BULETINUL Universităţii Petrol – Gaze din Ploieşti	Vol. LXVII No. 1/2015	15 – 19	Seria Tehnică

Applying Artificial Neural Networks in Gasoline Formulation. Case Study

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Abstract

Nowadays, the ecological commercial gasoline in the European Union must fulfill the EURO 6 and EN 228 standards. Because of its quickness, the possibility of commercial ecological gasoline properties estimation using the artificial neural networks is very attractive.

This paper discusses estimating the Research and Motor octane numbers for blending gasoline, using artificial neural network. The neural network was trained using a training database of 60 records. Because the database contains correlated data, the training was efficient, so the neural network offered accurate estimations for new samples of gasoline, non-existent in the training database.

Key words: *commercial gasoline, artificial neural network, properties estimation, gasoline formulation*

Introduction

One of the important problems of mankind is air pollution. According to the World Health Organization, air pollution caused in 2012 the death of 7 million people, worldwide [1]. An important contribution to the degree of air pollution is given by the emissions caused by gasoline burning in the internal combustion engines [12]. About 60 years ago, the number of vehicles was small, reason for which the effects of air pollution were not noticeable. With the constant increase of the number of vehicles, the degree of air pollution due to gasoline burning in the engine constantly increased.

The ecological commercial gasoline is obtained by blending its components, process known as *formulation* [13]. Component blending is being made using a *blending recipe*. The blending recipe is based on a mathematical blending model, model which can be determined based on the different properties of the gasoline components.

Nowadays, the commercial gasoline must fulfill the EURO 6 and EN 228 standards [4, 10].

A large number of mathematical blending models use artificial neural networks (ANNs) [2]. Because of the ANN flexibility, numerous and detailed research related to estimating gasoline properties were made.

F. Trivella and his collaborators used an ANN to estimate the gasoline octane numbers of the catalytic reforming gasoline of a refinery in Italy. Using the developed ANN, a system for automating the estimation process was created [16].

Nikos Pasadakis and his collaborators used as input data for the training database the octane numbers and the volume percentages of the most utilized 7 components in obtaining the commercial ecological gasoline, along with the octane numbers for 173 blendings, obtained using these components [15].

Côcco Lilian and her collaborators used ANN to correlate the chemical composition of the gasoline that is sold in Brazil and some of its properties, like the distillation curve and the Reid Vapor Pressure. 1284 gasoline samples were used for ANN training, and the estimation error was under 1% [8].

Paranghooshi and his collaborators used as input data for the training database the volumic concentrations of the most six used components from a series of gasoline types multiplied with the blendings' octane numbers [14].

Wen Yu and América Morales used two types of ANNs [17]. They divided the gasoline properties into *static properties* and *dynamic properties*, these two types of properties being modelled by using two types of ANNs: to model the static properties, a *feedforward* ANN was used and for modelling the dynamic properties, a *recurrent* ANN was used [3, 7].

This paper aims to present an estimation of the gasoline properties using ANNs. A case study regarding applying ANNs to gasoline formulation will be presented. The study presented in this paper can be adapted according to the necessities.

Experimental Part

As it was mentioned in the introduction, this paper presents a case study regarding applying ANNs in gasoline formulation.

Among the multitude of components utilized to obtain blending commercial ecological gasoline, in this study four of the most utilized components were taken into consideration: FCC gasoline, catalytic reforming (CR) gasoline, iC_5 fraction and bioethanol. The components' octane numbers are presented in Table 1.

Table 1. Research and Motor octane numbers of the components utilized in the experimental program

Component	**RON**	**MON**
FCC gasoline	94.0	83.7
CR gasoline	96.0	83.0
iC_5 fraction	94.3	87.6
Bioethanol	108.6	89.7

The presented case study's purpose is blending gasoline octane numbers estimation when both the components' octane numbers and the proportions in which the components are used in the blending are known. This study consists in estimating the octane numbers of a blending that has 39.2% vol. FCC gasoline, 39.2% vol. CR gasoline, 19.6% vol. iC_5 fraction and 2% vol. bioethanol.

In order to use the ANN to accomplish the case study's purpose, the ANN training with the help of a database is necessary, the database being called *training database*. In order to obtain the necessary data required by the training database, 60 blendings, using the four components listed above, were used.

To obtain the necessary blendings, 10 initial blendings, called *base blendings* were obtained. The base blendings' compositions are presented in Table 2. To each of these 10 base blendings, bioethanol in proportions of 2, 4, 6, 8 respectively 10% vol. was added [9]. To determine the components' and the blendings' octane numbers, the IROX 2000 device was used [5].

Table 2. The base blendings' compositions used in the experimental program

Blending number	Utilized proportions of each component (% vol.)		
	FCC Gasoline	**CR Gasoline**	***i*C_5 Fraction**
1	40	40	20
2	45	30	25
3	35	45	20
4	40	45	15
5	50	25	25
6	30	45	25
7	25	60	15
8	60	25	15
9	30	50	20
10	35	30	35

The experiments took place in laboratory conditions and the components were stored in safe conditions, to prevent altering their properties. During the experimental determinations, the IROX 2000 device was operated according to the instructions from its user manual [6].

The blendings’ octane numbers were introduced in the training database as *output data* or *target data*. The training database *input data* are the volumic percentages in which each component was used in the analyzed blendings.

ANN Creation and Training

To create and train the ANN, the *Neural Network Fitting Tool* module of Matlab R2012b software was used. This module facilitates the processes of creating and training an ANN. In order to create and train the ANN, the obtained experimental data were converted according to the specifications mentioned in the program’s help system [9, 11].

Training the ANN was made using the following parameters:

- The database data destination separation: 70% training data, 15% validation data and 15% test data;
- Number of neurons in the hidden layer: 10;
- Training algorithm: Levenberg-Marquardt algorithm.

Obtained Results and Discussions

To verify the estimations’ accuracy, offered by the created and trained ANN, the octane numbers for the blending specified in the case study description will be estimated.

In Table 3, the octane numbers determined according to the experimental plan and the octane numbers estimated using the ANN are presented for the blending specified earlier.

Table 3. The determined and the estimated octane numbers for the studied blending

RON		Difference	MON		Difference
Determined	**Estimated**		**Determined**	**Estimated**	
96.3	96.5	0.2	85.2	85.54	0.34

According to Table 3, the ANN’s highest estimation error was 0.34 octane units. It is worth mentioning that these estimation errors were obtained using a small training database, but the data's strong correlation offset this drawback. Because of this face, it can be stated that it is much more important to have a small database, with highly correlated data than a large database with low correlation between the data.

Conclusions

In this paper a case study of using an ANN to estimate the blending gasoline properties was presented. The estimation needed preparation of 60 blendings that have FCC gasoline, CR gasoline, iC_5 fraction and bioethanol, blendings of which the MON and RON were determined.

The experimental data were introduced into a training database, used to train the ANN. The ANN was created and trained using the *Neural Network Tool* module of the MatlabR2012b software.

The created and trained ANN's estimation error was tested using a blending of which the octane numbers were previously known. The maximum estimation error was of 0.34 octane units. This difference proves that a correctly trained ANN can offer accurate estimations of the properties for which it was trained for.

Due to their flexibility, the ANNs can be used to determine other properties than the octane numbers, other properties could be also used as input data for the training database.

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Aplicarea rețelelor neuronale artificiale în formularea benzinelor. Studiu de caz

Rezumat

În prezent, benzinele comerciale ecologice din Uniunea Europeană trebuie să îndeplinească standardele EURO 6 și EN 228. Datorită rapidității sale, posibilitatea estimării proprietăților benzinei comerciale ecologice utilizând rețelele neuronale artificiale este foarte atractivă.

Această lucrare discută posibilitatea estimării cifrelor octanice Research și Motor pentru benzina de amestec utilizând rețelele neuronale artificiale. Rețeaua neuronală a fost antrenată utilizând o bază de date de antrenament de 60 de înregistrări. Deoarece baza de date conține date corelate între ele, antrenamentul a fost eficient, deci rețeaua neuronală a oferit estimări precise pentru probe noi de benzină, neexistente în baza de date.