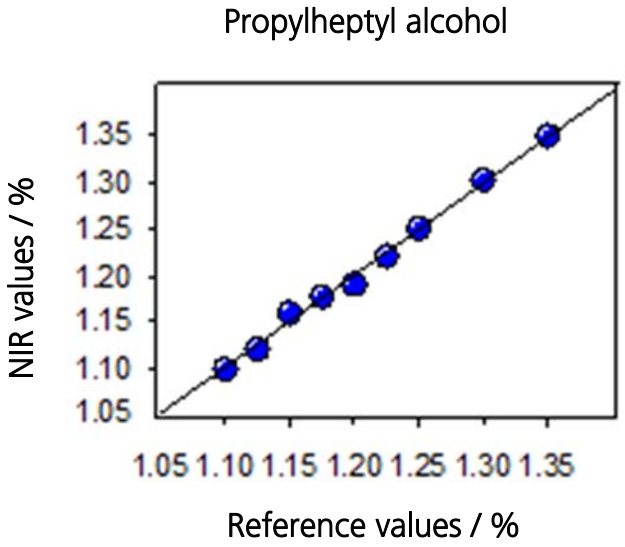
NIR Application Note NIR-29

Butyl glycol and propylheptyl alcohol in water-borne paint



This Application Note shows that Vis-NIR spectroscopy is ideally suited to quantify two important additives – butyl glycol and propylheptyl alcohol – in water-based paints. The determination of the additive content, commonly achieved with time-consuming conventional lab methods, can easily be performed by Vis-NIR spectroscopy. With a single measurement, Vis-NIR spectroscopy provides multiple parameters.

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Method description

Introduction

Paint industry is a worldwide growing business also as a result of increased development possibilities flying under the flag of "development by design". Paint industry nowadays develops and produces not only paints to protect and/ or to color objects, but also to induce a specific behavior to objects.
According to the main ingredient, paints can be divided into two classes: water-based and solvent-based paints. In earlier days, paints consisted on up to 65%, of occasionally harmful, organic solvents. Today, the market share is dominated by water-based paint, which makes only up to 10% of organic solvents. Besides water, solvents, and pigments, additives (like butyl glycol and propylheptyl alcohol) in low concentrations but high importance, are added to induce a desired behavior.
Butyl glycol is a commonly used highly volatile co-solvent for rheology control due to its ability to manipulate the evaporation time of paints.
Propylheptyl alcohol is mainly used as a plasticizer to meet demands on specific coating properties such as dry film appearance or substrate adhesion.
The control of those additives is of high importance to insure consistency of product quality. Particularly, in a goal-oriented production like paint industry, a fast, but strict analytical method is essential. Therefore, the determination of the additive content, commonly achieved with time-consuming conventional lab methods, can easily be replaced by Vis-NIR spectroscopy to give results of all parameters of interest within a single measurement operated even by untrained users.

Configuration

Tab. 1: Used equipment and accessories

Equipment	Metrohm code
NIRS XDS SmartProbe Analyzer	29211610
Vision Software 4.0.3	66069102

Fig. 1: A NIRS SmartProbe Analyzer equipped with a transflection probe was used to record the spectral data.

Experimental

A NIRS SmartProbe Analyzer (transflection measurement) was used to collect the spectral data of light gray and black paint samples containing two different additives, butyl glycol and propylheptyl alcohol. The samples were placed in a beaker and stirred constantly to avoid sedimentation of sooty particles in black paint and TiO_2 in light gray paint, respectively. Stirring also keeps the water-insoluble solvents homogenously distributed in the suspension.
Vision (Metrohm chemometrical software) with the algorithm of Partial Least Squares (PLS), was used to develop quantitative prediction models for butyl glycol and propylheptyl alcohol of each light gray and black paint, see Tab.2. Absorption bands over the full Vis-NIR range (400 – 2500 nm) were chosen to develop a good model. The spectral data were pretreated using a 1^{st} derivative with a segment size of 20 nm and a gap size of 1 nm. External validation on an independent data set was applied to verify the performance of the derived quantitative models.

Parameter	Concentration / %
Butyl glycol in black paint	0.900–1.150
Butyl glycol in light gray paint	0.800–1.100
Propylheptyl alcohol black paint	1.125–1.350
Propylheptyl alcohol light gray paint	0.900–1.100

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Results

Butyl glycol content in black paint:

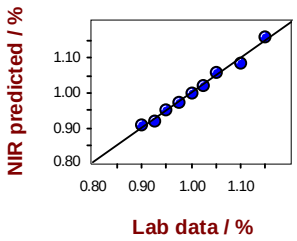

Fig. 2: Correlation of reference data to NIR predicted values as a result of quantitative method development of butyl glycol content in black paint.

Regression model	PLS with 2 factors
Wavelength range	500–1080 nm 1120–1950 nm
R^2	0.9904
SEC	0.0093
SEV	0.0095
F-value	310.6
PRESS	0.0804

Propylheptyl alcohol in black paint:

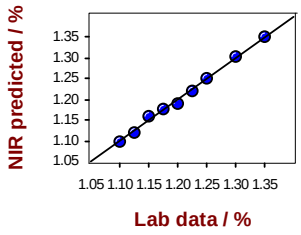

Fig. 3: Correlation of reference data to NIR predicted values as a result of quantitative method development of propylheptyl alcohol in black paint.

Regression model	PLS with 3 factors
Wavelength range	500–1080 nm 1120–1950 nm
R^2	0.9957
SEC	0.0068
SEV	0.0969
F-value	382.1
PRESS	0.0846

Butyl glycol content in light gray paint:

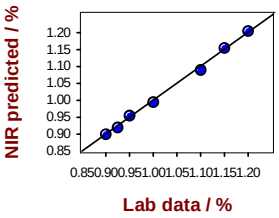

Fig. 4: Correlation of reference data to NIR predicted values as a result of quantitative method development of butyl glycol in light gray paint.

Regression model	PLS with 2 factors
Wavelength range	1120–1950 nm
R^2	0.9732
SEC	0.0216
SEV	0.0882
F-value	451.4
PRESS	0.0545

Propylheptyl alcohol in light gray paint:

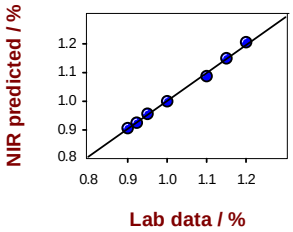

Fig. 5: Correlation of reference data to NIR predicted values as a result of quantitative method development of propylheptyl alcohol in light gray paint.

Regression model	PLS with 2 factors
Wavelength range	1120–1950 nm
R^2	0.9975
SEC	0.0072
SEV	0.0704
F-value	795.1
PRESS	0.0346

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External validation:

Sample name	Lab value / %	NIR value / %	Residual / %
Propylheptyl alcohol white	0.9361	0.9750	-0.0389
	1.0092	1.0000	0.0092
	1.0151	1.0500	-0.0349
	1.0498	1.0500	-0.0002
	1.1607	1.2000	-0.0393
Butyl glycol white	1.1035	1.0490	0.0545
	0.9160	0.8500	0.0660
	1.0962	1.1000	-0.0038
	0.8264	0.8500	-0.0236
	1.0036	1.1000	-0.0964
	0.9770	0.9500	0.0270
	1.0690	1.1000	-0.0310
Butyl glycol black	1.0297	0.9500	0.0797
	1.0413	0.9500	0.0913
	1.0092	1.1000	-0.0908
	0.9199	1.0250	-0.1051
Propylheptyl alcohol	1.1274	1.1750	-0.0476
	1.1884	1.1500	0.0384
	1.2182	1.2000	0.0181
	1.3018	1.3500	-0.0482

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