Estimating Ternary Blends Properties using ANNs Trained with Binary Blends

STEFAN SANDRU*, ION ONUTU

Petroleum-Gas University of Ploiesti, Department of Petroleum Engineering and Environmental Protection,39 Bucharest Blvd., 100520, Ploiesti, Romania

The present study aimed to estimate the physical properties of the diesel-diesel-biodiesel ternary blends, using artificial neural networks, also known as ANNs. The input data used to estimate the properties was the percentage in which each component was used to obtain the blend. Using two hydrofined diesel fuels from a local refinery and three biodiesel samples synthesized in the university laboratory, a total of 114 blends, both binary and ternary, were obtained. The ANN training database was comprised of exclusively 96 binary blends, from the total of 114. The predictions were made on the remaining 18 ternary blends. All the predictions were within the error mentioned in the standard, concluding the fact that the created ANNs had a rate of 100% accuracy.

Keywords: diesel-biodiesel blends, artificial neural network estimation

The artificial neural networks are best known for their uses in estimation, whether it is a fuels chemical and physical property or an engine's fuel consumption or emissions. The neural networks are an alternative to experimental testing because the estimation process takes a lot less time and it is a lot cheaper than the actual test. One of the biggest advantages of the neural networks is their random and evolutive character, which allows them to explore new solutions at each run. One of the few disadvantages that ANNs have is the large database required for training.

Doicin, B. et al. used ANN to estimate the octane number of the gasoline blends. Their ANN had 4 inputs with 2 outputs and it was trained using the Levenberg-Marquardt algorithm. Following the training of the network and after analyzing the regression plots and error histogram it was concluded that the network created was viable, which was proven by the accuracy of the returned results [1]. Artificial neural networks were also used by Matei, D. et al. to predict the performance of the Pd/SBA-15 catalyst in order to maximize the production of hydrogen by the steam reforming of the ethanol [2]. The study conducted by Aminian, A. and ZareNezhad, B. compared four prediction algorithms, in order to find the most suitable algorithm for the estimation of biodiesel viscosity. The authors compared SVM (Support Vector Machine), ANFIS (Adaptive Neuro Fuzzy Inference System) and ANN optimized using GA (Genetic Algorithm) and SA (Simulated Annealing). The best results were given by the ANN trained with Levenberg-Marquardt and optimized with GA [3]. Menon, P.R., and Krishnasamy, A. used both artificial neural networks and genetic algorithm to predict and optimize the characteristics of the biodiesel fueled engine. Using the models provided by the ANN, the authors reduced the extensive engine experiments. The ANN had a high regression coefficient, above 0.9, and less than 10% absolute error. Using both the GA and the ANN, the study also optimized the biodiesel composition [4].

In the study conducted by Kshirsagar, C.M. et al., neural networks were used to predict the output parameters of a Diesel engine, when it uses biodiesel synthesized from Calophyllum inophyllum. Tests were run at 5 different parameters in order to obtain the necessary data for the training database. The ANN predicted, with great accuracy the performance parameters as well as the emission parameters [5]. In order to determine the cetane number, a special engine is required and 700 mL of sample. Because of this, Kessler, T. et al. decided to develop an ANN with the purpose of predicting the cetane number for furan biodiesel additives. The authors also improved an existing model, using ANN, generalizing the model [6]. Using the values returned by the Diesel-RK software, Salam, S., and Verma, T.N. trained the ANN to estimate the engines combustion, performance and emissions. The results were satisfying, all errors falling within the required limits [7]. Ganesan, P. et al. used ANN to predict the performance and emissions of a diesel electric generator. The training database included the generator parameters: the capacity of the engine, the speed and torque. Analyzing the prediction, it was concluded that the developed ANN had a good accuracy [8]. ANN was used alongside GA by Taghavifar, H. et al. to investigate the behavior of fuel spraying in the engine. The experimental data was collected using CFD (Computational Fluid Dynamics) extrapolation. A correlation coefficient of 0.994 was obtained during the training of the ANN with the Levenberg-Marquardt algorithm. After applying the genetic algorithms, the correlation coefficient increased to 0.999 [9]. Hosseini, S.M. et al. compared in their study the ANN with a semi-theoretical model. The semi-theoretical model used rough hard-sphere theory for the correlation and prediction of dynamic viscosities. The neural network had multilayer perceptron comprising of one hidden layer. The performance of both semi-theoretical and ANN model was checked by predicting dynamic viscosities over the temperature range within 283–393 K and pressures up to 140 MPa with the average absolute relative deviation of 3.10% (for 648 data points) and 0.91% (for 796 data points), respectively. The ANN model developed herein, has been trained, validated and tested for the set of data gathered, pointing that the efficiency of the neural network model was found excellent on the entire dataset [10].

Experimental part

Obtaining the binary (diesel-biodiesel; diesel-diesel) blends

The three biodiesel samples used in this study were synthesized in the laboratory using two different mixing

* email: sandru0318@gmail.com

methods: mechanical stirring and ultrasound blending. The parameters used for the biodiesel production were:

-methanol to rapeseed oil molar ratio was 3.7:1, to which 2 g of basic catalyst, namely KOH, were added;

-the mixing time was:

-2 h for mechanical stirring;

-15 min for ultrasound blending at 37 kHz, with 100 W power;

-30 min for ultrasound blending at 80 kHz, with 100 W power.

The hydrofined diesel samples used in this study were received from the local refinery.

Using the two hydrofined diesel along with the three biodiesel samples, 96 binary blends were obtained as follows:

-each diesel type was blended with each biodiesel type having the following biodiesel concentrations: 0% (pure diesel), 1%, 3%, 6%, 9%, 12%, 15%, 18%, 20%, 30%, 50%, 70%, 80%, 100% (pure biodiesel).

-the two hydrofined diesel types were also blended with one another in the following concentrations: 0%, 1%, 3%, 6%, 9%, 12%, 15%, 18%, 20%, 30%, 50%, 70%, 80%, 82%, 85%, 88%, 91%, 94%, 97%, 99%, 100%.

The 18 blends on which the ANN was tested are a simulation of the real-world diesel fuel blends, from the percentage point of view. Hence the database used for training the ANN also has diesel-diesel blends.

Two physical properties were chosen to be evaluated and tested with the ANN:

-relative density at 20 °C, the pycnometer method according to STAS 35-73;

-kinematic viscosity at 40 °C (cSt), using the Ubbelohde type viscometer according to EN ISO 3104;

The 18 new blends, on which the ANN was tested are presented in table 1. The values presented in the table are in volume percentage.

Creating and training the Artificial Neural Network

Using the Neural Network Fitting Tool, a sub-application of the larger Matlab 2017b [11] software, two neural networks were created, one for each property. In figure 1 the structure of the two ANNs used in this study is presented. It is a two-layer feed-forward network that has 5 inputs, 10 neurons in the sigmoid hidden layer, 1 linear output neuron and 1 output.

The training database, comprised of 96 binary blends, was divided randomly:

-70% of the 96 blends were used for training the ANN;

-15% of the remaining 30%, were used to measure network generalization and to halt training when generalization stops improving;

-the last 15% was used for testing, in order to provide an independent measure of network performance during and after training. These values did not affect the overall performance of the ANN.

The neurons number will determine the networks complexity. If we work with a small number of neurons the network will not explore all the possibilities. Then again, if we choose a higher number of neurons than needed, a phenomenon called overtraining will appear and the correlation between variables will not be accurate. In order to choose the right training algorithm and number of neurons, all three training algorithms were tested

| Sample number	Diesel 1	Diesel 2	Biodiesel-mechanical stirring	Biodiesel-ultrasound 37 kHz	Biodiesel-ultrasound 80 kHz
1	20	79	1	—	—
2	30	67	3	—	—
3	40	54	6	—	—
4	50	41	9	—	—
5	60	28	12	—	—
6	70	15	15	—	—
7	20	79	—	1	—
8	30	67	—	3	—
9	40	54	—	6	—
10	50	41	—	9	—
11	60	28	—	12	—
12	70	15	—	15	—
13	20	79	—	—	1
14	30	67	—	—	3
15	40	54	—	—	6
16	50	41	—	—	9
17	60	28	—	—	12
18	70	15	—	—	15

Table 1
TESTING BLENDS
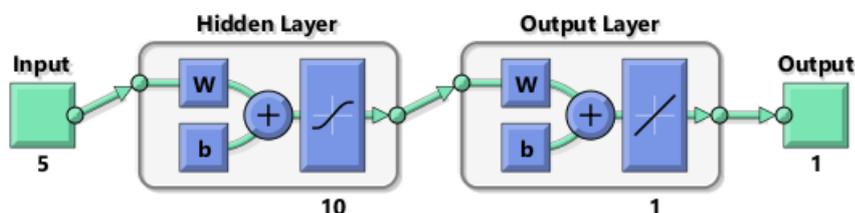
Fig. 1. Neural network structure

(Levenberg-Marquardt, Bayesian Regularization and Scaled Conjugate Gradient) with different neurons numbers.

To analyze the performance of the neural network, we have two options: the correlation coefficient R and the Error Histogram. The correlation coefficient R takes values between [0,1]. The closer R gets to 1, the stronger is the correlation between variables. If R is closer to 0, or even equal to 0, there is no correlation at all between the variables. The Histogram Error indicates the error in which the predictions returned by the ANN should fit.

In this study the error defined by the standards was used, not the error given by the Histogram Error, since the two might be different and the purpose is to evaluate the ANN according to the standard after which the determinations were made.

Results and discussions

The properties of the five types of fuel used in this study are presented in table 2.

Creating the ANN for the relative density at 20 °C

Using the Levenberg-Marquardt training algorithm with 10 neurons, the artificial neural network corresponding to relative density at 20 °C was created. The regression plots and correlation coefficient R can be found in figure 2.

Judging by the correlation coefficients and the way the points are fitted on the diagonal line, it can be said the ANN found a strong correlation between the variables.

Creating the ANN for kinematic viscosity at 40 °C

Using the same parameters as before, Levenberg-Marquardt with 10 neurons, the ANN for kinematic viscosity at 40 °C was created. The regression plots are illustrated in figure 3.

Figure 3 shows us a very good ANN, with a high correlation coefficient.

The predictions returned by the ANNs will be presented in tables. The errors used in evaluating the ANNs are taken from the standard used to determine the property, not the ones given by the neural network, since they might not be the same. The estimation might fit the neural network error, but not the error given by the standard, hence, the estimation did not meet the requirements.

Estimating relative density at 20 °C

The predictions for relative density are presented in table 3. An error of d"0.002 was chosen, according to the standard. As it can be seen, the artificial neural network had an accuracy of 100%, since all the predictions fell within the given error.

Estimating kinetic viscosity at 40 °C

The results returned by the ANN are presented in table 4. The chosen error was d"0.1, according to the standard. The values were rounded up to 1 decimal, to match the values in the standard, all the calculations being made in Excel. For example, for the first sample, the actual values are: First prediction: 2.52, Second prediction: 2.46; Average: 2.49, the Average being rounded up at 2.5. All the values fall within the error given by the standard.

Table 2
PHYSICAL PROPERTIES OF THE SAMPLES

| Test	Test method	Unit	Diesel 1	Diesel 2	Biodiesel-mechanical stirring	Biodiesel-ultrasound 37 kHz	Biodiesel-ultrasound 80 kHz
Relative density at 20 °C	STAS 35-73	-	0.838	0.837	0.883	0.885	0.883
Kinematic viscosity at 40 °C	EN ISO 3104	cSt	2.8	2.5	4.5	4.6	4.6
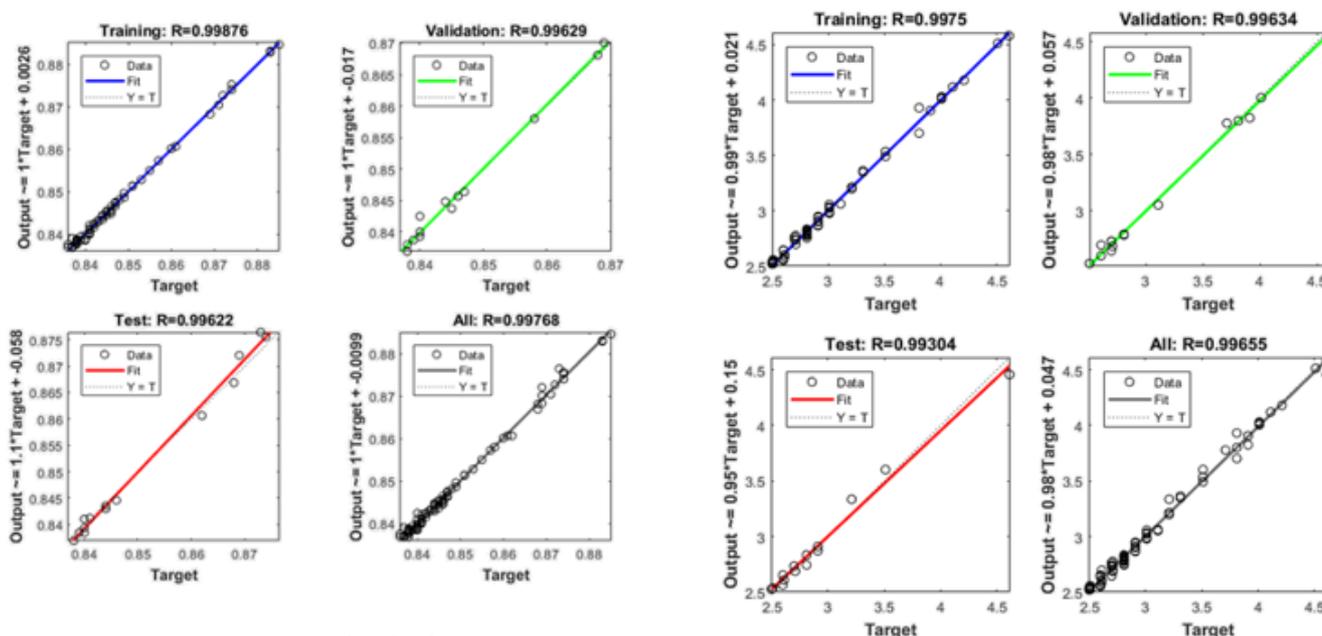
Fig. 2. Regression plots for density
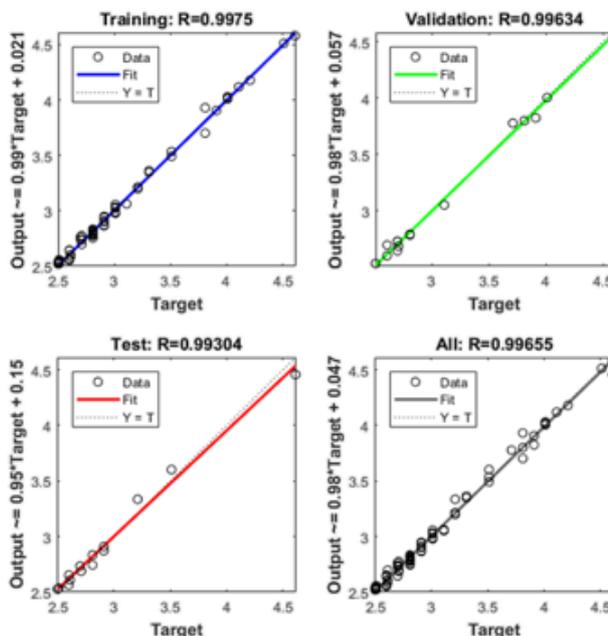
Fig. 3. Regression plots for viscosity

Sample number	First prediction	Second prediction	Average	Experimental values	Difference
1	0.838	0.838	0.838	0.839	0.001
2	0.840	0.839	0.840	0.841	0.001
3	0.842	0.840	0.841	0.841	0.000
4	0.843	0.841	0.842	0.842	0.000
5	0.844	0.843	0.844	0.845	0.001
6	0.845	0.844	0.845	0.846	0.001
7	0.838	0.838	0.838	0.839	0.001
8	0.839	0.839	0.839	0.840	0.001
9	0.840	0.840	0.840	0.842	0.002
10	0.841	0.841	0.841	0.843	0.002
11	0.842	0.844	0.843	0.845	0.002
12	0.844	0.844	0.844	0.845	0.001
13	0.837	0.838	0.838	0.838	0.000
14	0.839	0.839	0.839	0.840	0.001
15	0.840	0.840	0.840	0.842	0.002
16	0.841	0.841	0.841	0.843	0.002
17	0.844	0.846	0.845	0.847	0.002
18	0.845	0.844	0.845	0.846	0.001

Table 3
ESTIMATION RESULTS FOR DENSITY

Sample number	First prediction	Second prediction	Average	Experimental values	Difference
1	2.6	2.5	2.5	2.5	0.0
2	2.6	2.6	2.6	2.6	0.0
3	2.7	2.7	2.7	2.7	0.0
4	2.7	2.8	2.7	2.8	0.1
5	2.8	2.8	2.8	2.8	0.0
6	2.9	2.9	2.9	2.9	0.0
7	2.6	2.6	2.6	2.6	0.0
8	2.6	2.6	2.6	2.6	0.0
9	2.6	2.7	2.7	2.7	0.0
10	2.7	2.8	2.7	2.8	0.1
11	2.8	2.9	2.8	2.9	0.1
12	2.9	2.9	2.9	2.9	0.0
13	2.6	2.6	2.6	2.6	0.0
14	2.7	2.6	2.6	2.6	0.0
15	2.7	2.7	2.7	2.7	0.0
16	2.7	2.8	2.8	2.8	0.0
17	2.8	2.8	2.8	2.8	0.0
18	2.9	2.9	2.9	2.9	0.0

Table 4
ESTIMATION RESULTS FOR VISCOSITY

Conclusions

The aim of this study was to predict the physical properties of ternary blends, using artificial neural networks (ANNs) trained only with binary blends. In this paper 2 types of hydrofined diesel fuel, received from a local refinery and 3 types of biodiesel synthesized in university laboratory were used to obtain a total of 114 blends. 96 were binary blends, from which 77 blends were between diesel and biodiesel and 19 blends were between the 2 hydrofined diesel fuels. The remaining 18 ternary blends, used for prediction, are a simulation of the real-world blends where the diesel fuels have the majority in a blend, whereas the biodiesel is found in a low percentage, only up to 15%.

The predictions made using the ANN created in this study, returned flawless results, with an accuracy of 100%.

References

1. DOICIN, B., ONUTU, I., Rev. Chim. (Bucharest), **65**, no. 5, 2014, p. 559
2.MATEI, D., DOICIN, B., CURSARU, D.L., Digest Journal of Nanomaterials and Biostructures, **11**, no. 2, 2016, p. 443
3. AMINIAN, A., ZARENEZHAD, B., Renewable Energy, **120**, 2018, p. 488
4. MENON, P.R., KRISHNASAMY, A., Energy and Fuels, **32**, no.11, 2018, p. 11607
5. KSHIRSAGAR, C.M., ANAND, R., Applied Energy, **189**, 2017, p. 555
6. KESSLER, T., SACIA, E.R., BELL, A.T., MACK, J.H., Fuel, **206**, 2017, p. 171
7. SALAM, S., VERMA, T.N., Energy Conversion and Management, **180**, 2019, p. 496
8.GANESAN, P., RAJAKARUNAKARAN, S., THIRUGNANASAMBANDAM, M., DEVARAJ, D., Energy, **83**, 2015, p. 115
9. TAGHAVIFAR, H., KHALILARYA, S., JAFARMADAR, S., Energy, **71**, 2014, p. 656
10. HOSSEINI, S.M., PIERANTOZZI, M., MOGHADASI, J., Fuel, **235**, 2019, p. 1083
11.***https://www.mathworks.com/products/deep-learning.html; last accesed: December 2018