The Influence of Spectral Characteristics on the Accuracy of Concentration Quantitatively Analysis by Near Infrared Spectroscopy

HuiQuan Wang, Hui Wang, Zhe Zhao, JingHong Miao, JinHai Wang

PII: S1350-4495(18)30445-6
DOI: https://doi.org/10.1016/j.infrared.2018.09.001
Reference: INFPHY 2683

To appear in: *Infrared Physics & Technology*

Received Date: 16 June 2018
Revised Date: 1 September 2018
Accepted Date: 1 September 2018

Please cite this article as: H. Wang, H. Wang, Z. Zhao, J. Miao, J. Wang, The Influence of Spectral Characteristics on the Accuracy of Concentration Quantitatively Analysis by Near Infrared Spectroscopy, *Infrared Physics & Technology* (2018), doi: https://doi.org/10.1016/j.infrared.2018.09.001

The Influence of Spectral Characteristics on the Accuracy of Concentration Quantitatively Analysis by Near Infrared Spectroscopy

HuiQuan Wang [1,2,3],Hui Wang[1], Zhe Zhao [1,2,3]*, JingHong Miao[1,2]*and JinHai Wang[1,2]

1. School of Electronics and Information Engineering, Tianjin Polytechnic University, Tianjin 300387, China
2. Tianjin Key Laboratory of Optoelectronic Detection Technology and Systems, Tianjin 300387,China
3. School of Precision Instrument and Opto-Electronics Engineering, Tianjin University, Tianjin 300072, China

Abstract: In order to solve the problem of measurement blindness caused by the lack of detectability analysis in the near-infrared spectroscopy (NIRS), two important parameters including Equivalent Signal Noise Ratio (*ESNR*) and Overlapping Coefficient (*OC*) are proposed in this manuscript. According to the proportion of the component absorbance to the total absorbance and the overlap degree between near-infrared spectral curves of the components, the above parameters can achieve quantitative analysis of the concentration of components tested based on NIRS. The research combines the theoretical simulations and ethanol concentration experiments.The quantitative relationship between above two parameters and spectral analysis error is discussed by the partial least squares (PLS) modeling NIRS. The estimated *RMSE* of ethanol concentration obtained by theoretical analysis of this study was 0.30%, and the actual *RMSE* of near-infrared spectroscopy was 0.32%. The relative error is 6.67%, and the results are consistent.This study provided an effective and rapid prediction method for the quantitative analysis of NIRS, and optimized the theory of the detectability analysis of NIRS, which is a significant guidance for the quantitative analysis of the concentration measured by NIRS.

Keywords: overlapping coefficient; equivalent signal noise ratio; spectrum analysis; detectability

1 Introduction

Near-infrared spectroscopy (NIRS) is widely used in the inspection and monitoring of food[1,2], medicine[3,4], environment[5,6], chemical engineering and other fields[7,8]. Compared with visible spectroscopy, fluorescence spectroscopy, Raman spectroscopy and other analytical methods, near-infrared spectroscopy has the advantages of non-destructive, environmental protection, and convenient operation. NIRS characteristic absorption peaks and spectral line overlaps severely, and mathematical models need to be established by chemometric methods. Therefore, improving the analysis accuracy is the most important issue in the field of spectral analysis. Researchers mainly study the improvement of the accuracy of NIRS from the following three aspects. First, develop a higher-performance spectrum acquisition instrument to obtain better spectral data[9,10]; Second, use appropriate spectral pre-processing methods to improve spectral

Fund Project：National Natural Science Foundation of China (No. 61705164)，China Postdoctoral Science Fund 61st Batch
About the Author：Huiquan Wang, e-mail:huiquan@tjpu.edu.cn.
* Communication contact: e-mail: zhaozhe@tjpu.edu.cn.