducted by measuring the NIR spectra of a series of styrene / acrylonitrile / MEK samples of known concentration. A quantitative model was then developed using Partial Least Squares Regression (PLSR) which will allow the measurement of future samples based only on their NIR spectrum. A set of mixtures of known concentrations were analyzed with a Guided Wave NIR-O full spectrum analyzer using a 10 mm pathlength cell connected connected to the spectrometer via fiber optics. Guided Wave analyzer systems use fiber optics to allow the sample probe to be located in remote locations away from the spectrophotometer itself.

The Results

The NIR spectra of styrene, acrylonitrile, and MEK are shown in Figure 2. The mixture samples were used in Partial Least Square Regression (PLSR) models for each of the three components. The calibration results are summarized in Table 1 with predicted versus measured plots shown in Figures 3, 4, and 5. The NIR-O dual-beam spectrometer is an excellent choice for online, real-time measurements for hydrocarbon mixtures such as the one presented here.

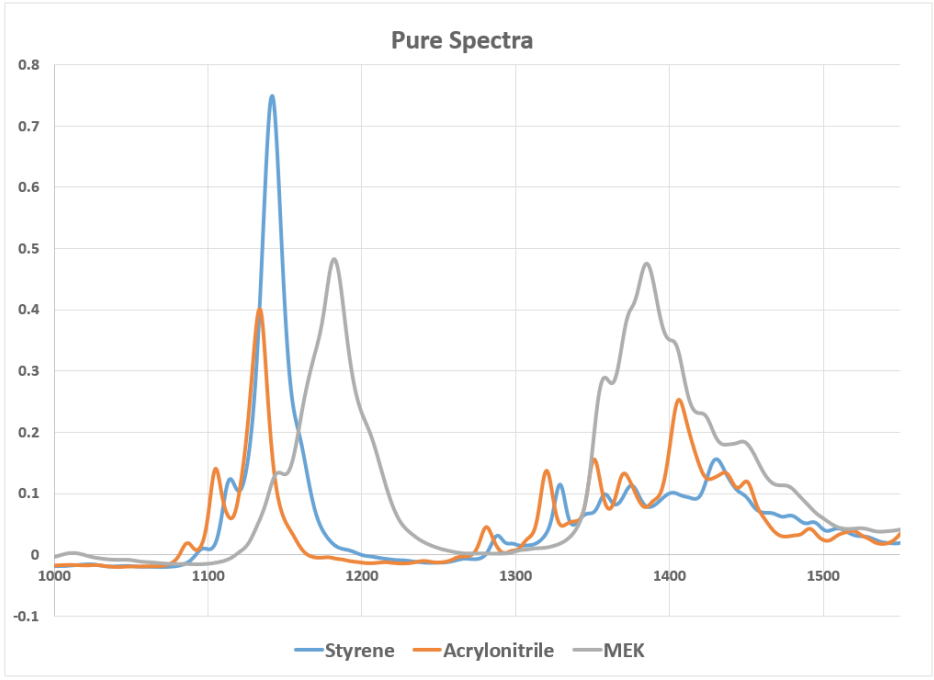

Figure 2. NIR Spectral Data

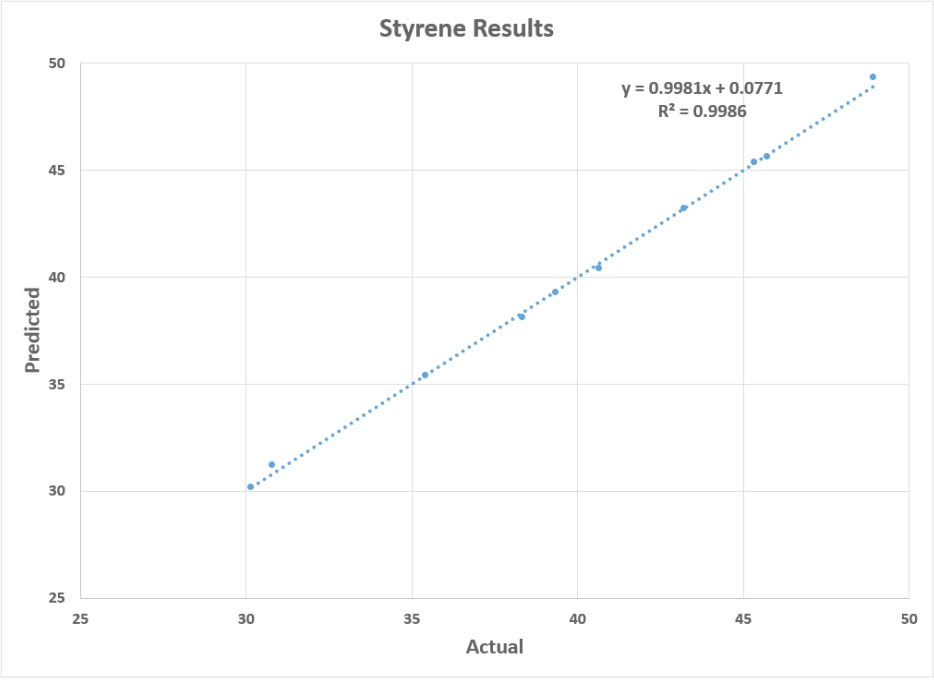

Figure 3. Styrene

Parameter	Range (wt %)	RMSEP (rms error) wt %	R^2
Styrene	30 - 50	0.22	0.999
Acrylonitrile	0 - 19	0.16	0.999
MEK	40 - 60	0.10	0.999

Table 1 Analysis Results

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Literature: 3086-19-10-16

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The Conclusion

Real-time monitoring of polymer feed concentrations can be achieved with both Guided Wave analyzers; the NIR-O Full Spectrum NIR spectrometer or the ClearView db photometer. By collecting these data, process engineers in the polymer plant can make informed decisions on process optimizations to ensure product quality. The proof of concept study presented in this application note illustrates that Guided Wave process analyzers can detect changes in concentrations as little as 0.1 %wt.

NIR-O™ Guided Wave's Spectrometer NIR Online Process Analyzer

ClearView db™ Photometer NIR Online Process Analyzer Enclosure Options

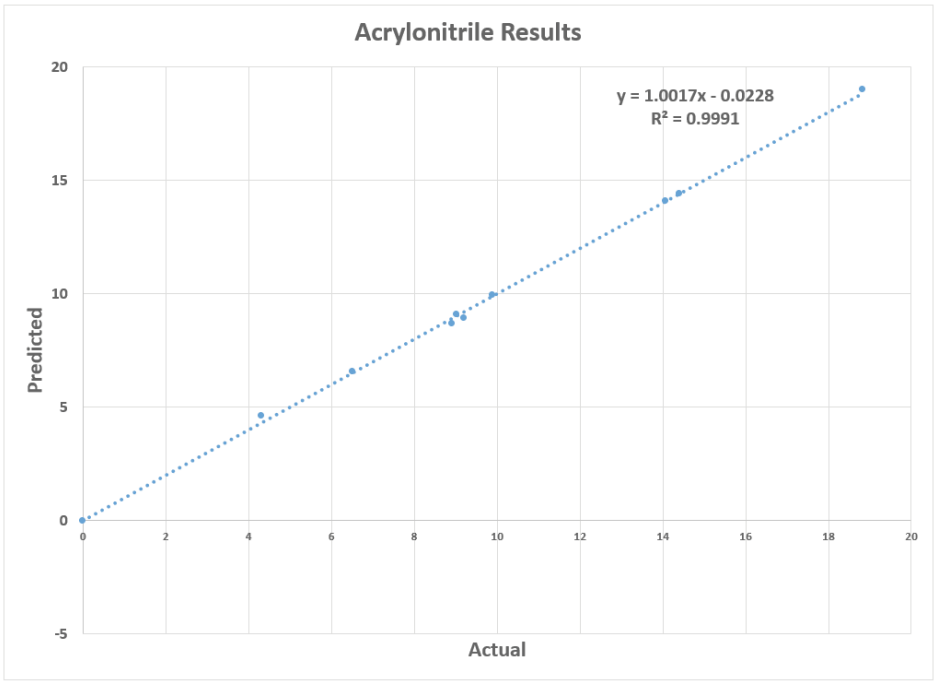

Figure 4. Acrylonitrile

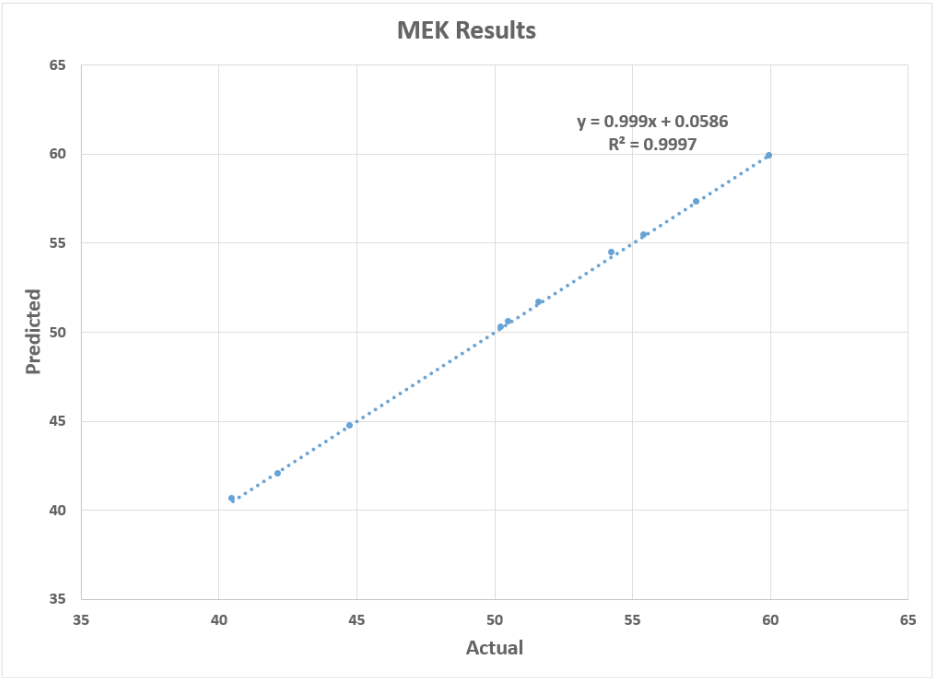

Figure 5. MEK