

Abstract

Evaluation of a new process near infrared analyser and a calibration strategy for on-line determination of quality properties of gasoline

Celio Pasquini^{1*}, Jarbas José Rodrigues Rohwedder¹ and Aerenton Ferreira Bueno²

¹Department of Analytical Chemistry, Chemistry Institute, State University of Campinas - UNICAMP, Campinas - SP – Brazil

²Henrique Lage Refinery – REVAP – PETROBRAS – São José dos Campos – SP - Brazil

*Corresponding author: pasquini@iqm.unicamp.br

Introduction

Recently, a new concept of a process analyser based on near infrared spectrometry has been proposed. The analyser precludes the usual two spectrophotometer approach adopted by most of the process NIR analyser schemes described so far. The NIR spectrophotometer has been designed to be removed from the process case and taken to the laboratory to construct the multivariate models. The instrument is then returned to the case and the models developed are used as obtained, without any model transfer operations. The described approach to calibration and the new process analyser are evaluated in this work.

Materials and Methods

The NIR spectrophotometer was constructed using an array of 255 PbS sensors adapted to receive the dispersed beam of a symmetric Czerny-Turner optical arrangement optimised to work in the 1600 – 1900 nm spectral region. Twin flow cells with a 1.5 mm optical path were employed; one to contain the gasoline while the other was kept empty and acted as reference in order to obtain the absorbance spectra of the samples. The spectrophotometer has few moving parts and they are robust enough to allow the instrument to be transported without any alteration in its spectral performance. Samples of gasoline (n = 60), collected during six months in the production line of the refinery, were used for construction in the refinery laboratory of PLS models for prediction of distillation point temperatures (10, 50, and 90%), MON, RON, IAD and aromatics, olefins, saturates, benzene contents and density. The instrument was returned to the process site where another 20 samples were randomly analysed during one month and simultaneously collected, analysed by the standard methods and employed in the external validation of the models.

Results and Discussion

The models constructed in the laboratory for the quality properties of the gasoline reported above all showed a very good performance with RMSEPs obtained after full cross-validation within the reproducibility of the standard ASTM recommended methods. The external validation performed with the spectrophotometer operating in the process shows results with RMSEP of external prediction statistically indistinguishable from those obtained in the laboratory environment.

Conclusion

The newly-adopted strategy to construct and employ a process NIR analyser has been successfully demonstrated for gasoline quality monitoring allowing the conclusion that the approach can avoid model transfer problems by calibrating the movable spectrophotometer in the laboratory and returning the unit to the process to operate the same models without any alteration.