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Prediction of physico-chemical properties of Colombian heavy crude oil and vacuum residues from mass spectrometry (MALDI-TOF), vibrational spectroscopy (FT-IR and Raman) and chemometry

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In recent years there has been a growing trend to process heavier crude at refineries around the world. One of the main byproducts in the oil refinement process is the vacuum residues, which are very difficult to manipulate and characterize due to their high viscosity and high compositional complexity. Characterizing these kinds of feedstocks (vacuum bottoms and heavy crudes) is essential for designing of refinement schemes that maximize their yields and obtain quality products. Generally, their characterization is performed by standard analytical methods. These methods are often time-consuming, elaborate and costly and require a large amount of sample and solvents. The main objective of this work was to develop an alternative methodology to determine, in a simple, fast and reliable manner, different physicochemical properties of Colombian heavy crudes and vacuum residues. This methodology consisted in combining spectroscopic techniques (Infrared and Raman) and MALDI-TOF mass spectrometry with the chemometric method partial least squares regression (PLS). PLS chemometric models for calibration and validation were developed to predict API gravity, Conrad son RCC carbon residue, aromatic hydrocarbon content (tetra, penta, hexa and hepta + aromatic compounds) from vacuum residues and heavy crude from Colombia. The efficiency of the models was evaluated by means of the standard error of calibration (SEC) and prediction (SEP) and correlation coefficient R2. The high correlation found between the reference values and those predicted by IR, Raman and mass demonstrates the credibility of the proposed method. In addition, the results revealed that the two loads investigated when using the PLS multivariable calibration method can be included in the same model.

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