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# Determination of Physical Properties of Crude Oil Distillates by Near-Infrared Spectroscopy and Multivariate Calibration

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**Abstract :** Petroleum refineries are a highly complex process industry with continuous production and high operating costs. Physical separation of crude oil starts with the crude oil distillation unit, continues with various conversion and purification units, and passes through many stages until obtaining the final product. To meet the desired product specification, process parameters are strictly followed. To be able to ensure the quality of distillates, routine analyses are performed in quality control laboratories based on appropriate international standards such as American Society for Testing and Materials (ASTM) standard methods and European Standard (EN) methods. The cut point of distillates in the crude distillation unit is very crucial for the efficiency of the upcoming processes. In order to maximize the process efficiency, the determination of the quality of distillates should be as fast as possible, reliable, and cost-effective. In this sense, an alternative study was carried out on the crude oil distillation unit that serves the entire refinery process. In this work, studies were conducted with three different crude oil distillates which are Light Straight Run Naphtha (LSRN), Heavy Straight Run Naphtha (HSRN), and Kerosene. These products are named after separation by the number of carbons it contains. LSRN consists of five to six carbon-containing hydrocarbons, HSRN consist of six to ten, and kerosene consists of sixteen to twenty-two carbon-containing hydrocarbons. Physical properties of three different crude distillation unit products (LSRN, HSRN, and Kerosene) were determined using Near-Infrared Spectroscopy with multivariate calibration. The absorbance spectra of the petroleum samples were obtained in the range from 10000 $cm^{-1}$ to 4000 $cm^{-1}$, employing a quartz transmittance flow through cell with a 2 mm light path and a resolution of 2 $cm^{-1}$. A total of 400 samples were collected for each petroleum sample for almost four years. Several different crude oil grades were processed during sample collection times. Extended Multiplicative Signal Correction (EMSC) and Savitzky-Golay (SG) preprocessing techniques were applied to FT-NIR spectra of samples to eliminate baseline shifts and suppress unwanted variation. Two different multivariate calibration approaches (Partial Least Squares Regression, PLS and Genetic Inverse Least Squares, GILS) and an ensemble model were applied to preprocessed FT-NIR spectra. Predictive performance of each multivariate calibration technique and preprocessing techniques were compared, and the best models were chosen according to the reproducibility of ASTM reference methods. This work demonstrates the developed models can be used for routine analysis instead of conventional analytical methods with over 90% accuracy.

**Keywords :** crude distillation unit, multivariate calibration, near infrared spectroscopy, data preprocessing, refinery
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