Classification of fuels using multilayer perceptron neural networks


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Abstract. Electrical impedance data obtained with an array of conducting polymer chemical sensors was used by a neural network (ANN) to classify fuel adulteration. Real samples were classified with accuracy greater than 90% in two groups: approved and adulterated.

Keywords: Neural network, fuel adulteration, interdigitated electrodes, poly(3-methylthiophene), poly(3-hexylthiophene), MLP.

PACS: 07.07.Df Sensors (chemical, optical, electrical, movement, gas, etc.)

INTRODUCTION

Fuel adulteration is a major concern in Brazil. The local governmental agency detects from 2 to 6% of problematic samples yearly, which is a lot considering Brazil’s market size. Besides, as gasoline may have different properties depending on its source and the myriad of adulteration possibilities is even more vast, array of sensors based on “global selectivity concept” [1,2] seems to be more suitable methodology to detect problems in fuel.

The global selectivity concept encompasses the cross-sensitivity of non-specific chemical sensors and the use of multivariated data analysis methods as a way to provide “fingerprints” for samples of different chemical composition. The chemical sensors can employ different types of sensoactive materials, whose electrical responses are dependent on the physico-chemical characteristics of the media they get in contact with. Conducting polymers are per excellence suitable sensoactive materials, since their electrical conductivity is highly influenced by the environmental conditions and they can be easily processed in the thin film form by different techniques. Moreover, a vast number of conducting polymers with different structures and chemosensitivity are available.

In the present contribution, we employ an artificial neural network (ANNs) with multi-layer perceptron (MLP) [2,3] to classify data of fuel samples. ANNs are distributed computing systems composed by units connected by weighted links, simulating the structure and functioning of the brain. Data from real samples obtained with an array of conducting polymer sensors were analyzed. Impedance data of each sensor were used to discriminate and classify adulteration of gasoline and ethanol fuels using principal component analysis (PCA) and ANN.

EXPERIMENTAL AND METHODS

Fuel samples collected from gas stations and previously analyzed by a certified laboratory were discriminated and classified with an array of conducting polymers sensors [4,5]. The sensors were made of poly(3-methylthiophene) (PMTh) and poly(3-hexylthiophene) (PHTh) films deposited by chronopotenciometry and chronoamperometry [5]. The array was composed by four sensors with polythiophene films and one plain sensor. Impedance data were collected with the sensor array immersed in 25 mL fuel samples at 25°C by using a Solartron 1260A impedance analyzer.

Data were initially processed by PCA in order to discriminate groups of samples (40 fuel samples). Afterwards, a MLP ANN was developed (mais detalhes) and employed to classify samples in two groups: approved or adulterated.
RESULTS

Impedance spectroscopy data of different mixtures of gasoline and ethanol and ethanol and distilled water were taken. The sensors respond to differences in the fuel composition. Figure 1 shows the response of a polythiophene sensor, which could be modeled by an equivalent circuit (inset) as proposed by Taylor [6]. All circuit elements are affected (Figure 2) by changes on the fuel composition. Thus, data of different properties such as dielectrics, double-layer, and interface characteristics could be used to analyze the fuel samples.

![Figure 1](image1.png)

**FIGURE 1.** Impedance spectrum (Nyquist plot) of a polythiophene sensor submitted to a fuel sample, as quoted. The inset shows a model equivalent circuit for the sensor.

![Figure 2](image2.png)

**FIGURE 2.** Circuit elements of the polythiophene sensor as a function of the fuel sample composition.

The PCA analysis (Figure 3) shows that approved fuels tend to group together while adulterated ones are sparser. The MLP ANN analysis was done with several configurations (learning rate, units in hidden layer, etc) and using the 5 fold cross-validation technique. Performances better than 90% were achieved.

![Figure 3](image3.png)

**FIGURE 3.** PCA plot of 40 gasoline samples analyzed with the conducting polymer sensor array.

CONCLUSIONS

The use of an ANN allowed to discriminate and classify real fuel samples according to their chemical composition, in two groups: approved and adulterated. Moreover, better performances can be achieved improving the ANN algorithm which is under current investigation.

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