Prediction of Different Crude Oil Properties from FTIR Data with Statistical Methods, Deep and Shallow Neural Networks

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Keywords: FTIR, Crude Oil Properties, Statistical Methods, Deep Neural Network, Shallow Neural Network, Chemometric Methods

Abstract:

In recent years, Fourier Transform InfraRed (FTIR) spectrometry has been widely used to estimate different characteristics and contents of materials in many fields. Even though numerous works have been published in this area, it has still been difficult to suggest a global method that can predict the properties of crude oils from different resources based solely on FTIR data. In this study, we compare the application of several methods in order to predict particular important properties (i.e., viscosity, density, total sulfur content, total acid number, etc.) of crude oil samples from seven different Canadian oil fields. We employed chemometric methods such as Partial Least Squares regression (PLS) and principal component regression (PCR) and compared the results to the performance of neural networks (NN) with a different number of layers. These methods were evaluated by calculating the coefficient of determination (R2) and prediction root mean squared errors (RMSE). Although less complicated statistical methods like PCR and PLS could lead to excellent predictions for some properties, we found that neural networks could improve the results in other properties. In addition, the prediction accuracy of some properties, like viscosity, was improved by classification before the application of regression methods.

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Prediction of Different Crude Oil Properties from FTIR Data with Statistical Methods, Deep and Shallow Neural Networks

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ABSTRACT

In recent years, Fourier Transform InfraRed (FTIR) spectrometry has been widely used to estimate different characteristics and contents of materials in many fields. Even though numerous works have been published in this area, it has still been difficult to suggest a global method that can predict the properties of crude oils from different resources based solely on FTIR data. In this study, we compare the application of several methods in order to predict particular important properties (i.e., viscosity, density, total sulfur content, total acid number, etc.) of crude oil samples from seven different Canadian oil fields. We employed chemometric methods such as Partial Least Squares regression (PLS) and principal component regression (PCR) and compared the results to the performance of neural networks (NN) with a different number of layers. These methods were evaluated by calculating the coefficient of determination (R^2) and prediction root mean squared errors (RMSE). Although less complicated statistical methods like PCR and PLS could lead to excellent predictions for some properties, we found that neural networks could improve the results in other properties. In addition, the prediction accuracy of some properties, like viscosity, was improved by classification before the application of regression methods.

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INTRODUCTION

An accurate determination of specifications of crude oil as the essential source of the world's fossil fuel is vital in the oil industry. Since petroleum is a complex mixture of organic compounds, its quality is mostly evaluated by physicochemical properties [1]. These properties are of high interest for addressing many reservoir engineering and operational process problems.

American Society for Testing and Materials (ASTM) and American Petroleum Institute (API) have standard methods for reporting crude oil analysis. So, these properties are ideally determined experimentally on actual fluid samples via elaborate laboratory procedures, which are mostly expensive and not too eco-friendly.

Accordingly, it is of high value to propose methods for both reliable and rapid evaluation of crude oils, which can estimate properties without any sample preparation so more eco-friendly, and with less labor work. In this work, we propose the best chemometric methods and neural networks using FTIR spectroscopy for simultaneously reliable and rapid determination of crude oil properties.

Owing to rapid and significant advances in multivariate statistics and machine learning techniques, it is now possible to estimate many properties of interest (that are difficult or costly to measure) using other relatively simpler, faster, and less expensive measurements. Analytical procedures which are less dependent on sample size [2] are now available for mapping out the relationship between the easily available measurements, such as Fourier Transform InfraRed (FTIR), and the difficult to obtain measurements, such as the viscosity of crude oil.

METHODS

Stepping towards incorporating FTIR data into physicochemical properties, we studied the data of one hundred and seven crude oil samples obtained from seven different Canadian oil fields that a petroleum company in Canada supplied. They obtained the FTIR spectra corresponding to these samples using a Thermo Fisher FTIR microscope. They also measured several physicochemical properties of these crude oil samples using appropriate analytical instruments. The company wants to develop robust models that can only provide accurate estimates of the physicochemical properties utilizing FTIR data, thus avoiding the need for elaborate, expensive, and time-consuming laboratory procedures.

We analyzed the application of several methods to predict particular important properties of crude oil samples by randomly dividing data into training, calibration, and test sets. We employed chemometric methods such as Partial Least Squares regression (PLS) and principal component regression (PCR) and compared the results to the performance of neural networks (NN) with a different number of layers. We evaluated these methods by calculating the coefficient of determination (R^2) and prediction root mean squared errors (RMSE).

These results have been partially reported in a separate study involving eighty-two crude oil samples focused on predicting viscosity and density with chemometric methods [1].

DISCUSSION

This study focuses on the importance of spectra data in predicting the physicochemical properties of crude oil samples from different oil fields. We suggest the best methods, including chemometric ones, like PLS and PCR, and varying depth neural network ones, to calculate several important crude oil properties, like viscosity, density, total acid number, total sulfur content, etc., disrespect of analyzing a light oil or a heavy one.

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