

APPLICATION NOTE

Water in Acetic Acid and p-Xylene Using a ClearView® db Photometer

Purpose

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

Measurement Background

The spectra of this 3-component mixture are complex. Initial visual inspection suggests that a complete spectrum and PLS (Partial Least-Squares) multivariate analysis are required.

Experimental

The spectra were taken with a full spectrum NIR process spectrometer and low-OH optical fibers. Thirteen samples were analyzed at 50 °C in a 5 mm quartz cuvette.

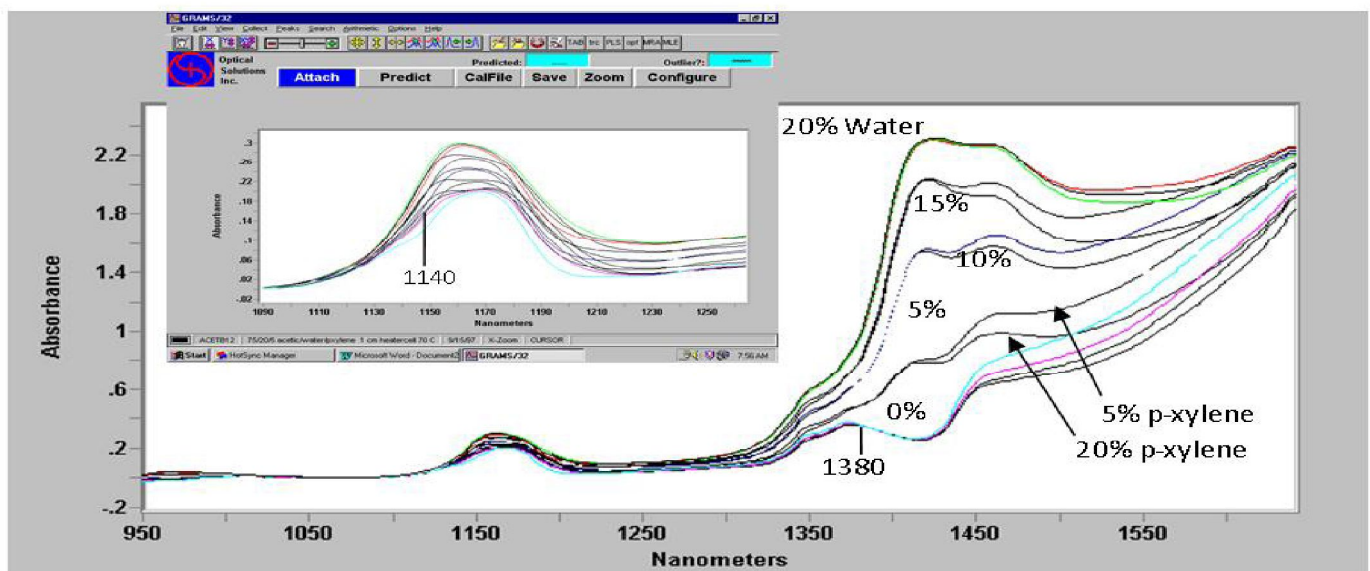


Figure 1

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	-0.19	-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

Results

A PLS model was created. The results show reasonable predictions in Table 1. 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 also presented in table 1, show a standard error for the calibration near 0.3% (vol.) for each component, which is better than the PLS results.

Conclusion

Our GUIDED WAVE™ ClearView® db Dual-Beam Photometer can provide quantitative analyses of water, p-xylene and acetic acid using 1390nm, 1140nm, 1380 nm and 1080 nm (reference) filter. For more detailed information regarding system specifications and the ClearView db analyzer please contact a Process Insights sales or technical specialist.

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