Rapid identification and assay of crude oils based on moving-window correlation coefficient and near infrared spectral library

Chu Xiaoli*, Xu Yupeng, Tian Songbai, Wang Jing and Lu Wanzhen

Research Institute of Petroleum Processing, Beijing, 100083, P.R. China *Corresponding author: cxlyuli@sina.com

Introduction

Crude oil assay plays a very important role in petroleum exploitation, trading and processing. As a fast and viable measurement solution, spectroscopic methods such as NMR, Raman, IR, and NIR have been developed¹⁻³ since the corresponding spectra reflect the complete molecular composition of the petroleum and petroleum products. Unlike gasoline or diesel analysis, crude oil assay may involve hundreds of chemical, physical and performance parameters for a whole sample and its sub-fractions. Therefore, development and maintenance of a large number of regression models built by traditional multivariate calibration methods such as PLS one by one is not practical. The aim of this study was to develop a new method to provide a complete crude oil assay based on a NIR spectral library using pattern recognition techniques.

Materials and Methods

Samples

From 1998 to 2010, 265 crude oil samples were collected from our crude oil evaluation group in the Research Institute of Petroleum of SINOPEC. Those samples originated from more than 200 crude oil fields distributed within China and elsewhere around the world. The detailed assay data for each crude oil sample collected were determined by traditional analytical methods according to conventional assay strategy.

Near infrared spectroscopy

Near infrared spectroscopy measurements were carried out at room temperature on a Thermo Antais II FT-NIR spectrometer. Spectral resolution was 8cm⁻¹ and 64 scans were accumulated over the range 3500 cm⁻¹ to 10000 cm⁻¹ for each spectrum. A quartz glass transmittance cell with 1.0mm light path was employed.

Traditional pattern recognition methods, based on distance or correlation coefficient etc., do not easily identify crude oil samples because some parts of the crude oil NIR spectra are highly similar. Therefore, a new spectral searching method, named moving window correlation coefficient, which can distinguish between highly similar crude oils accurately, is proposed in this paper.

Results and Discussion

The main parameters of the moving window correlation coefficient method were discussed and selected in this study. Two very similar crude oils (Arab middle crude oil and Arab heavy crude oil) were selected from the NIR spectral library according to their detailed assay data. The results show that the moving window correlation coefficient method can distinguish the NIR spectra of very similar crude oils. Three new crude oil samples (Merry 16 crude oil, Tahe heavy crude oil and Daqing crude oil) collected in 2010 were selected as validation samples to evaluate the developed method. The NIR spectral library and assay database also contain these three crude oil types but from the years 2008, 2006 and 2009. This means that the three test samples were not the same as those of the same type in NIR spectral library. The recognition results indicated that the spectra in the NIR spectral library which were most similar to the new three samples were the same types.

Conclusion

A rapid identification and assay strategy for crude oil was proposed based on the moving window correlation coefficient method and NIR spectral library combined with a crude oil assay database. This strategy can quickly provide detailed assay data of an unknown crude oil if the assay database contains the crude oil. If the assay database and NIR spectral library do not contain the unknown crude oil, the assay data of the crude oil most similar to the sample can be recommended for reference.

Reference paper as:

C. Xiaoli, X. Yupeng, T. Songbai, W. Jing and L. Wanzhen (2012). Rapid identification and assay of crude oils based

on moving-window correlation coefficient and near infrared spectral library, in: Proceedings of the 15th International Conference on Near Infrared Spectroscopy, Edited by M. Manley, C.M. McGoverin, D.B. Thomas and G. Downey, Cape Town, South Africa, pp. 112-113.