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Gasoline quality prediction using gas chromatography and FTIR spectroscopy: An artificial intelligence approach

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Abstract

This paper reports on analysis of 45 gasoline samples with different qualities, namely, octane number and chemical composition. Measurements of data from gas chromatography and IR (FTIR) spectroscopy are used to gasoline quality prediction and classification. The data were processed using principal component analysis (PCA) and fuzzy C means (FCM) algorithm. The data were then analyzed following the neural network paradigms, hybrid neural network and support vector machines (SVM) classifier. The IR spectra were compressed and denoised by the discrete wavelet analysis. Using the hybrid neural network and multi linear regression method (MLRM), excellent correlation between chemical composition of the gasoline samples and predicted value of the octane number was obtained. About 100% correct classification for six different categories of the gasoline was achieved, each of which has different qualities.

Keywords: Gasoline classification; Octane number; Neural networks; Wavelet analysis; SVM classifier

1. Introduction

The antiknock performance of a gasoline is its ability to resist detonation, a form of abnormal combustion. Detonation occurs when the air–fuel mixture reaches a temperature and/or pressure at which it can no longer keep from self-igniting. Two types of abnormal combustion are common: the first is detonation, as previously mentioned, and the other is preignition.

Research octane number (RON) is determined in a standardized engine. This is a very expensive method but still the only accepted one. Very soon scientists began to look for a correlation between the tendency of hydrocarbon-based fuels to knock and the composition of these fuels. With the help of kinetic models, possible reaction mechanisms were established. Later on the calculation of octane numbers from IR and NIR spectral data was done. Octane number has also been correlated with carbon or hydrocarbon types [1,2] measured by gas chromatography, high performance liquid chromatography, or nuclear magnetic resonance [3]. The octane number prediction out of these models gave good and reproducible results, but only for fuels with a very similar composition. Most of the correlation models published were developed with multiple linear or nonlinear regression techniques, which require the user to specify a priori a mathematical model of the empirical correlation. The neural network approach is an alternative way of solving the problem. Unlike multiple linear or nonlinear regression techniques, which require a predefined empirical model, the neural network can identify and learn the correlative patterns between the input and corresponding output values once a training set is provided.

In this paper, the application of gas chromatography and IR (FTIR) data in combination with different pattern-recognition engines (PCA, FCM, neural networks) to predict the octane number of gasoline is reported. The selforganizing hybrid network and SVM network were used.

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2. Method

Forty-five unleaded gasoline samples were selected for this study. These samples covered a wide range of gasoline properties. The following methods were applied to the chemical and physical and chemical structure analysis:

- *Research octane number (RON).* The test procedure was performed according to PN-82/C-04112 standard. This parameter was measured by comparing of antiknock performance of tested fuel with antiknock performance fuels in conditions described in this standard. The octane number of the fuel samples was determined by burning the gasoline in an engine under controlled conditions, e.g. of spark timing, compression, engine speed, and load, until a standard level of knock occurs.
- *Gas chromatography*. The determination of hydrocarbon composition was performed according to the test procedure based on the ASTM D 5134. This test method provides the procedure to determine total chemical group composition of tested samples (e.g. *n*-paraffins, *i*-paraffins, naphthenes, olefins and aromatics). In addition, several hundred chemical compounds presented in tested samples were determined. The mass percent of the five hydrocarbon types and ethanol identified by GC were used as neural network inputs.
- *FTIR spectroscopy.* The determination of hydrocarbon composition was performed according to the test procedure worked in Central Petroleum Laboratory using a spectrometer type MAGNA-IR 750 NICOLET. All the spectra of samples were registered and analyzed by two compatible programs: OMNIC 1.2a and QUANTIR 1.20 at the following conditions:

Number of sample scans 32, sample cell KBr (25), resolution about 2 cm^{-1} and spectral range 4000–400 cm^{-1}. The measurements were performed in nitrogen atmosphere. One spectrum was recorded as data-vector which has 1868 independent variables (individual spectral channels). The dimension of the spectrum vectors was reduced to 231 approximation coefficients by wavelets technique using 3-level decomposition and 5-db wavelet function [4]. These 231 approximation coefficients after the features extraction were reduced to six independent features. The features extraction was performed using three different methods: PCA technique, test of the maximal variance of the peak absorption and chemical interpretation of the optical transitions (peaks of the absorption). Finally, one spectrum was represented as vector with six components. These six-component vectors were used as neural network inputs.

Repeatability and reproducibility of the analytical techniques used in this work were within the requirement of the standard ASTM methods for the specific analysis.

All network calculations in this study were performed using MATLAB 6.5 software, originally developed software for the selforganizing hybrid neural network [5] and SVM neural network [6] as well. The experimental data were processed using principal component analysis (PCA), fuzzy C means analysis (FCM), wavelet analysis and neural network (SVM) classifier.

3. Hybrid neural network as a signal processor

To solve the complex estimation tasks, the neural network of the hybrid structure presented in Fig. 1 was applied. The first part of the network is the selforganizing Kohonen layer, the second one is the feedforward network called multilayer perceptron (MLP) which is trained in the supervised mode. The hybrid neural structure consisting of the selforganizing layer performing the role of recognition and classification and the second cascaded subnetwork in the form of multilayer perceptron, performing the role of estimator. The perceptron subnetwork is fed up with the signals generated by the selforganizing layer. The important point of the proposed organization of signal processing is the reliability and acceleration of the whole pattern recognition process. The procedure of learning the hybrid network is split into two separate phases: the selforganization of the Kohonen layer (the generalized Kohonen algorithm was used here) and afterwards the supervised learning of the MLP subnetwork. Thanks to the separation of both phases, the complexity of the learning has been significantly reduced and learning process accelerated. This procedure is not straightforward, since qualitative and quantitative aspects are merged together with a degree of complexity generally dependent on the number of components composing the chemical pattern and on the degree of non-linearity of the problem.

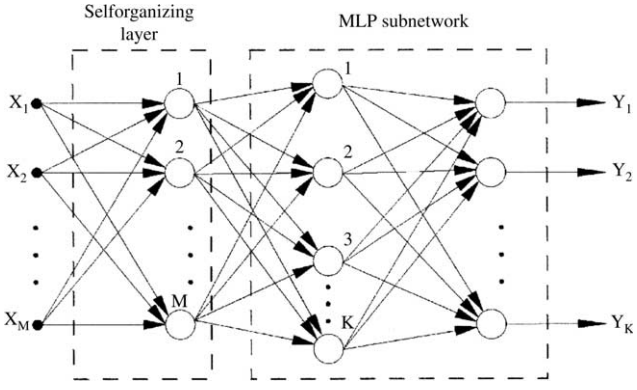

Fig. 1. Structure of the hybrid neural network.