Octane Number Estimation Using Neural Networks

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The octane number is one of the most important properties of commercial gasoline, offering important information regarding the anti-knock resistance of the fuel. The experimental determination of the octane number is made according to the ASTM D 2699 standard. The procedure is slow and requires a large quantity of reagents. Because of these reasons, the estimation of thhe octane number through various methods is used. In this papaer, from the methods of the octane number, the method which uses neural networks was chosen. In this variant, the estimation of the octane number is made by correlating some properties of the gasoline components with the octane number. One of the advantages of using neural networks for the estimation of the octane numbers is that the estimated values are obtained in a short amount of time.

Keywords: octane number, neural networks, octane number estimation, artificial intelligence

The octane number was introduced in 1927 and measures the gasoline anti-knocking resistance [1]. The method for the determination of the octane number is specified in the ASTM D2699 standard and consists in comparing the anti-knocking properties of the fuel with those of a mixture between n-heptane and iso-octane, with an identical anti-knocking behaviour [2].

According to the standard, the determination of the Research and Motor octane numbers is made using standard engine. The biggest drawbacks of this method are the time length of the determination and the fact that the obtained results are useful as long as the properties of the gasoline components remain constant. Because of these drawbacks and due to the technological progress in automation of the commercial gasoline reformulation, the estimation of the octane number of the commercial gasoline became very attractive.

The values of the octane number depend in a non-linear way of the mixture composition. Because of this reason, estimation methods which are more complex than those based on linear equations are required. The estimation methods of the octane number must preserve the estimating capacity, no matter how much the properties of the gasoline components may vary. More evolved estimation methods are used as basic tools for determination of the optimum blending recipe, which guarantees the specified octane number. The objective functions of these evolved methods can be maximum benefit, minimum production cost, price or component availability.

Over time, many methods for estimating octane numbers were developed. A few of these methods use the structural group contribution [3], modelling of the interactions between the gasoline components [4], Raman spectroscopy [5] or interaction coefficients [6].

A class of estimation methods is based on the flexibility and accuracy of the artificial neural networks. The neural networks represent a branch of the Artificial Intelligence, which is accepted as a new computing technology [7]. The principle behind the neural networks is the simulation of the structure and functioning of the biological neural networks. The simulation efficiency depends on the neural networks structure and how efficiently is the network trained [8].

In the estimation algorithm of the neural networks, which has input and output data, one or more properties of the gasoline components can be chosen as input data.

An example of estimating octane numbers using neural networks is shown in [9]. The researchers used a neural network to estimate the octane number of catalytic reforming gasoline from a refinery in Italy. To accomplish the desired goal, the authors used the data obtained in the past, in the refinery, and estimated the octane numbers and the content of naphthenic and aromatic hydrocarbons of the catalytic reforming gasoline. Based on the obtained neural network, a controlling system which automates the entire estimation process was developed. This system allows data entering into the training database, and neural network training after the database update to be made in a short amount of time.

Another way of using the neural networks for estimating the octane number is used by Nikos Pasadakis and his collaborators [10]. The authors used as input data for the neural network the Research and Motor octane numbers, the volumic percentage of 7 most used components for obtaining the commercial gasoline, components obtained from a refinery in Greece, along with the octane numbers of 173 other mixtures of these components.

The octane number of blending gasoline can be estimated from the structure of its components. An example is showed in [11]. In his study, the molecular structures of over 200 components of the commercial gasoline were correlated with their octane numbers through a neural network.

The estimation of the gasoline octane number using neural network can be achieved using gas chromatography also [12, 13]. The results of the chromatographic analysis of each analyzed gasoline were correlated with their octane numbers using a neural network. The differences between the determined and the estimated values for the octane number, for the same gasoline, are less than 0.5 octanes.

Another way of octane number estimation of blending gasoline was experimented by E. Paranghooshi and his collaborators [14]. In this study, the authors used as input data for the neural network the volumic concentration of the most used six components from a series of mixtures, values multiplied by the mixtures octane numbers.

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Table 1
COMPONENTS OF THE STUDIED BLENDING GASOLINES AND THEIR OCTANE NUMBERS

Component	RON	MON
FCC gasoline	94.0	83.7
Catalytic reforming gasoline	96.0	83.0
iC_5 fraction	94.3	87.6
Bio-ethanol	108.6	89.7

This paper aims to present a way of using the neural networks for estimating the Research and Motor octane numbers. The entire cycle of creating, training and using a neural network will be presented. In the end, the estimated octane numbers will be compared with those determined experimentally, for identical gasoline, being discussed the obtained results and the neural network performance.

Experimental part

The individual data, used for neural network training, were obtained experimentally. The neural network is created, trained and used with the help of a computer, with Mathworks Matlab R2012b installed [15].

Obtaining the data for the training database

To obtain the training data, 60 mixtures containing FCC gasoline, catalytic reforming gasoline, iC_5 fraction and bio-ethanol were prepared. The octane numbers of the utilized components are presented in table 1.

To obtain the required mixtures, first the initial mixtures were obtained. Their compositions are presented in table 2. Bio-ethanol, in proportions of 2, 4, 6, 8 respectively 10% vol. was added to each of these 10 initial mixtures. The octane numbers of all the prepared mixtures were determined using the IROX 2000 device [16].

The mixtures were obtained in the laboratory, in working conditions, in which the components were kept safe, to prevent the alteration of their properties.

The experimental data necessary to create the training database are the proportions, expressed in volumic percentage, in which the components are blend (the input data of the neural network) and the Motor and Research octane numbers of the blending (the output data of the neural network).

The results of the experimental determination were converted into a matrix form, required by the neural network. Blending proportions were stored into a matrix with 4 rows and 60 columns, which will be named matrix *P* and the octane numbers of the studied blends were stored into a matrix with 2 rows and 60 columns, which will be named matrix *C*. The two matrices have the general forms (1) and (2):

$$P = \begin{pmatrix} \%vol\ FCC\ gas., blend\ 1 & \%vol\ FCC\ gas., blend\ 2 & \dots \\ \%vol\ cat.ref.gas., blend\ 1 & \%vol\ cat.ref.gas., blend\ 2 & \dots \\ \%vol\ iC_5\ fraction, blend\ 1 & \%vol\ iC_5\ fraction, blend\ 2 & \dots \\ \%vol\ bio-ethanol, blend\ 1 & \%vol\ bio-etanol, blend\ 2 & \dots \end{pmatrix} \quad (1)$$

$$C = \begin{pmatrix} RON, blend\ 1 & RON, blend\ 2 & \dots \\ MON, blend\ 1 & MON, blend\ 2 & \dots \end{pmatrix} \quad (2)$$

Table 2
INITIAL MIXTURES USED, ALONG WITH BIO-ETHANOL, TO OBTAIN THE MIXTURES WHICH WILL FORM THE TRAINING DATABASE

Number	Proportions used from each component (volumic percentage)		
	FCC gasoline	Catalytic reforming gasoline	iC_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

Conversion of the obtained data

Fragments of matrices *P* and *C*, used for training the neural network are presented in the matrices (3) and (4):

$$P = \begin{pmatrix} 40 & 39.2 & 38.4 \\ 40 & 39.2 & 38.4 \\ 20 & 19.6 & 19.2 \\ 0 & 2 & 4 \end{pmatrix} \quad (3)$$

$$C = \begin{pmatrix} 95.9 & 96.3 & 96.9 \\ 85.1 & 85.2 & 85.4 \end{pmatrix} \quad (4)$$

Creating and training the neural network

The creation of the neural network was made using the *Neural Network Fitting Tool*, which is a component of Matlab R2012b. This module is presented as a *wizard*, its purpose being the automatic and fast creation and training of the neural network. The parameters that were used in this module for creating the neural network are:

- input data for the training database: matrix *P*;
- output data for the training database: matrix *C*;
- separation by destination of the data from the training database: 70% training data, 15% validation data and 15% test data;
- number of neurons from the hidden layer: 10. The tests conducted with a superior number of neurons showed that an increase of this number, in this context, is not necessary. On the contrary, a network with 100 neurons in the hidden layer got over-trained. Over-training is an unwanted phenomenon, which can occur during the training phase of the neural network. The consequence of over-training is that the network offers very accurate estimations for the input data that belong to the training database but very poor estimations for other input data.

The structure of the generated neural network, used to estimate the octane number is presented in figure 1.

The training of the neural network was done using the same module, *Neural Network Fitting Tool*. The training was made using a random distribution of the data into the three data types, the training algorithm used was Levenberg-Marquardt.

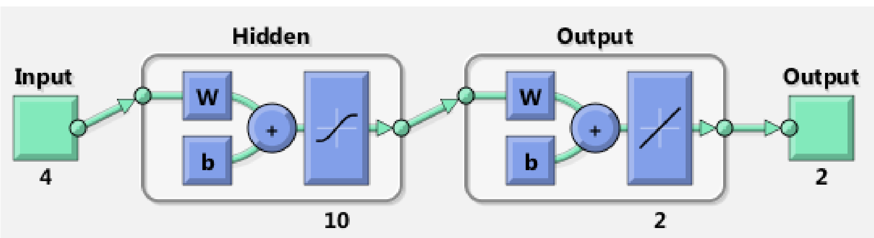

Fig. 1. Structure of the generated neural network for the estimation of the octane number

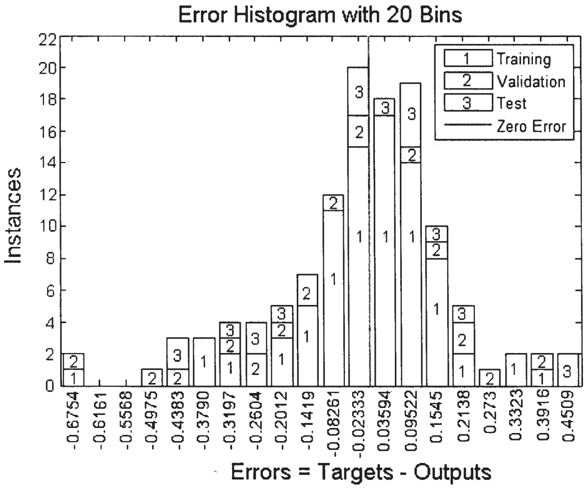

Fig. 2. The error histogram of the neural network training, using the created training database

To evaluate the neural network training efficiency, two evaluation methods were used: the error histogram and the evaluation of the training data correlation, using the Neural Network training Regression function, provided by the same module.

After the training of the neural network, the results provided by the error histogram are represented in figure 2.

Figure 2 represents the fact that the data from the training database have a very good correlation. The errors presented are in between [-0.67, 0.45] % and the majority of the data have an error in the interval [-0.02, 0.09] %, values very close to 0.

The data correlation from the training database are presented in figure 3:

The evaluation criterium of training efficiency provided by this method is the data correlation degree, noted as R. The data correlation degree is a real, positive, subunit number. If R has the value of 1 then there is a perfect correlation between the training data, a value of R equal with 0 represents that the data from the training database are at random.

Figure 3 shows that each training data type has a correlation degree of over 99%. This result, along with the result presented in figure 2, shows that, related to the training database, the neural network will show an accurate estimation of Motor and Research octane number.

The created and trained neural network can be saved as an editable script file. The neural network is saved, in the script file, as a variable, which can be called later. By default, this variable is called *net*.

Using the neural network

Using the neural network created in Matlab R2012b is done according to the following steps:

- the matrix that has the proportions in which the components are blend is being created. The matrix will be created using the syntax presented in matrix P, from equation (1).
- in the command window of Matlab R2012b the variable *net* will be called, passing as a parameter the matrix created in step 1;
- the result is also shown as a matrix, its syntax being identical with the syntax of the matrix C from equation (2).

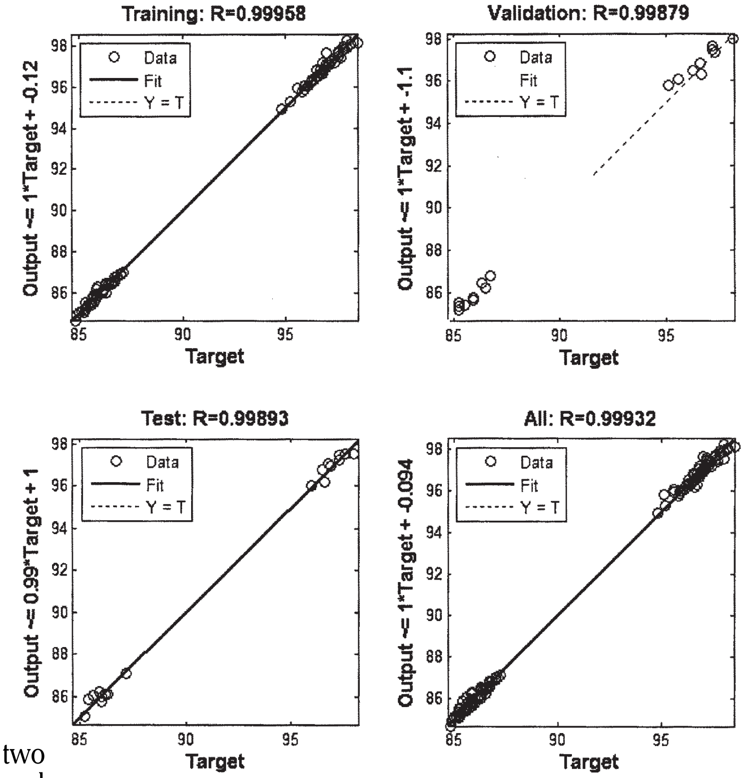

Fig. 3. The correlation degree of the data from the training database, correlation determined using regression analysis

Results and discussions

To verify the accuracy of the estimations shown by the created and trained neural network, the Motor and Research octane numbers of the mixtures presented in matrix P will be estimated. According to the experimental determinations, the Motor and Research octane numbers of the mixtures from matrix P are represented in matrix C.

The matrix that will be passed as a parameter to the neural network is the matrix (5):

$$Ex = \begin{pmatrix} 40 & 39.2 & 38.4 \\ 40 & 39.2 & 38.4 \\ 20 & 19.6 & 19.2 \\ 0 & 2 & 4 \end{pmatrix} \quad (5)$$

Using the neural network is made according to the syntax:

X = net (Ex)

In the syntax above, X is the matrix that will store the output values provided by the neural networks. The output values provided by the neural network are presented in the matrix (6):

$$X = \begin{pmatrix} 96.02 & 96.50 & 96.90 \\ 85.11 & 85.54 & 85.85 \end{pmatrix} \quad (6)$$

The differences between the results obtained through experimental determination of the octane numbers of the mixtures from matrix P, results shown in matrix C and the results shown by matrix X, are presented in matrix D (7):

$$D = \begin{pmatrix} 0.1250 & 0.2014 & 0.0070 \\ 0.0179 & 0.3460 & 0.4557 \end{pmatrix} \quad (7)$$

According to matrix D, the neural network offered accurate estimations, the largest difference being of about 0.5 octanes. The neural network performance is very good, despite the fact that the training database used is relatively small. The small number of data was compensated by the strong correlation. It is always better to have a small, database with strongly correlated data than having a large database with weakly correlated data.

Conclusions

The neural network represents a fast, flexible and efficient method for estimating the octane number of the blending gasoline. The estimation of the octane numbers is made from one or more component properties.

The neural network performance depends of its training efficiency. To evaluate the training efficiency, two criteria were used: the error histogram and the correlation degree of the data. For a highly efficient training, it is necessary to have a large number of training data that are strongly correlated. If it is not possible to create or to obtain a training database with a large number of training data, a smaller database with highly correlated data can also be used. The correlation criteria is the most important, an evidence being matrix (7).

To obtain an increase in the estimation accuracy, periodically introducing new training data into the training database is recommended, to improve the database. A re-training of the neural network with the new database is required, for the changes to take effect.

The method of estimating the octane number using neural networks can be used in optimization algorithms to determine the blend composition, so that the octane number condition is met, fulfilling in the same time the refinery needs related to components cost and availability.

The neural networks can be used also to estimate other properties of blending gasoline: vapour pressure, density, etc. The data required by the neural network, in this case, will be the components properties, as input data and the gasoline properties which need to be estimated as output data. It is also required to create a new database, which contains the necessary data for the neural network training. The procedure for the creation, training and using the neural network remains identical.

References

1.*** Industrial Engineering Chemistry, 1927. **19**: p. 145;
2.*** ASTM D2699. (http://www.astm.org/Standards/D2699.htm).
3.ALBAHRI, T.A., Structural Group Contribution Method for Predicting the Octane Number of Pure Hydrocarbons and Their Mixtures. Fuel Chemistry Division Preprints, 2002. **47**(2): p. 531-532.
4.CHORNG, H. T., COON, J.E., A Generalized Interaction Method for the Prediction of Octane Numbers for Gasoline Blends. 1998.
5.FLECHER, P. E., et al., Determination of Octane Numbers and Reid Vapour Pressure in Commercial Gasoline Using Dispersive Fiber-Optic Raman Spectroscopy. Spectrochimica Acta Part A, 1997. **53**: p. 199-206.
6.MORRIS, W.E., Optimum Blending Gives Best Pool Octane. Oil& Gas Journal, 1986.
7.KUMAR, K., THAKUR, G.S.M., Advanced Applications of Neural Networks and Artificial Intelligence: A Review. Information Technology and Computer Science, 2012. **6**: p. 57-68.
8.DOICIN, B., ONUTU, I., STANICA-EZEANU, D. Provocari si Tendinte in Fabricarea Benzinelor Auto Comerciale. Simpozionul International “Proprietatile Chimiei Pentru o Dezvoltare Durabila”, Bucuresti, 2012.
9.TRIVELLA, F., ALBERTI, A., BRAMBILLA, A., Estimation of Gasoline Octane Number From A Catalytic Reformer Using Artificial Neural Networks. Artificial Intelligence in the Petroleum Industry, 1995: p. 323-328.
10.PASADAKIS, N., GAGANIS, V., FOTEINOPOULOS, C. Octane number prediction for gasoline blends. Fuel Processing Technology, 2006(2006): p. 505-509.
11.MEUSINGER, R. Determination of Octane Numbers of Gasoline Compounds From Their Chemical Structure by C13 NMR Spectroscopy and Neural Networks. Fuel, 2001. **80**: p. 613-621.
12.LIU, M.Y. et al., Determination of Octane Number of Gasoline by Double ANN Algorithm Combined With Multidimensional Gas Chromatography. Sixth International Conference on Natural Computation (ICNC), 2010. **3**: p. 1640-1642.
13.VAN LEEUWEN, J.A., JONKER, R.J., GILL, R Octane number prediction based on gas chromatographic analysis with non-linear regression techniques. Chemometrics and Intelligent Laboratory Systems, 1994. **25**(1994): p. 325-340.
14.PARANGHOOSHI, E., SADEGHI, M.T., SHAFIEI, S. Prediction of Octane Number and Additives for Gasoline Blends Using Artificial Neural Networks. 6th International Congress on Chemical Engineering, 2011.
15.*** MathWorks. (http://www.mathworks.com/).
16.*** IROX 2000 Gasoline Analyzer. (http://www.grabner-instruments.com/products/fuelanalysis/irox2000.aspx)

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