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New NIR spectroscopy coupled with chemometric methods for detection and quantification of ethanol adulteration in premium 91 gasolines

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Ethanol, due to its high octane rating of 108, is often added as adulterant to premium 91 gasoline fuels to boost up its octane rating to 96 or more but it does not provide the same power to engine as that of super-premium 96 gasoline fuels. In this study a novel sensitive Near Infra-Red (NIR) spectroscopy combined with multivariate is employed to detect and quantify ethanol adulteration in premium 91 gasoline fuels. Standard samples of premium 91 octane gasolines were collected from Oman Oil Refineries and Petroleum Industries Company (ORPIC). The premium 91 samples were then intentionally spiked with ethanol at various levels. NIR spectroscopy was employed for the analysis of all samples in the near-infrared region, absorption mode, in the range 700-2500 nm. Then the multivariate methods such as the Principal Component Analysis (PCA), the Partial Least Square Discriminant Analysis (PLSDA) and the Partial Least Square regression (PLS) analysis were used to interpret the obtained NIR spectral data. PLSDA model was developed to distinguish between the pure gasoline samples and those intentionally-adulterated by ethanol. For PLSDA model the obtained R-square value was 97% with 0.0769 RMSE. A PLS model was also developed to quantify the levels of ethanol adulterant in premium 91 gasoline samples. The obtained PLS regression model has an r-square value of 99% with 1.88 RMSECV values which is very close to the predicted RMSEP value i.e. 1.58 and R2 value of 99% for one factor loading.

Biography

Fazal Mabood has his expertise in development of new robust spectroscopies coupled with chemometrics for analysis of clinical, food, meat, plant, petrochemical and pharmaceutical samples. He has worked on new design of experiment (DoE), application of factor analysis and PCA algorithms in chemistry, waste polymer recycling. He has completed his Post-doctorate on application of different factor analysis algorithms in chemistry from Dalhousie University, Canada, Doctor of Philosophy (PhD in Chemistry) from University of Peshawar and Master of Science (MSc in Chemistry) from University of Peshawar.

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