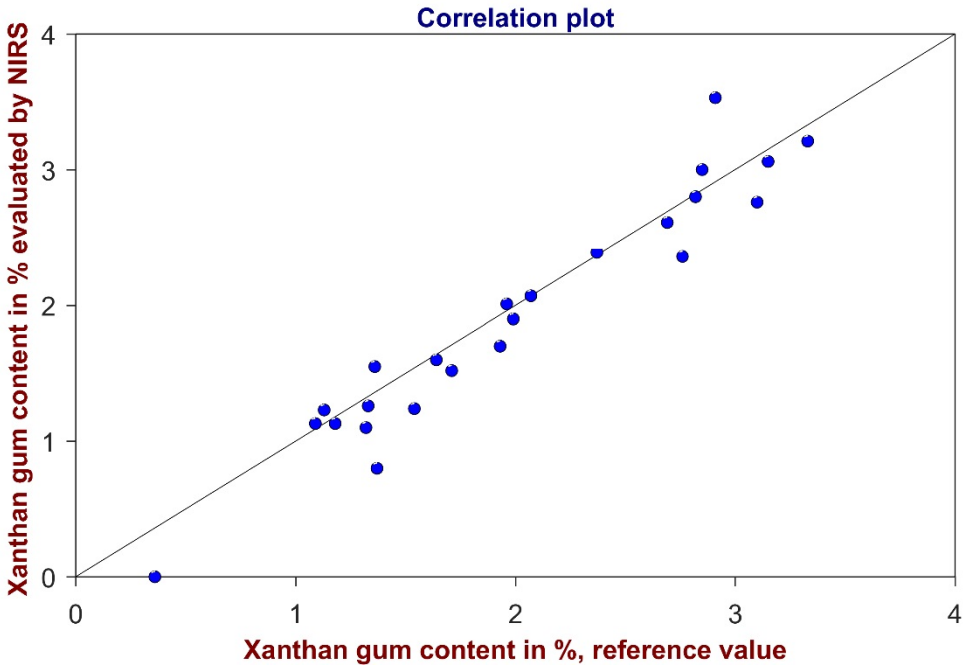
NIR Application Note NIR–52

Simultaneous determination of xanthan gum, optical density, and glucose in aqueous solutions by Vis-NIRS



Near-infrared spectroscopy (NIRS) was used as an analysis method for quality control of aqueous xanthan gum solutions. Quantitative models for the determination of optical density, glucose, and xanthan gum were developed, enabling fast and reliable quality control.

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Method description

Introduction

Xanthan gum is a natural polysaccharide with a wide range of applications in the cosmetic and pharmaceutical industry. As even small amounts in water increases drastically the viscosity of the solution, xanthan gum is used as a natural thickener in different personal care products such as lotions, shampoos, liquid soaps or toothpaste. Furthermore, its addition prevents the separation of emulsions or helps to suspend solid particles. Xanthan gum is also used in the pharmaceutical industry as an excipient.
The main physical and chemical parameters of interest for this application field are the optical density and the concentrations of xanthan gum and of impurities like glucose. As shown herein, these quality parameters can be simultaneously determined by Vis-NIR spectroscopy in less than one minute without sample preparation.

Experimental

The set of customer samples used consisted of more than 100 samples. The samples were collected from more than 20 different fermenters within a 4 week time period. Near-infrared spectra were acquired using Metrohm XDS RapidLiquid Analyzer (Fig. 1). The samples were placed in 4 mm disposable glass vials and measured in transmission mode over the full Vis-NIR wavelength range of 400–2500 nm. The temperature was kept constant at 40 °C. The software package Vision Air 2.0 Complete was used for data acquisition, data management, and development of the quantification method (Tab. 1).

Tab.1: Used equipment and software.

Equipment	Metrohm order code
NIRS XDS RapidLiquid Analyzer	2.921.1410
NIRS 4 mm disposable glass vials	6.7402.010
Vision Air 2.0 Complete	6.6072.208

Fig. 1: The NIRS XDS RapidLiquid Analyzer was used for spectral data acquisition over the full range from 400 nm to 2500 nm.

75% of samples were used for the calibration. Residual 25% of samples were used for the validation. The spectra were pre-treated using 2nd derivative. A Partial Least Squares Regression (PLS) or Multiple Linear Regression (MLR) was performed over the specific spectral regions.

Results

The correlation plots in Fig. 2–4 show high correlation between the parameters determined by the reference analytical method (x-axis) and the predicted values (y-axis) from Vis-NIR spectroscopy. The good correlation results are confirmed by the high coefficients of determination and very low standard errors of calibration, cross-validation and prediction (SEC, SECV and SEP)

Glucose

Tab.2: Results of the quantitative method development for glucose.

Concentration range	0–4.5%
Method	PLS
Number of factors	5
Wavelength range	626–694 and 1662–1744 nm
Pretreatment	2nd derivative
SEC	0.26%
SECV	0.28%
SEP	0.34%
R^2	0.9623

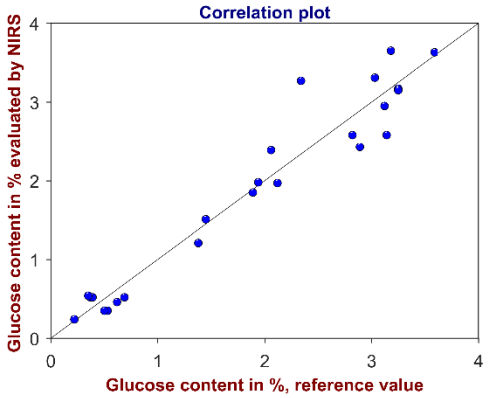

Fig. 2: Validation of the method for the determination of glucose content. The correlation plot shows reference values versus glucose values evaluated by Vis-NIR spectroscopy. High coefficient of determination (R^2 = 0.9623) and low standard error of prediction (SEP = 0.34%) demonstrate that the method is suitable for its intended use.

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Method description

Xanthan gum

Tab.3: Results of the quantitative method development for xanthan.

Concentration range	0–5%
Method	PLS
Number of factors	4
Wavelength range	1662–1744 nm
Pretreatment	2nd derivative
SEC	0.19%
SECV	0.20%
SEP	0.35%
R^2	0.9431

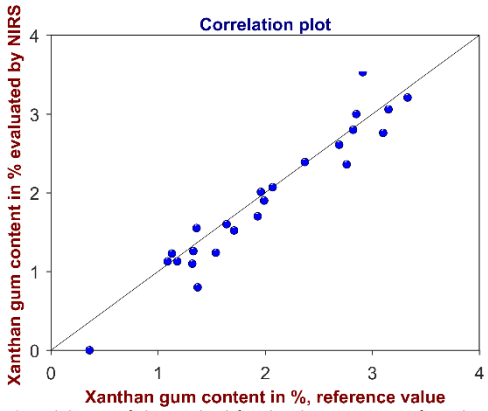

Fig. 3: Validation of the method for the determination of xanthan gum content. The correlation plot shows reference values versus xanthan gum values evaluated by Vis-NIR spectroscopy. High coefficient of determination (R^2 = 0.9431) and low standard error of prediction (SEP = 0.35%) demonstrate that the method is suitable for its intended use.

Optical density (OD)

Tab.4: Results of the quantitative method development for optical density.

Concentration range	0–12
Method	MLR
Wavelength	893 and 967 nm
Pretreatment	2nd derivative
SEC	0.63
SECV	0.71
SEP	0.90
R^2	0.9052

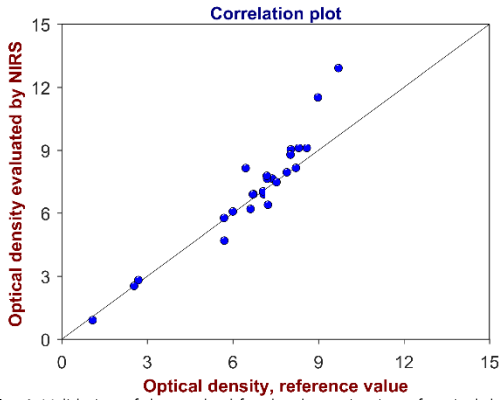

Fig. 4: Validation of the method for the determination of optical density. The correlation plot shows reference values versus optical density values evaluated by Vis-NIR spectroscopy. High coefficient of determination (R^2 = 0.9052) and low standard error of prediction (SEP = 0.90) demonstrate that the method is suitable for its intended use.

Summary

A Metrohm NIRS XDS RapidLiquid Analyzer was used as a feasibility study for the simultaneous determination of glucose and xanthan gum content as well as optical density in aqueous xanthan gum solutions. The calibration models of the Vis-NIR method provide results with acceptable standard errors and accuracy. Thus, it has been demonstrated that Vis-NIR spectroscopy has is a suitable high throughput quality control analysis method for the production of aqueous xanthan gum solutions. In combination with the intuitive Vision Air Software, this approach is a time- and cost-saving solution for routine analysis of aqueous xanthan gum solutions and it can even be successfully employed by inexperienced operators.

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