Process Insights
Premium Insights Into Process

GuidedWave

Application Note:

Water in Acetic Acid & p-Xylene with a ClearView® db Filter Photometer

Challenge

Can quantitative analysis be done with a multiple wavelength filter photometer?

Background

The spectra of this 3-component mixture are complex. Initial visual inspection suggests that a complete spectrum and multivariate analysis (PLS – partial least-squares) are required.

Experimental

Spectra were taken with an InGaAs diode array spectrometer and low-OH optical fibers. Thirteen samples were analyzed at 50°C in a 5 mm quartz cuvette.

Zpurge Unit
Class I, Division 2

ExProof Unit
Class I, Division 1

General
Purpose Unit

ClearView db Enclosure Options

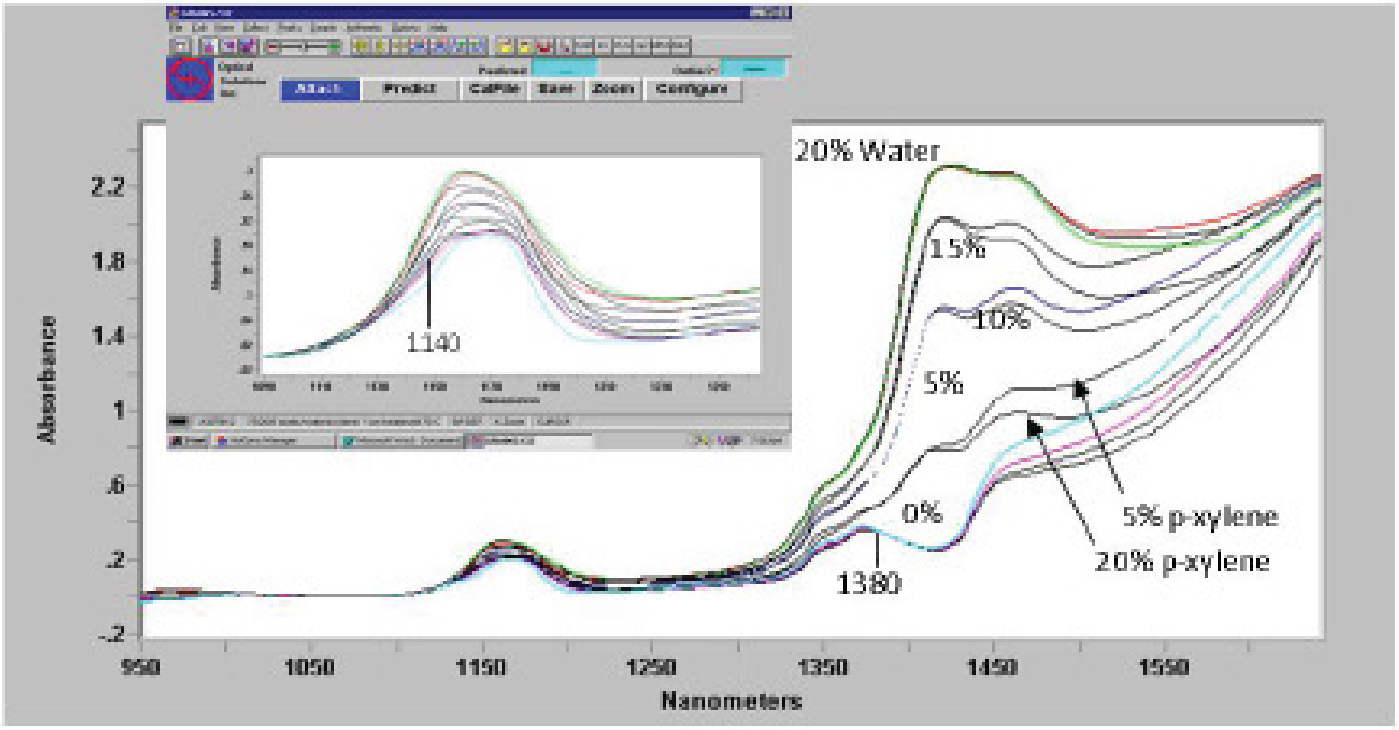

Figure 1

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Results

A PLS model was created. The results show reasonable predictions in the table below. PLS uses the complete spectrum for quantitative analysis. It is apparent from the spectra, however, that water can be analyzed near 1380 nm, independent of p-xylene or acetic acid content. Multiple linear regression (MLR) systematically investigates which wavelength or wavelengths provide a statistically acceptable calibration. The MLR results confirmed that water can be determined solely at 1390 nm, and that acetic acid and p-xylene can be determined using two wavelengths at 1140 and 1380 nm.

The results are also presented in the table below, showing a standard error for the calibration near 0.3% (vol.) for each component, which is better than the PLS results.

Conclusion

ClearView db fiber-optic filter photometer system can provide quantitative analyses of water, p-xylene and acetic acid using 1390nm, 1140nm, 1380 nm and 1080 nm (reference) filters.

Sample	Acetic Acid	Residual PLS	Residual MLR	Water	Residual PLS	Residual MLR	p=Xylene	Residual PLS	Residual MLS
1	70	1.32	0.34	10	-0.39	-0.38	20	-0.85	-0.32
2	70	-0.36	-0.30	20	0.19	0.13	10	0.04	0.04
3	80	0.56	0.39	20	0.34	0.33	0	-0.84	-0.48
4	100	1.25	0.35	0	-0.36	-0.09	0	-0.85	-0.25
5	90	0.07	0.09	0	-0.18	-0.09	10	0.08	-0.08
6	80	0.00	0.13	0	-0.09	-0.11	20	-0.01	0.19
7	80	-0.38	-0.18	10	-0.43	-0.35	10	0.91	0.43
8	90	-1.20	-0.82	5	0.60	0.59	5	0.58	0.16
9	70	-0.31	-0.08	15	-0.14	-0.19	15	0.35	0.01
10	75	-0.11	-0.05	5	0.75	0.45	20	-0.64	-0.17
11	75	-0.20	0.04	20	-0.53	-0.31	5	0.83	0.36
12	85	0.18	-0.03	15	0.32	0.30	0	-0.72	-0.14
13	85	-0.35	0.00	0	-0.18	-0.14	15	0.51	0.03
Std. Error:		0.66	0.36		0.36	0.32		0.64	0.28
Adj. R^2:		0.994	0.999		0.998	0.999		0.992	0.999

Table 1

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a Process Insights Brand
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