

Strategy for introducing NIR spectroscopy and multivariate calibration techniques in industry

M.S. Larrechi, M.P. Callao

Analytical methods based on near infrared spectroscopy (NIR) and multivariate calibration techniques have important characteristics for industrial applications because they are quick and can be used to make direct determinations and extract information from several parameters from one single measurement. They can also be used in on-line applications. However, they have not been used in industry as much as one might expect because the validity of the calibration model must be assured when the signal is transformed. There are chemometric techniques for tackling every problem, but there are no specific guidelines about which procedure to use. In this article, we describe a practical strategy for introducing these methods. We discuss the relative merits of the various univariate and multivariate control techniques and describe how they might be used. We also discuss the standardisation of the calibration models and describe how to obtain robust models at low experimental cost. Finally, we illustrate our strategy with a practical case study from the petrochemical industry.

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Keywords: Multivariate statistical process control (MSPC); Near infrared spectroscopy (NIR); Petrochemical industry; Robust model; Standardisation

M.S. Larrechi, M.P. Callao*
Departament de Química
Analítica i Química Orgànica,
Universitat Rovira i Virgili, Pl.
Imperial Tàrraco, s/n, E-43005
Tarragona, Spain

1. Introduction

NIR combined with multivariate processing techniques has been widely studied in recent years. There have been important applications, for example in the agricultural industry [1], the pharmaceutical industry [2] and the petrochemical industry [3].

In the petrochemical industry, the method made a strong impact when it was used to determine the number of octanes in different types of petrol [4]. The method is interesting because a wide variety of samples can be measured without the need for pre-treatment and because the determinations can be made quickly. Both of these are highly desirable features for on-line applications.

However, NIR has not been fully introduced in the above areas as an alternative to conventional analytical methods. We believe this may partly be because it is sensitive to factors such as temperature, the ageing of the source, and small instrumental disturbances that can affect the validity of the models over time. This suggests that the system needs to be controlled. It may also be because the goodness of the results depends on whether the samples analysed are of the same type as those used as calibration samples. Outliers in prediction should therefore be easily detected.

These problems (control, suitability of the system if a change is detected, and outlier detection) have been widely studied [5–7]. Such studies have illustrated the chemometric approaches to solving the problems, but, in our opinion, they have always dealt with just one of the problems and have been too theoretical. We think that these techniques need general practical guidelines that can be applied to each particular field.

Another problem is that these methods are normally implemented by specialised personnel but are used on a day-to-day basis by operators who are unfamiliar with the science on which they are based. It would be useful, therefore, if they contained means by which the operators could feel that they were involved in analysing the results they helped to produce.

We are developing NIR methods for use in the petrochemical industry [8–10]. In this article, we use this experience to discuss a practical strategy for using these methods effectively. As an example, we will discuss the determination of the ethylene

*Corresponding Author. Tel.: +34 977 559 559; Fax: +34 977 559 566;
E-mail: callao@quimica.urv.es

Application Of Multivariate Calibration And Nir

Josef Brandt, Ivar Ugi



Application Of Multivariate Calibration And Nir:

Multi- and Megavariate Data Analysis Basic Principles and Applications L. Eriksson, T. Byrne, E. Johansson, J. Trygg, C. Vikström, 2013-07-01 To understand the world around us as well as ourselves we need to measure many things many variables many properties of the systems and processes we investigate Hence data collected in science technology and almost everywhere else are multivariate a data table with multiple variables measured on multiple observations cases samples items process time points experiments This book describes a remarkably simple minimalistic and practical approach to the analysis of data tables multivariate data The approach is based on projection methods which are PCA principal components analysis and PLS projection to latent structures and the book shows how this works in science and technology for a wide variety of applications In particular it is shown how the great information content in well collected multivariate data can be expressed in terms of simple but illuminating plots facilitating the understanding and interpretation of the data The projection approach applies to a variety of data analytical objectives i e i summarizing and visualizing a data set ii multivariate classification and discriminant analysis and iii finding quantitative relationships among the variables This works with any shape of data table with many or few variables columns many or few observations rows and complete or incomplete data tables missing data In particular projections handle data matrices with more variables than observations very well and the data can be noisy and highly collinear Authors The five authors are all connected to the Umetrics company www.umetrics.com which has developed and sold software for multivariate analysis since 1987 as well as supports customers with training and consultations Umetrics customers include most large and medium sized companies in the pharmaceutical biopharm chemical and semiconductor sectors

Handbook of Near-Infrared Analysis Donald A. Burns, Emil W. Ciurczak, 2007-09-07 Fast inexpensive and easy to use near infrared NIR spectroscopy can be used to analyze small samples of virtually any composition The Handbook of Near Infrared Analysis Third Edition explains how to perform accurate as well as time and cost effective analyses across a growing spectrum of disciplines Presenting nearly 50% new and re

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or controlling blending as well as practical concerns for mixing processes NIR spectroscopy as applied to traditional granulation drug layering and film coating of beads or granules Pharmaceutical assays including qualitative analysis quantitative analysis determination of actives in tablets and capsules and considerations for intact dosage form analysis Steps involved in the validation and acceptance of an NIR spectroscopy method including quality assurance qualification and verification of instruments and the International Conference on Harmonization ICH guidelines Medical applications including those related to blood glucose measurements tissue and major organ analysis fetal analysis and cancer research Providing comprehensive coverage of NIR spectroscopy from theory mathematics application and mechanics of NIR analysis the book supplies ample references to facilitate further research into this burgeoning field

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Near-Infrared Spectroscopy H. W. Siesler,2002-02-15 Over the last few years near infrared NIR spectroscopy has rapidly developed into an important and extremely useful method of analysis In fact for certain research areas and applications ranging from material science via chemistry to life sciences it has become an indispensable tool because this fast and cost effective type of spectroscopy provides qualitative and quantitative information not available from any other technique This book offers a balanced overview of the fundamental theory and instrumentation of NIR spectroscopy introducing the material in a readily comprehensible manner A considerable part of the text is dedicated to practical applications including sample preparation and investigations of polymers textiles drugs food and animal feed However special topics such as two

dimensional correlation analysis are also covered in separate chapters Written by eight experts in different fields this book presents an introduction to the current state of developments and is valuable to spectroscopists and to practitioners applying NIR spectroscopy as a daily analytical tool **Transfer of Multivariate Calibration Models** Hans Barring,2001

Real-time Analysis of Light Alkenes at Elevated Temperatures and Pressures by Fiber-optic Near Infrared Spectroscopy Engin Deniz Yalvac,1996 *Near Infrared Spectroscopy* Anthony M. C. Davies,Phil Williams,1996

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