Abstract

Comparison of near infrared and mid-infrared spectroscopy for heavy oil characterisation and evaluation of different combination methods

Jérémy Laxalde[1,2], Noémie Caillol[1]*, François Wahl[1], Nathalie Schildknecht, Cyril Ruckebusch[2] and Ludovic Duponchel[2]

[1]IFP Énergies Nouvelles, Établissement de Lyon, Rond-point de l'échangeur de Solaize, BP 3, 69360 Solaize
[2]LASIR, CNRS, Université Lille 1 – Villeneuve d'Ascq, France
*Corresponding author: noemie.caillol@ifpenergiesnouvelles.fr

Introduction

Predictive chemometric models are developed as an alternative to heavy oil reference methods. This work focuses on SARA quantification (saturates, aromatics, resins and asphaltens). Both NIR and MIR spectroscopy are used in literature for this purpose, and classical PLS models developed and compared. No work has evaluated the potential of NIR and MIR combination for the characterisation of heavy oils. The aim of this methodology is to point out the complementarities of NIR and MIR spectroscopy in order to improve model interpretability and predictive ability. Several methods for combination were tested and compared.

Materials and Methods

Samples (n = 230) were selected to thoroughly cover existing concentration ranges, crude oil origins and different processes for the improvement of heavy oil quality. Reference values of investigated properties were obtained from normalised reference methods (ASTM). NIR spectra were recorded at 100°C using the Bomen Resid-IR. A ThermoOptek Nicolet spectrometer equipped with a heated attenuated total reflectance (ATR) accessory was used for the acquisition at 100°C of MIR spectra. Classic optimisation of PLS models for both MIR and NIR spectra was performed. For the evaluation of NIR and MIR combination, several methods were investigated and compared in terms of spectra interpretability and predictive ability.

Results and Discussion

The main issue for classical model optimisation was the correction of the baseline slope in NIR spectra which corresponds to the tail of the electronic absorption band in the visible region caused by transitions of asphaltens molecules (aggregated compounds). The best results were obtained using the weighted least square baseline correction. When comparing NIR and MIR, NIR generally gives the best models. However, results point out the existence of useful information in MIR spectra. Therefore, NIR and MIR combination methods were evaluated. Compared to a basic concatenated method, elaborated strategies (H-PLS, MB-PLS and S-PLS) improved the modelling approach by assigning an adequate number of latent values for the decomposition of each spectral block. As a result, noise was reduced and relevant descriptors were used in the final model. Model interpretability was also improved by indicators which indicate how the initial blocks participate in the final model (such as % explained variance, scores and loadings which are available for both initial and final descriptors).

Conclusion

NIR and MIR were successfully employed for heavy oil characterisation. NIR led to more efficient classical PLS models than MIR. The potential of several methods for their combination was evaluated.

Reference paper as:
J. Laxalde, N. Caillol, F. Wahl, N. Schildknecht, C. Ruckebusch and L. Duponchel (2012).Comparison of near infrared and mid-infrared spectroscopy for heavy oil characterisation and evaluation of different combination methods (abstract), 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, p. 205.