



Estimation of Total Organic Carbon in Source Rocks by Using Back-Propagation Artificial Neural Network and Passay Method-A Case Study

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ARTICLE INFO	ABSTRACT
<p>Article History: Received: 31 December 2019 Revised: 17 May 2021 Accepted: 18 May 2021</p> <p>Article type: Research</p> <p>Keywords: Levenberg–Marquardt Training Algorithm, Multi-layer Perceptron, Organic Carbon (TOC), Petrophysical Logs, Total Passay Method</p>	<p>The purpose of this study is to calculate Total Organic Carbon (TOC) values of the Iranian field using a combination of sonic and resistivity logs (Passay method) and neural networks method in the conditions where the core analysis or well-log measurement does not exist. We compared the resultant TOC with the ones obtained from the geochemical analysis. To correlate between the total organic carbon data and petrophysical log, which are available after logging, Multilayer Perceptron Artificial Neural Network is used. After analyzing 100 cutting samples by using rock -Eval pyrolysis, geochemical parameters have achieved. By using the multi-layer perceptron with Levenberg–Marquardt training algorithm, the TOC with correlation coefficient 0.88 and MSE 1.443 have been provided in the intervals without analyzed samples. Finally, the TOC was estimated by using separation of resistivity and the sonic log, although, with the favorable results in some other fields, the estimation had a correlation Coefficient of 51% in this field. Comparing the performance of the multi-layer perceptron with Levenberg–Marquardt training algorithm (with an accuracy of 88%) and results of the Passay method (with an accuracy of 51%) indicated that the neural network is more accurate and has better consistency compared with the empirical formula.</p>

Introduction

Source rocks, commonly shale and limestone, contain significant amounts of organic matter [1]. Detection of organic matter by using logging tools. Based on physical characteristics of source rock, including lower density, slower sonic velocity or higher sonic transit time, frequently higher uranium content, higher resistivity, and higher hydrogen and carbon concentrations, they are distinguishable from surrounding rocks. Therefore, the logs used for source rock evaluations are density, sonic, gamma-ray, neutron, and resistivity [2]. In source rock, evaluation of three main characteristics is used to detect the petroleum potential of the formation: the amount of rock organic matter, quality of organic matter, and degree of maturity

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of its organic content. The quantity of organic matter is called total organic carbon (TOC). The capability of the source rock to generate petroleum is determined by (the percentage of hydrogen and TOC quantity of kerogen [3]). To determine the -mentioned characteristics, geochemical analysis is used. By considering, the log data can be taken at low intervals so that they can be considered as continuous data from oil wells. Sampling operations are done on drilling cuttings of every well at intervals more than 5 m, relevant geochemical experiments were performed on the samples. Hence, there are some intervals between checkpoints that remain unanalyzed. Local studies are expensive and time-consuming, and there is the possibility of losing rich samples or sampling poor and ineffective layers. Therefore, researchers have tried to find a quantitative and qualitative relationship between TOC content and logging data.

Given the low density of the organic carbon (~ 1.0-1.4 g/cc), the presence of TOC in the formation affects several physical properties. For instance, high TOC leads to a reduction in the bulk density of the formation. Given the TOC presence, source rock intervals generally show apparent high resistivity in comparison with non-source rock intervals. In other words, organic matters are not electrically conductive. Besides, high TOC content in a formation leads to an increase in gamma-ray due to the radioactive material contamination (e.g. Uranium). Furthermore, the transit time increases, and consequently, the acoustic velocity decreases by the high presence of TOC [4].

The TOC is measured in the laboratory by using pyrolysis, microscopy, and pyrolysis-gas chromatography methods. However, in several studies, new methods have been developed to estimate the TOC from well logs, because of the availability of logs compared to core samples. Moreover, the continuous recording leads to eliminating the statistical uncertainties of limited sampling [2-7]. The construction of the TOC log also allows for rapid identification and classification of potential organic-rich zones, determination of zones that should be sampled for specialized geochemical analysis allowing for a determination of the TOC vertical distribution in the formation as an input to basin evaluation models [8].

An artificial neural network (ANN) is a computing machine that is inspired by biological neural networks. The ANN training is based on some input data, the result of the input data, and finding a logical connection among them. Then, the ANN can predict the results of any given input data. Generally, they are comprised of neurons, connections, weights, and propagation functions. Nowadays, ANN is attributed as an efficient approach to predict complex industries, including; data handling, electronic, civil engineering, and mechanic engineering.

For example, ANN used to establish a combination of process input parameters to maximize material removal rate (MRR) and minimize surface roughness (SR) and tool wear rate (TWR) [9], and find the best result for shear stress and vertical strain and behavior of rubbers [10], to achieve o earthquake parameters [11], and to decrease the number of required computation steps for searching process on sparse datasets [12].

In this research, the authors tried to find a prediction model to estimate the TOC in Source Rocks by using the back-propagation ANN and Passay method.

Alizadeh et al. [13] tried to predict the total organic carbon (TOC) content of the source rock by using probabilistic neural networks and seismic markers. They used well logs and 3D-seismic data not only to detect hydrocarbon reservoirs but also to evaluate the geochemical parameters.

Total Organic Carbon

The TOC is the amount of organic carbon in source rock expressed as a percentage by weight. There are three methods for measuring and estimating the TOC. In the first method,

direct measurements in the laboratory are used. In the second method, direct measurement using a well logging tool is implemented. The last one is based on the estimation by the neural network method [14]. Two widely used empirical approaches have been developed to estimate the TOC from the logging data quantitatively. The first was developed in Devonian shale using bulk density logs and was later refined in the Bakken shale [3, 6, 15]. Based on the response of the bulk density measurement to low-density organic matter ($\sim 1.0 \text{ g/cm}^3$), the Schmoker's method [3] computes TOC as follows:

$$TOC\% = \frac{154.497}{\rho_b} - 57.261 \quad (1)$$

where ρ_b is the bulk density (g/cm^3), and the TOC is reported in the weight percentage. This equation assumes a constant mineral composition and porosity in the formation. Although the method was developed and refined based on specific environments, it is often used for the TOC estimation in various shale formations. The second method used in this research was performed based on a method introduced by Passey et al. [16]. In this method, two sonic and resistivity logs were implemented. When we have fine-grain and non-source rocks, these two logs are matched together to show the baseline. Every deviation from the baseline represents organic matter-rich intervals. The deviation can be measured by $\Delta \log R$ formula at each depth.

$$\Delta \log R = \log \left(\frac{R}{R_{baseline}} \right) + 0.02 \times (\Delta t - \Delta t_{baseline}) \quad (2)$$

where R is resistivity measured in $\Omega \text{ m}$ by the logging tool, $\Delta \log R$ is curve separation measured in logarithmic resistivity cycles, $\Delta t_{baseline}$ is the transit time when the curves are baseline in non-source rocks, $R_{baseline}$ is resistivity corresponding to $\Delta T_{baseline}$ value, and Δt is the measure transit time in $\mu\text{S.ft}^{-1}$.

The deviation of $\Delta \log R$ relates to the TOC and is a function of maturity. The level of organic maturity (LOM) is calculated by analysis of different samples (vitrinite reflectance, thermal alteration index, and T_{max}) or by estimating burial and thermal history. The formula used for calculating $\Delta \log R$ by sonic and resistivity logs is:

Exxon used the following empirical formula to calculate TOC in organic-rich source rocks from $\Delta \log R$.

$$TOC \% = (\Delta \log R) \times 10^{(2.297 - 0.1688 \times LOM)} \quad (3)$$

In Eq. 3, the TOC is in weight percentage. The LOM is the level of maturity in which $LOM = 7$ corresponds to the early maturity of kerogen type I and $LOM = 8-9$ corresponds to the maturity of kerogen type II [16].

Rock-Eval Pyrolysis

Rock-Eval pyrolysis provides information on the quantity, type, and thermal maturity of the organic matter. Pyrolysis is a widely used degradation technique that allows breaking complex subsidence into fragments by heating it under an inert atmosphere. Rock-Eval data are expressed in mg/g of rock and contain four basic parameters [17]:

- 1) S_1 represents the quantity of free hydrocarbons in the rock and is roughly analogous to the solvent extractable portion of the organic matter.
- 2) S_2 represents the number of hydrocarbons released by the kerogen in the sample during pyrolysis.
- 3) S_3 is related to the amount of oxygen present in the kerogen.
- 4) T_{max} is the temperature in which the maximum rate of generation (of the S_2 peak) occurs and can be used to estimate thermal maturity.

In addition, the ratio of S_2/S_3 gives a general indication of kerogen quality (type) and reveals whether oil or gas is likely to be generated. The ratio of $S_1/(S_1+S_2)$, or the productivity index (PI), is an indication of the relative amount of free hydrocarbons (in place or migrated) that exists in the sample. PI increases with maturity, from near zero for immature source rock to 0.15 in post-mature one. Hydrogen index (HI) and oxygen Index (OI) values are expressed in mg of hydrocarbons (S_2 peak) or carbon dioxide (S_3 peak) per gram of organic carbon. When they are plotted versus each other on a Van Krevelen-type diagram, information on kerogen type and maturity can be acquired. Potential yield indicates the produced yield of hydrocarbon from source rock at optimum maturity that exhibits a measure of the quality of source rock.

The Multilayer Perceptron Neural Network

A neural network is inspired by human biology. Each neural network is composed of a set of neurons connected with some neurons in the network. It receives a signal from other neurons and transforms to outside using a transfer function. The multilayer perceptron (MLP) is a feed-forward artificial neural network. The MLP is composed of a set of layers that the first one is called the input layer, while the last one is called the output layer. A set of layers between these two layers are called hidden layers. It is shown that one hidden layer is enough for better approximations and the neural network will react better [18]. The MLP uses the supervised learning mode where both input and desired output are available. The MLP is a feed-forward network consisting of units arranged in layers, with only forward connections to units in subsequent layers. The connections have weights associated with them. Each signal traveling along a link is multiplied by its weight. The input layer, which is the first layer, has input units that distribute the inputs to units in subsequent layers. In the following (hidden) layer, each unit sums its inputs and adds a threshold. Afterward, the resultant nonlinearly transforms the sum, known as called the net function, to produce the unit output, called the activation. The output layer units often have linear activations, so output activations equal the net function values. The units in the hidden layers are called hidden units [19, 20].

Many training algorithms have been developed and the Back-propagation is one of the classical algorithms [18]. Traditional back propagation algorithms have some drawbacks, such as being stuck into local minimum and low convergence speed. The Levenberg Marquardt training algorithm comes to resolve these ambiguities. The Levenberg Marquardt (LM) training algorithm approximates Newton's method for the ANN. The LM technique is the best algorithm for optimization problems applied to the ANN [21].

Materials and Methods

In this study, two wells from one of the southern Iranian fields were selected to measure the amount of the TOC. After running appropriate logs, potential source rock zones have been identified based on petrophysical data. Based on the obtained results, the TOC was computed by the $\Delta \log R$ method. Afterward, the computed TOC was compared with calculated TOC by using Rock-Eval 6 and neural networks the schematic of the total organic matter of analyzed rocks shown in (Fig 1).

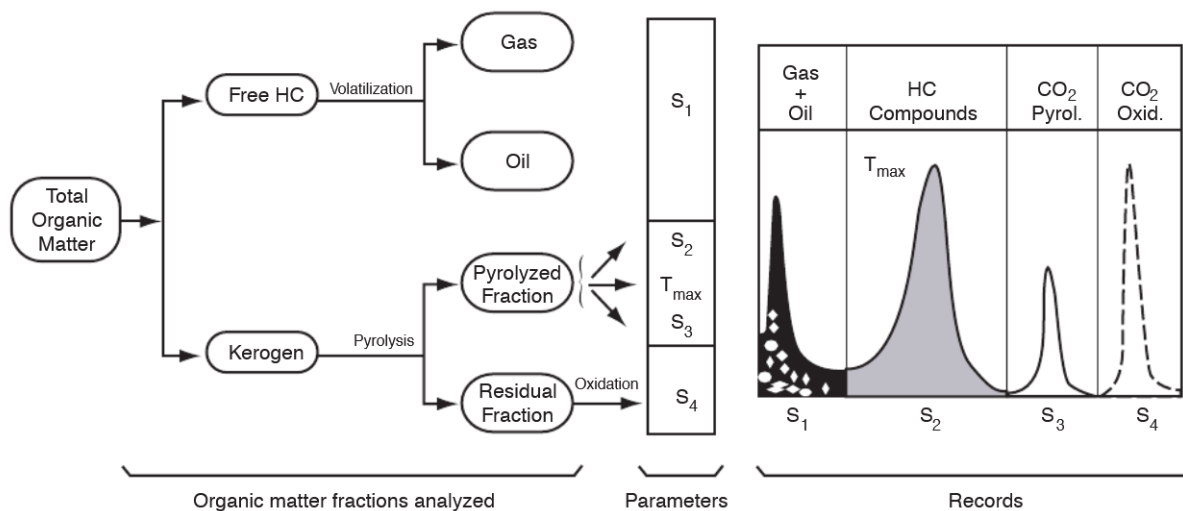


Fig. 1. the schematic of the total organic matter of analyzed rocks [22]

In this study, we used MATLAB software version 2012-b and its neural network functions. Mean square error (MSE) was considered as a network performance function. To increase the efficiency of the neural network model, a sensitivity analysis was conducted on the number of neurons in the network. The results of the sensitivity analysis on the number of hidden neurons are shown in Table 1. Based on Table 1, the best performance of a three-layer neural network is nine neurons in the hidden layer. To find the best training function in a neural network, a sensitivity analysis was performed. The results of the sensitivity analysis are shown in Table 2. As can be seen in Table 2, the best performance among neural network training functions (algorithms) to adjust weights and biases is Levenberg-Marquardt (training). The Levenberg-Marquardt training algorithm comes to resolve back-propagation problems.

Table 1. Sensitivity analysis on the number of hidden neurons

Number of hidden neurons	Mean square Error	R ²
1	8.4717	0.6789
3	7.0043	0.7015
5	4.9411	0.7845
7	6.1213	0.7548
9	1.6124	0.8035
11	3.0015	0.7957
13	6.8974	0.7011

Table 2. Sensitivity analysis on the type of training function

Training function	MSE
Batch gradient descent(traingd)	14.11
Variable Learning Rate (traingda)	9.82
Variable Learning Rate (traingdx)	7.74
Batch Gradient Descent with Momentum (traingdm)	12.32
Levenberg- Marquardt (trainlm)	5.12

The three-layer structure, which contains an input layer, a hidden layer and an output layer, consists of 8 neurons in the input layer, include spectral gamma ray (SGR), corrected gamma ray (CGR), neutron porosity (NPHI), sonic log (DT), density log (RHOB), resistivity of later log deep (RLLD), Photoelectric absorption properties log (PEF), and total porosity logs, 9 neurons in the hidden layer, and one neuron in the output layer, which contains TOC data. Also, the Tan-Sigmoid transfer function is considered between the input and hidden layers. The purlin linear transfer function is considered between the hidden and the output layers (Fig. 2).

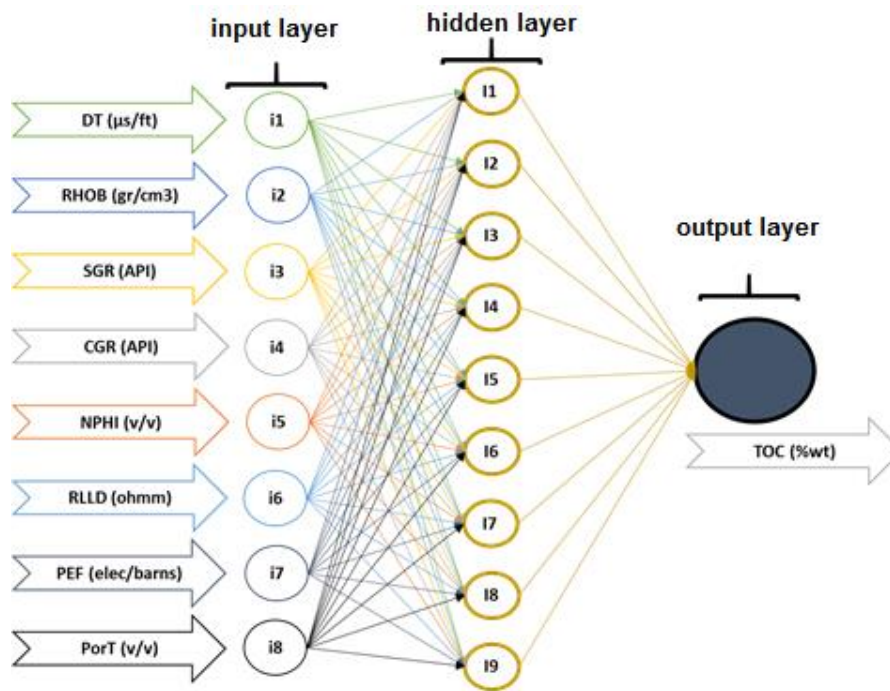


Fig. 2. MLP with Levenberg–Marquardt training algorithm Structure

Results and Discussion

The TOC includes kerogen and bitumen, which may occur together in petroleum source rocks and represent organic matter in a rock sample. Generally, source rocks have a minimum of 1.0 wt. percentage TOC contents. To generate petroleum, the carbon needs to be associated with hydrogen in source rock. The amount of hydrocarbon produced during pyrolysis (S_2) is a useful parameter for the evaluation of the source rock potential. A freed amount of S_2 during the pyrolysis less than 4.0 mg HC/g rock indicates a source rock having a low hydrocarbonization potential, whereas higher amounts exhibit a high source rock hydrocarbonization potential [23].

In this section, the first part discusses the Rock-Eval analysis and calculation of S_1 , S_2 , TOC, and HI parameters. The next part is devoted to investigating the efficiency of the method developed by Passay et al. and the inspection of the results obtained using ANN.

Evaluation of Hydrocarbonization Potential

To study the hydrocarbonization potential, first, the S_1 , S_2 and TOC amounts produced from the rock-eval pyrolysis of the samples were compared with the normal values [23]. For this objective, the aforementioned parameters were plotted in the hydrocarbonization potential diagram (Fig. 3). The diagram plots the changes of S_1+S_2 versus the TOC. According to the hydrocarbonization potential diagram, all studied samples had high and very high hydrocarbonization potentials.

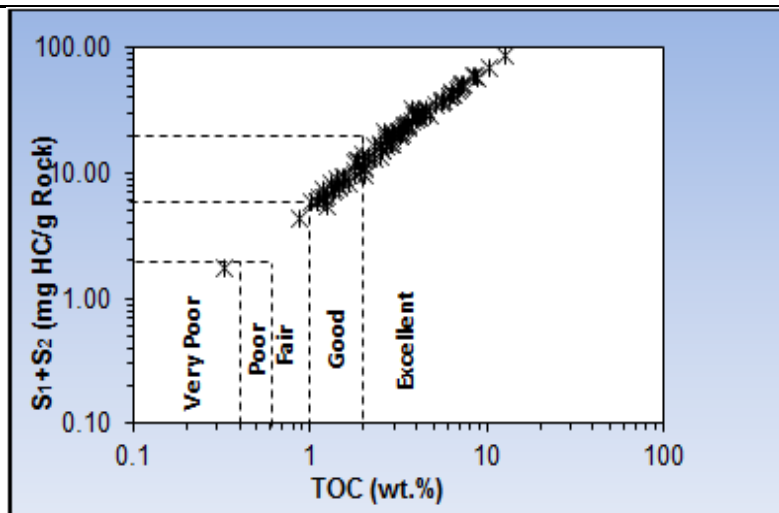


Fig. 3. S1 + S2 vs. TOC, showing Hydrocarbon Potential Evaluation

Determination of Kerogen Type and Maturation of Organic Matter

The S_2 versus TOC diagrams were used to determine the kerogen type. Plotting the points on the diagram indicated that most of the samples belong to the range of kerogen type II (Fig. 4).

Among different parameters derived from the pyrolysis, the T_{max} index reveals the thermal maturity of organic matter. T_{max} is directly proportional to the depth and thermal maturity degree of kerogen. The hydrogen index (HI), the TOC/ S_2 ratio, is a key source rock variable used in quantitative modeling of volumetric and phased extraction of the hydrocarbons. Besides, the HI also defines the kerogen type. The diagram of hydrogen index (HI) versus T_{max} is utilized to determine the organic compounds of the source rock.

Furthermore, the graph is functional for evaluating the thermal maturity of the source rocks. As Fig. 5 demonstrates, by sketching the diagram, it could be deduced that the organic compounds of the studied formation take place in the range of type II kerogen. Moreover, the points clarify that from the thermal maturity point of view, the hydrocarbons are immature and belong to the beginning of the oil window.

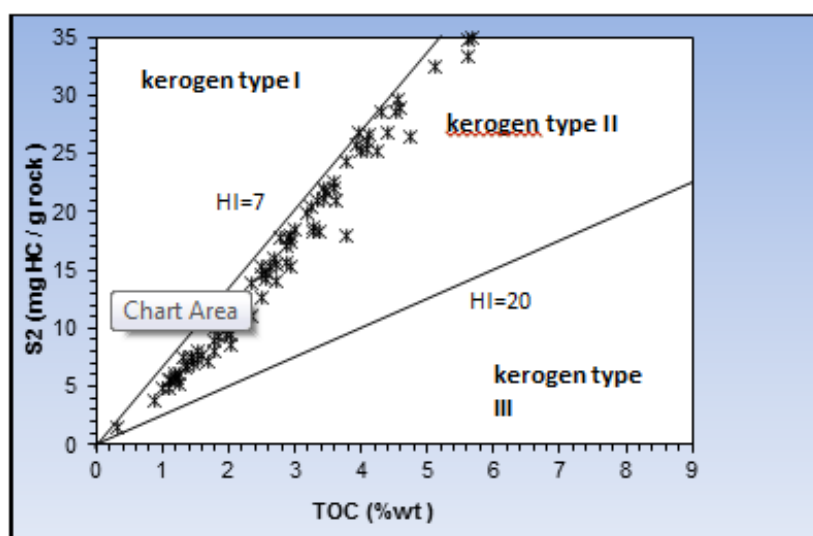


Fig. 4. S2 vs. TOC, showing the type of kerogen [24]

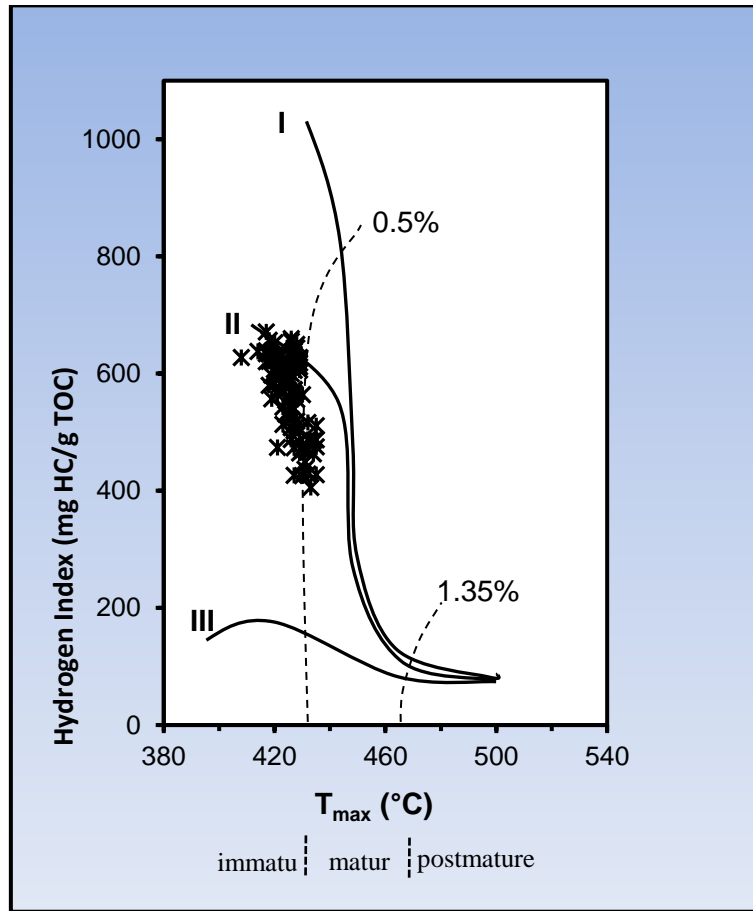


Fig. 5. Determination of thermal maturity and formation's kerogen type by the aid of HI and T_{max} [24]

To assess the generation potential and the hydrocarbon type, the diagram of hydrogen index (HI) plotted against TOC (Fig. 6) was used. By plotting the points of the diagram, it was understood that the formation lies in the oil zone, exhibiting high and very high production potentials.

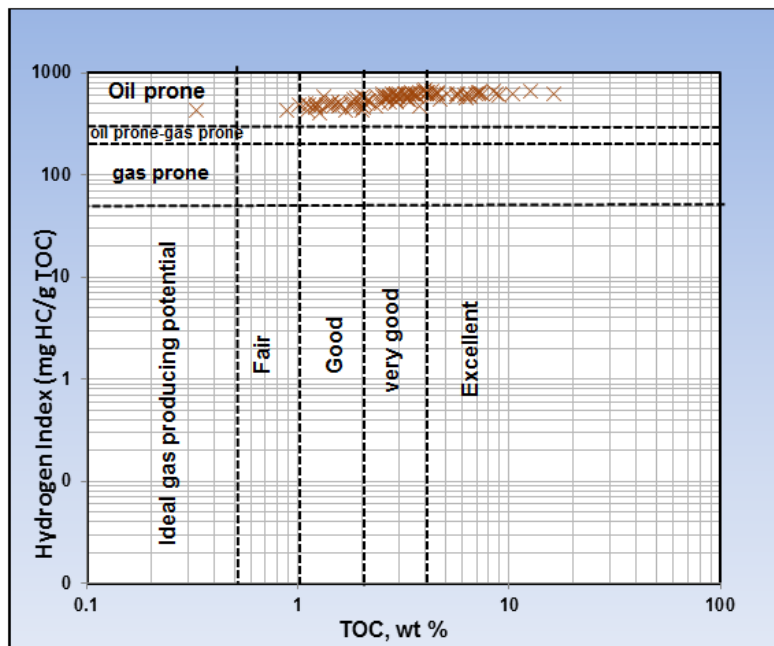


Fig. 6. Hydrogen index vs. TOC, showing type of Organic Matter [24]

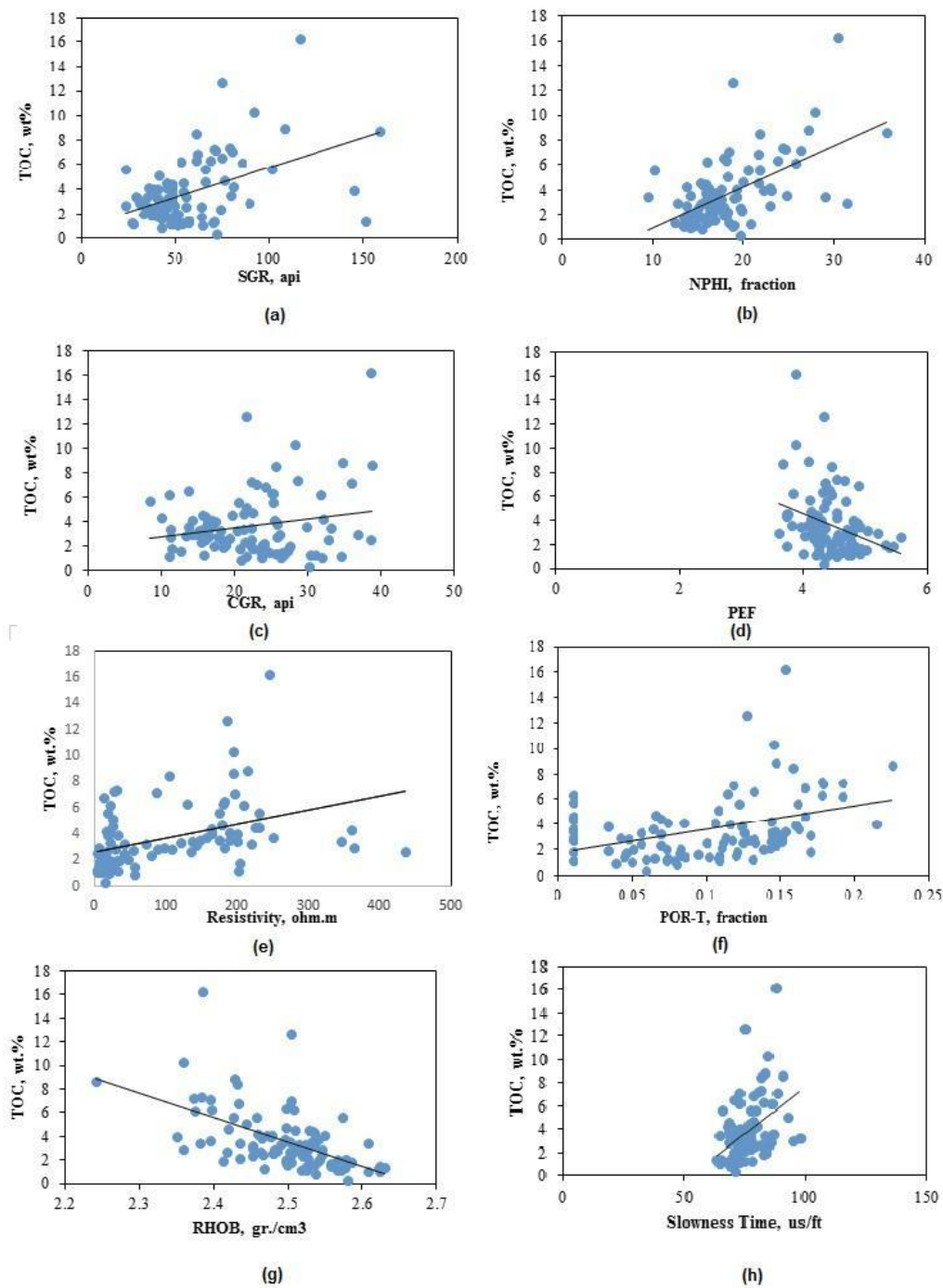


Fig. 7. Plots of (a) Sum Gamma Ray (b) Neutron Porosity (c) Corrected Gamma Ray (d) Photoelectric (e) Resistivity (f) Total Porosity (g) Density (h) Sonic, versus TOC

Correlation Coefficient between Total Amount of Organic Carbon and Various Logging Data

The relation between the TOC and petrophysical characteristics in one of southern Iranian field is shown in Fig. 7. The rocks, which are rich in organic compounds, usually have high radioactive activities. For instance, the gamma-ray of these rocks refers to higher values than shales and limes, which are not sourced rocks. As Figs. 7a and 7c demonstrate that the TOC increment results in the increment of summed gamma ray and corrected gamma ray in terms of the API. According to the direct proportional relationship between the organic content of the rock and corresponding porosity, an increment of the neutron porosity increases the TOC

content. The latter is illustrated in Fig. 7b. The inverse relationship between TOC and PEF, as Fig. 7d shows, is due to the inverse relationship between the photoelectric factor (PEF) and the organic content of the rock. As shown in Fig. 7e, an increment of the total amount of organic carbon causes a rise in the rock resistivity. This fact refers to the direct relationship between the latter parameters. Figs. 7f and 7g, by considering the inverse relationship between the amount of the formation bulk density and the organic content of the rock, indicate a direct relation between TOC and the porosity, and an inverse relation between the TOC amount and the density. According to Fig. 7h, referring to the direct relation of the organic content with the sonic wave traveling time, Δt rises with the rise of the TOC amount.

The Comparison between Experimental Values and Predicted Values Based by Passay's Model:

The Comparison between the Experimental values of Total Organic Carbon Amounts and the Predicted Amounts based by Passay's Model

Based on the results of the $\Delta \log R$, Fig. 8 shows the correlation between total organic carbon predicted by the Passay method and the actual total organic carbon.

Fig. 8 shows the regression between the total organic carbon amounts predicted by Passay's model and their experimental values. As Fig. 8 demonstrates, the regression coefficient between experimental and predicted TOC is not acceptable. Therefore, using this method to obtain the TOC results might carry a high error.

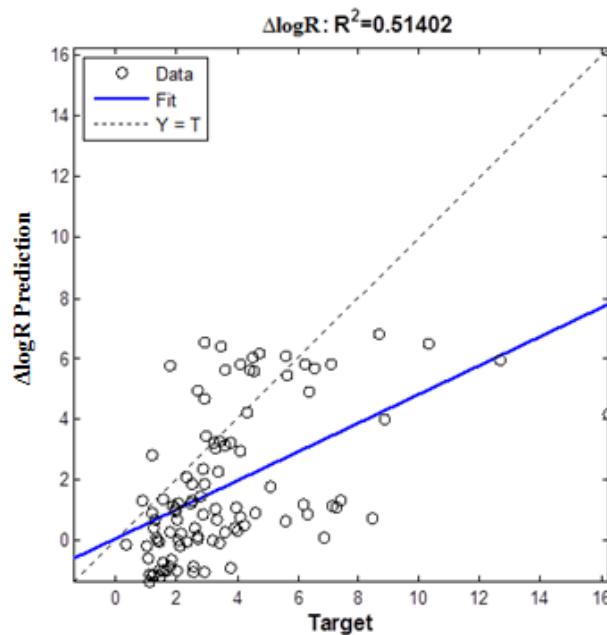


Fig. 8. Cross-plot showing correlation coefficient between actual TOC and TOC obtained from Passay method

The Comparison between Experimental and Passay's Model Predicted Values of TOC in Terms of Depth

Fig. 9 shows the comparison between predicted TOC by the Passay method and experimental TOC vs. depth. As can see in Fig. 9 in the depth of 2280-2470 and 2530-2540 the actual data is higher than the predicted data furthermore, in these depths, the deviation was high and in the depth of 2500-2530 and 2540-2580 the actual data is lower than the predicted data and the

deviation was low. Although formation heterogeneity caused much error for predicting of total organic carbon in wells, this method is suitable for shale formation. In addition, because the *LOM* must be predicted accurately, it can be the source of the error. Thus, the Passay method is not considered as an algorithm method for this formation.

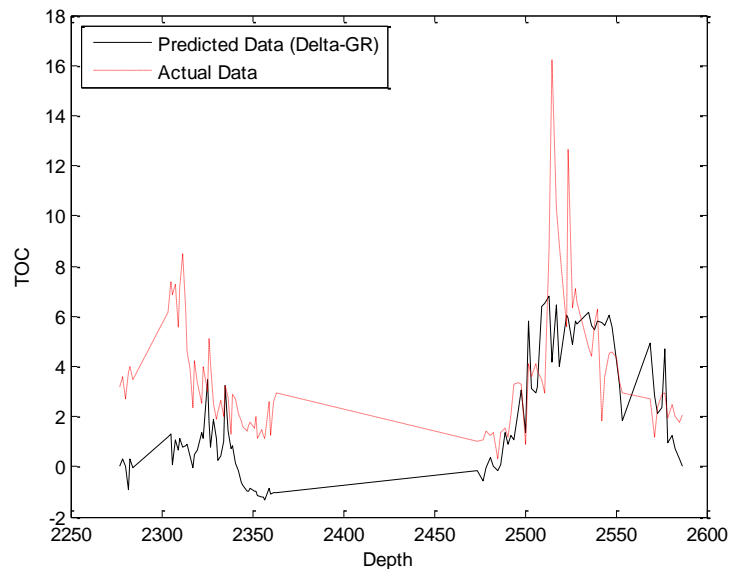


Fig. 9. Comparison between actual TOC and predicted TOC from Passay method vs. depth

The Comparison between Experimental and Predicted Values using the Neural Network Model

Comparison of Regression between the Amount of Total Organic Carbon and Predicted Total Organic Carbon by the Neural Network

Fig. 10 illustrates the linear regression between experimental and predicted values using the neural network model for all data. The correlation coefficient between experimental and estimated data, as Fig. 10 reveals, is equal to 0.88411, which is an acceptable value.

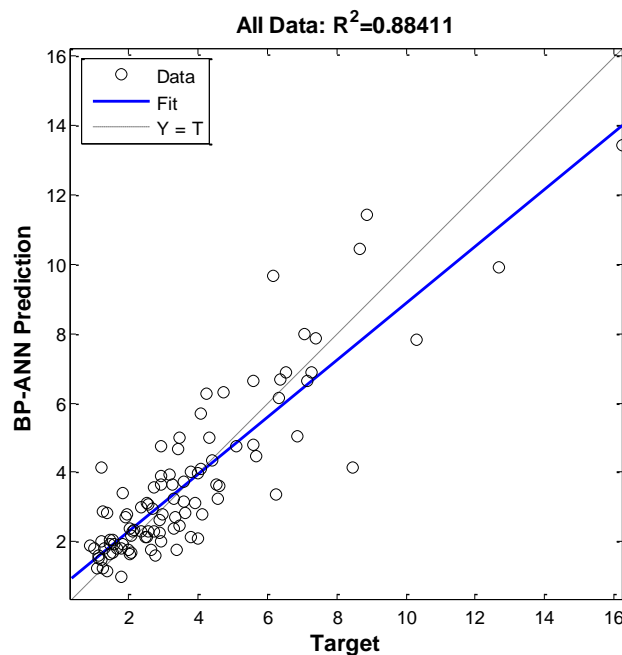


Fig. 10. Cross-plot showing Correlation coefficient between actual TOC and predicted TOC using the MLP with Levenberg–Marquardt training algorithm for all data

Fig. 11 exhibits the linear regression between experimental TOC values and the predicted TOC values based on the neural network model for the test data. The regression coefficient between experimental and estimated values during the neural network test time equals 0.80535, which is an acceptable value.

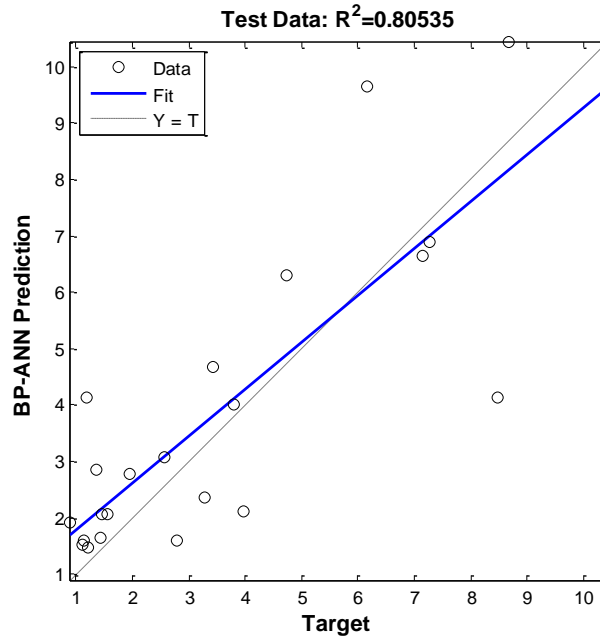


Fig. 11. Cross-plot showing Correlation coefficient between actual TOC and predicted TOC using the MLP with Levenberg–Marquardt training algorithm for Test data

Fig. 12 presents the linear regression between the experimental values of the TOC and the predicted ones obtained with the aid of the neural network model for the train data. According to Fig. 12, the regression coefficient between experimental and estimated data during the neural network test time equals 0.93341, which is an acceptable value.

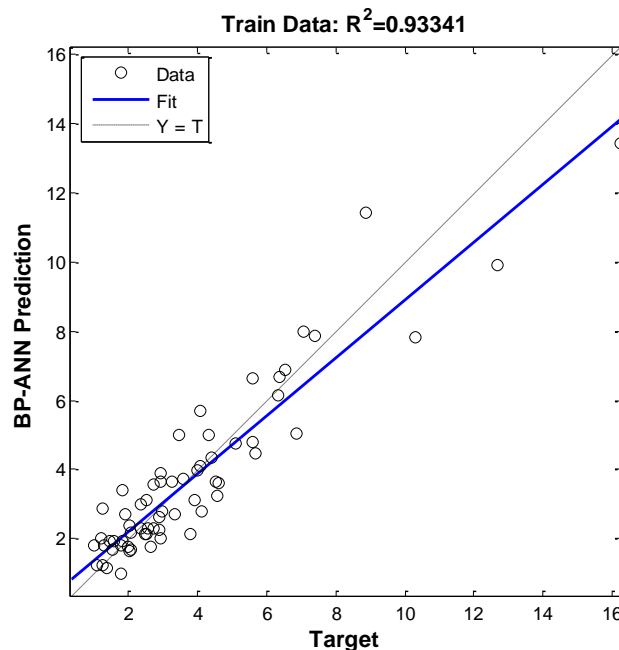


Fig. 12. Cross-plot showing Correlation coefficient between actual TOC and predicted TOC using the MLP with Levenberg–Marquardt training algorithm for train data

Comparison between the Amount of Total Organic carbon and Predicted TOC by the ANN

Fig. 13 shows the comparison between the amounts of TOC and predicted ones by the ANN vs. corresponding depth. About Fig. 13, in most part of the diagram the predicted is higher than the actual data and there is a negligible difference between predicted and actual models, so the deviation is low. So, we can use the ANN model for predicting the TOC in these wells.

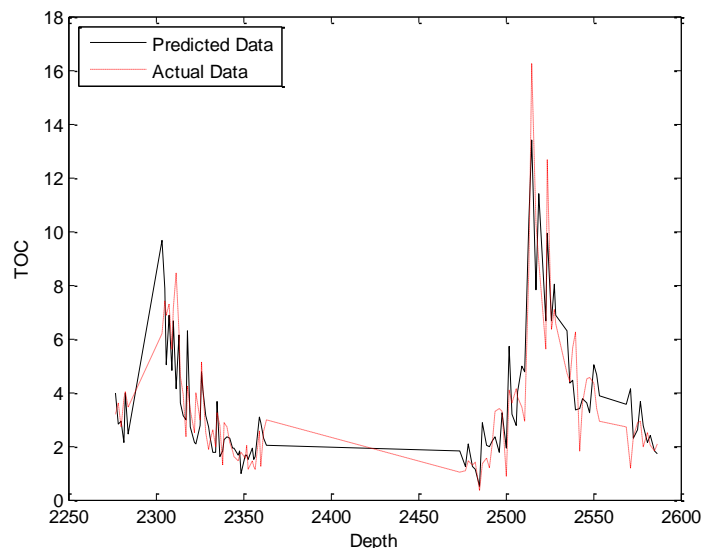


Fig. 13. Comparison between actual TOC and predicted TOC using the MLP with Levenberg–Marquardt training algorithm

Histogram of Error Distribution of MLP with Levenberg –Marquardt Training Algorithm for All Data

Fig. 14 shows the histograms of error distribution for all data in the neural network model. As shown in this figure, the high error distribution is minor, reflecting the proper efficiency of the neural network model in order to predict the TOC using the petro physical diagrams.

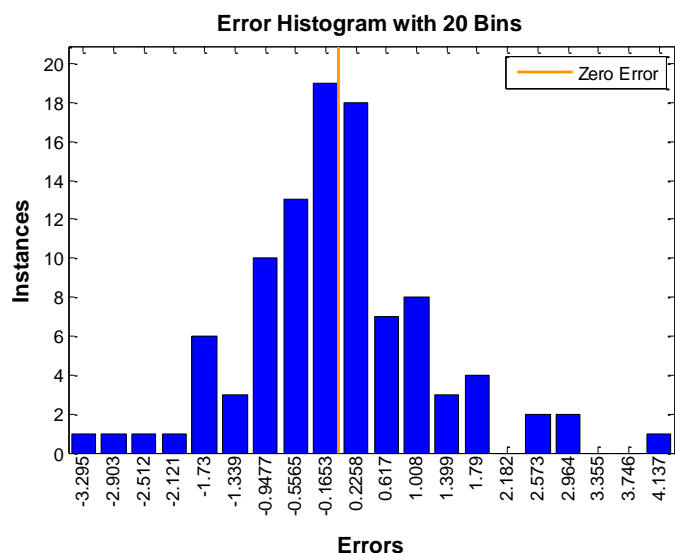


Fig. 14. Histogram of error distribution of MLP with Levenberg –Marquardt training algorithm for all data

Correlation between Actual TOC and Predicted TOC by ΔLogR Method and MLP with Levenberg–Marquardt Training Algorithm

Fig. 15 shows the graphical matching between predicted TOC by the neural network model and Passay model compared to the actual values of the data. Based on the results, the three-layer neural network model has better performance than the Passay model. Therefore, the three-layer perceptron neural network performs well for predicting the TOC content.

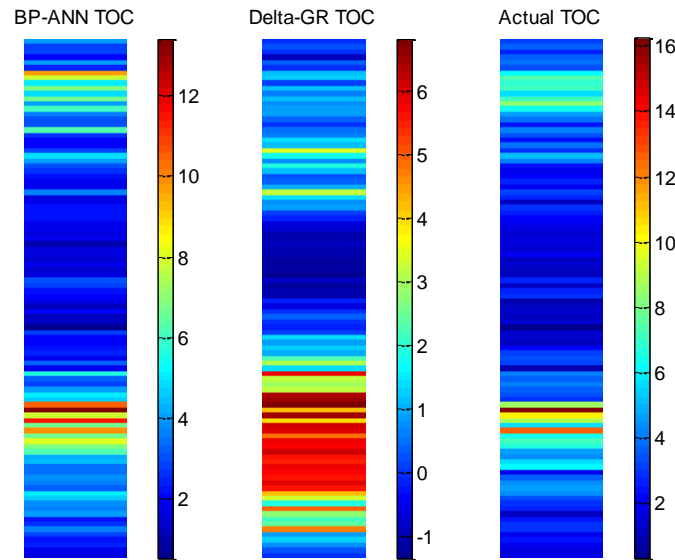


Fig. 15. Graphical correlation between actual TOC and predicted TOC by ΔLogR method and MLP with Levenberg–Marquardt training algorithm for all data

Conclusion

This study shows that the artificial neural networks model predicts the TOC with a correlation coefficient of 82%, without requiring complex mathematical modeling. However, this model has more errors regarding the data with low-frequency. The results-driven from this model are better correlated with measured data than the ones driven from ΔlogR . Because the ΔlogR equation is only suitable for shale rocks and their application for carbonic rocks arises, unreliable results, but the neural network can be used in both cases. The LOM values must be estimated exactly in the ΔlogR method. Otherwise, results will be remarkably wrong despite ΔlogR method, in the ANN method, the LOM values are less important and used only to correct relative LOM values.

Nomenclature

ΔlogR	Deviation of each depth
$\Delta t_{\text{baseline}}$	Transit time
Δt	Measure transit time
LOM	level of maturity
R_{baseline}	Resistivity corresponding to $\Delta T_{\text{baseline}}$
R	Resistivity
S_1	Quantity of free hydrocarbons
S_2	Hydrocarbons released by the kerogen
S_3	Oxygen present in the kerogen.

TOC	Total organic carbon
T _{max}	Maximum temperature generation

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