

Prediction of the Total Organic Carbon Using Artificial Neural Networks and the Spectral Gamma-Ray Logs

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Abstract

Characterization and accurate estimation of the hydrocarbon reserve in unconventional reservoirs are important because of the high cost associated with developing these resources. One of the most important parameters for characterization of the unconventional resources is the total organic carbon (TOC). This study is aimed to optimize the artificial neural networks (ANN) model for TOC estimation based on gamma-ray log, a combination of spectral gamma-ray logs. The ANN model was optimized using 750 datasets collected from well-A in Devonian shale. The optimized model was then tested on 226 datasets from Well-B and validated on 73 datasets from Well-C. The optimized model outperformed the previously developed correlations in predicting the TOC for validation data, where it predicted the TOC with an average absolute percentage error (AAPE) of 11.9% only, while other correlations predicted the TOC with AAPE of over 20%.

Introduction

Total organic carbon (TOC) is a critical parameter required for estimation of the hydrocarbon reserve of unconventional resources, TOC is affected by several parameters such as the maturity, carbon content, and gas adsorption; which affects the organic porosity of the reservoir, the wettability and pore structure of the reservoir rock also affect the TOC content of the reservoir ([Ross and Bustin, 2007](#)). Therefore, an accurate method for TOC estimation is required to accurately predict the reserve of the unconventional reservoir.

TOC is currently evaluated either through conducting extensive laboratory experiments that predict the TOC accurately, but they are costly, time-consuming, as well as it is very difficult to obtain a continuous profile of the TOC along the drilled hole by conducting this extensive laboratory work. Other researchers developed regression-based empirical correlations to evaluate the TOC on a specific formation ([Schmoker, 1979](#); [Passey et al., 1990](#); [Wang et al., 2019a](#); [Zhu et al., 2019a](#)). These correlations require modifications to make it possible to be applied in formations different than the one used to develop it.

By assuming that TOC is directly related to the formation density, and the change in the bulk formation density is only affected by the change in the TOC while assuming the density of the

other formation components is constant, Schmoker (1979) came up with the first empirical correlation for TOC prediction in Devonian shale. The weight percent of the TOC could be calculated based on the volumetric percentage calculated using the Schmoker correlation in Eq. (1), more detail about TOC conversion from volumetric to weight percentage is available in Schmoker (1979).

$$TOC(vol. \%) = \frac{(\rho_B - \rho)}{1.378} \quad (1)$$

where ρ_B represents the bulk formation density (g/cm^3), and ρ denotes the organic matter free rock density (g/cm^3).

In 1980, Schmoker revised his correlation to make it applicable to the Bakken formation, Schmoker (1980) calculated the TOC as a weight percentage using Eq. (2).

$$TOC(wt. \%) = \frac{[(100\rho_o) - (\rho - 0.9922\rho_{mi} - 0.039)]}{[(R\rho)(\rho_o - 1.135\rho_{mi} - 0.675)]} \quad (2)$$

where ρ_o is the organic matter density (g/cm^3), R is the organic matter to organic carbon weight percentage ratio, ρ_{mi} denotes the grain and formation fluid average density (g/cm^3).

The most commonly used correlation for TOC estimation is called $\Delta\log R$ model, summarized in Eq. (3) and Eq. (4), This model was developed by Passey et al. (1990). $\Delta\log R$ model is based on properly scaled resistivity and sonic transit time logs. It is important to mention that $\Delta\log R$ could be calculated using density log or sonic log.

$$\Delta\log R = \log_{10} \left(\frac{R}{R_{baseline}} \right) + 0.02 \times (\Delta t - \Delta t_{baseline}) \quad (3)$$

$$TOC = \Delta\log R \times 10^{(2.297 - 0.1688 \times LOM)} \quad (4)$$

where $\Delta\log R$ denotes the separation between the resistivity and sonic transit time logs, R and Δt are the resistivity of the target formation ($\Omega \cdot m$) and the sonic transient time ($\mu s/ft$), respectively, $R_{baseline}$ and $\Delta t_{baseline}$ denote the base formation resistivity and sonic transit time both corresponding to an organic lean shale, and LOM is the level of maturity.

As indicated in Eq. (3), $\Delta\log R$ model considers 1:50 linear relationship between the formation porosity and logarithmic resistivity, because of this assumption $\Delta\log R$ model is applicable only to a limited range of data with a specific relationship between the porosity and resistivity. Another drawback of this model is that it was developed assuming constant properties of the formation, this could not be applied to organic-rich shale which is characterized by an extreme variation for different resource plays. The use of LOM in estimating the TOC which was considered by this model is not recommended since it leads to problems in practice.

The predictability of TOC using Schmoker and $\Delta\log R$ was evaluated by Charsky and Herron (2013) on data collected from four wells. The results showed that the TOC was estimated with a high average absolute difference of 1.6 wt% for Schmoker and 1.7 wt% for $\Delta\log R$ model. To improve the accuracy of predicting the TOC for Devonian shale, Wang et al. (2016) suggested a revised $\Delta\log R$ model which uses gamma-ray (GR) log in addition to resistivity and sonic or density logs as inputs. Eq. (5) and Eq. (6) could be used to calculate $\Delta\log R$ based on sonic or density logs, respectively, and TOC could be estimated using Eq. (7).

The main advantage of Wang's models is that he did not use the approximation of the linear relationship between sonic and resistivity logs. Another positive point about this model is that LOM replaced T_{max} or R_o as shown in Eq. (7).

$$\Delta\log R = \log_{10} \left(\frac{R}{R_{baseline}} \right) + \frac{1}{\ln 10} \frac{m}{(\Delta t - \Delta t_m)} \times (\Delta t - \Delta t_{baseline}) \quad (5)$$

$$\Delta\log R = \log_{10} \left(\frac{R}{R_{baseline}} \right) + \frac{1}{\ln 10} \frac{m}{(\rho_m - \rho)} \times (\rho - \rho_{baseline}) \quad (6)$$

$$TOC = [\alpha \Delta \log R + \beta (GR - GR_{baseline})] \times 10^{(\delta - \eta T_{max})} \quad (7)$$

where m is the cementation exponent, Δt_m and ρ_m denote the matrix sonic transit time and density in ($\mu s/ft$) and (g/cm^3), respectively, $\rho_{baseline}$ represents the baseline density corresponding to $R_{baseline}$ (g/cm^3), α , β , δ and η are formation constants which must be determined, the maturity indicator T_{max} is in $^{\circ}C$, $GR_{baseline}$ is the baseline gamma-ray value of shale (API).

After comparing the original and revised $\Delta \log R$ models in Devonian shale, the results showed that the revised models accurately predicted the TOC with a coefficient of determination (R^2) greater than 0.92 while R^2 for the between the actual TOC and that predicted using the original $\Delta \log R$ model was 0.82 (Wang et al., 2016).

Recently with advances in the fourth industrial revolution, artificial intelligence tools were extensively applied in different applications related to the petroleum industry. Artificial intelligence tools were successfully implemented for estimation of the formation pore and fracture pressure (Ahmed et al., 2019a; 2019b), real-time prediction of the changes in drilling fluid properties (Elkatatny, 2017; Abdelgawad et al., 2019), optimization of drilling hydraulics (Wang and Salehi, 2015), prediction of the TOC (Mahmoud et al., 2017a; 2019a 2020a; Zhu et al., 2018; 2019b; Wang et al., 2019b; Siddig et al., 2021), prediction of the recovery factor (Mahmoud et al., 2017c; 2019d), estimation of rock mechanical parameters (Mahmoud et al., 2019c; 2020b; 2022a; 2022b), characterization of the heterogeneous hydrocarbon reservoirs (Mohaghegh et al., 1994), prediction of the formation porosity (Gamal et al., 2021), evaluation of the integrity of wellbore casing (Salehi et al., 2009; Al-Shehri, 2019), optimization of rate of penetration (Al-AbdulJabbar et al., 2018; Osman et al., 2021; Gamal et al., 2022), prediction of the formation tops (Elkatatny et al., 2021; Mahmoud et al., 2021), and others.

Recently, one of the most accurate correlations for estimation of the TOC was suggested by Mahmoud et al. (2017b). This correlation was based on the weights and biases of the optimized artificial neural networks (ANN) and it predicts the TOC from the GR, deep resistivity (DR), sonic transit time (DT), and formation bulk density (RHOB). When applied to evaluate TOC on Devonian shale, Mahmoud correlation outperformed Wang correlations.

One year later, Elkatatny (2019) optimized the ANN model for TOC estimation using the self-adaptive differential evolution algorithm, Elkatatny's model outperformed Mahmoud's model in TOC estimation for Devonian formation.

Shi et al. (2016) suggested the use of spectrum gamma-ray (SGR) logs in addition to GR, RHOB, neutron porosity, and compressional wave slowness for TOC prediction. The results indicate that TOC prediction was improved when this combination of inputs was used to predict the TOC through the application of the extreme learning machines.

In this study, ANN model was optimized to estimate the TOC based on the bulk GR, SGR logs, and a newly developed term that accounts for TOC from linear regression analysis (TOC_r).

Methodology

Data Preprocessing

Before training the ANN model, the data were preprocessed to remove any unrealistic data and outliers. All zeroes and 999 values were removed from the inputs to neglect the unrealistic values, then the outliers which are the parameters with values not within the range of ± 3.0 standard deviation were also removed from the training data. After this preprocessing stage 750, 226, and 73 datasets from Well-A, Well-B, and Well-C, respectively, were remaining and considered valid to develop the ANN model.

The optimized model and its design parameters are highly affected by the training data. The main factors to be considered are the statistical features of the training data. As long as

the training is performed on different data that have almost the same statistical features as the current training data, it is expected that the optimized design parameters of the hidden layers, neurons, and others will not vary significantly. For this reason, the statistical features for the training data are reported in Table 1, these features determine the applicable range for the optimized ANN model, and hence, the developed correlation.

Table 1. The statistical description of 750 datasets from Well-A and used to optimize the ANN model.

Statistical Parameter	Gamma-Ray ($^{\circ}$ API)	Potassium (wt%)	Thorium (ppm)	Uranium (ppm)	TOC (wt%)
Minimum	22.9	0.13	1.97	1.39	0.75
Maximum	298	4.06	17.0	22.6	5.66
Median	100	1.50	9.12	5.73	3.16
Skewness	0.87	2.07	-0.50	0.04	-0.90
Standard Deviation	40.3	0.63	2.57	3.33	1.30

As shown in the cross-plots of Figure 2, both GR and potassium have moderate correlations of 0.64 and 0.60, respectively, with the TOC. While the relationship of both the thorium and uranium with the TOC have low correlations of 0.24 and 0.29, respectively.

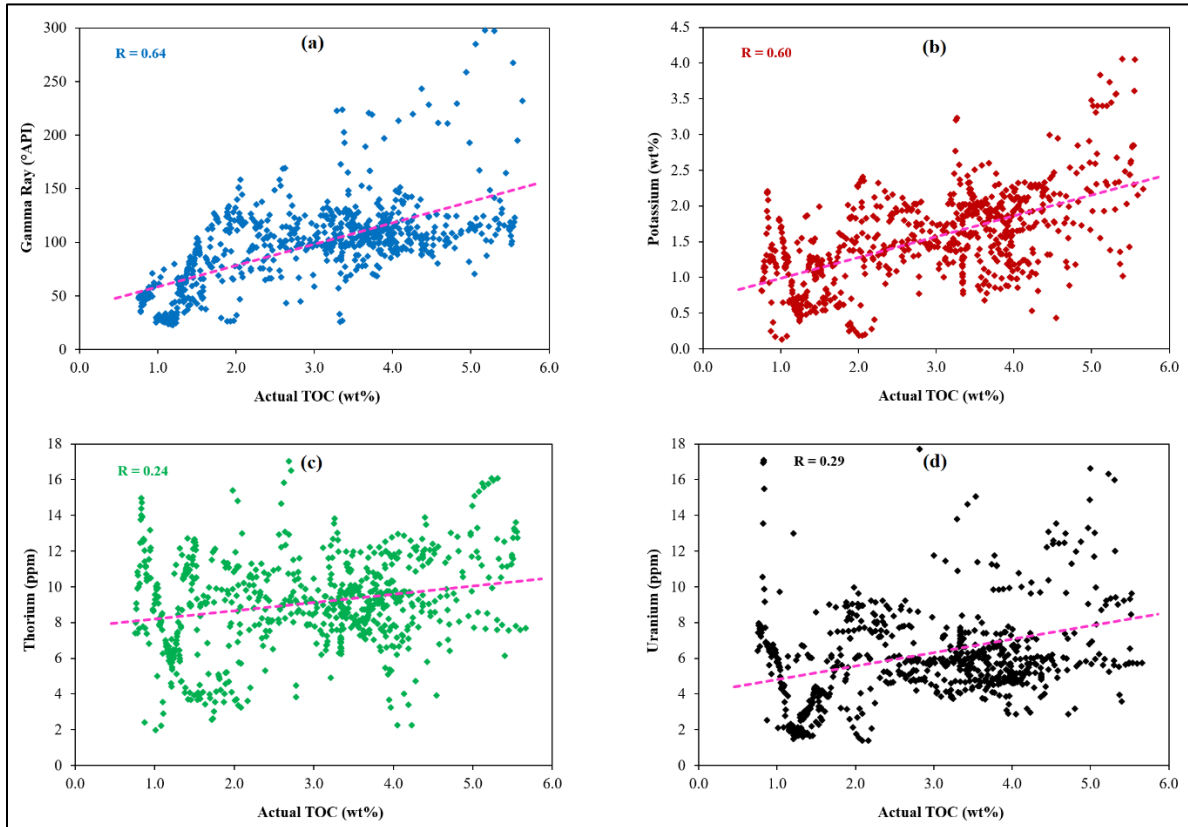


Figure 1: Cross-plots of the (a) GR, (b) potassium, (c) thorium, and (d) uranium, with the actual TOC for the 750 data points collected from Well-A.

Defining the Regression-Based TOC Parameter

The correlation between the inputs and output is one of the main parameters controlling the predictability of the optimized ANN model, so in this study linear regression analysis was conducted to define a new parameter named regression-based TOC or TOC_r . The TOC_r is a function of the logarithmic GR, the ratio of the potassium to thorium, and the uranium logs, this function is defined based on regression analysis to approximate the actual TOC.

The inputs for the TOC_r were identified based on regression analysis and their correlation coefficients (R's), Figure 3 shows the cross-plots of the actual TOC and the three input parameters considered to calculate the parameter TOC_r . As indicated in this figure, the logarithm of the GR, potassium-to-thorium ratio, and uranium logs have R's of 0.68, 0.57, and 0.29 with the TOC, respectively. These three parameters were then considered to define the new parameter TOC_r which is defined in a general form as in Eq. (5).

$$TOC_r = a \log(GR) + b \frac{K}{Th} + c Ur + d \quad \text{Eq. (1)}$$

Where TOC_r is the linear regression-based TOC (wt%), GR is the GR (°API), K is the potassium (%), Th is the thorium (ppm), Ur is the uranium (ppm), the coefficients a, b, c, and d are constants which could be determined based on linear regression.

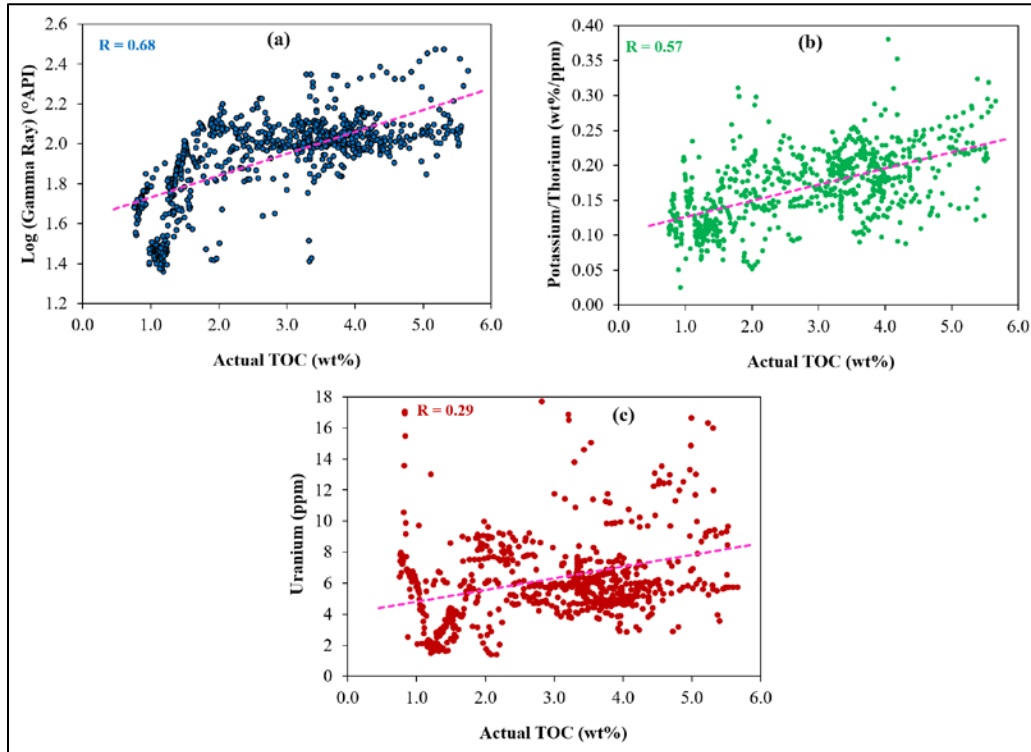


Figure 2: Cross-plots of the (a) logarithm of GR, (b) potassium to thorium ratio, and (c) uranium, with the actual TOC for the 750 data points collected from Well-A.

Linear regression analysis was conducted to define these coefficients, for this purpose, the 750 training data points were used, and the linear regression was conducted using the regression tool in Excel software. The results of this analysis showed that the coefficients a, b, c, and d are equal to 3.235, 7.420, 0.038, and -4.960, respectively. Substituting these coefficients back into Eq. (5), then the final expression for the parameter TOC_r will be as in Eq. (6).

$$\text{TOC}_r = 3.235 \log(\text{GR}) + 7.420 \frac{\text{K}}{\text{Th}} + 0.038 \text{Ur} - 4.960 \quad \text{Eq. (2)}$$

Then Eq. (6) was used to calculate the TOC_r for the data. As shown in Figure 4 this new parameter is highly correlated with the TOC (R of 0.74). The next step is to optimize the ANN model, in this step the use of the new parameter (i.e. TOC_r) also with the four well logs of the GR, potassium, thorium, and uranium as inputs to optimize the ANN model.

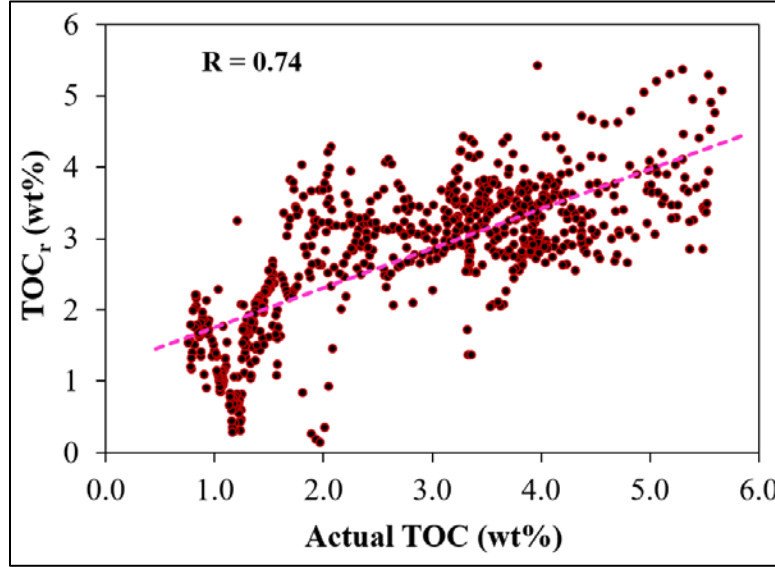


Figure 3: The cross-plot of the linear regression-based TOC and actual TOC for the 750 data points collected from Well-A.

Optimization of the Artificial Neural Networks Model

750 datasets of the different input parameters collected from Well-A were used to optimize the ANN model to estimate the TOC. These input parameters include the bulk GR and SGR logs of potassium, thorium, and uranium as well as the TOC_r parameter as calculated using Eq. (6). Figure 5 compares the inputs collected from Well-A and considered to train the ANN model.

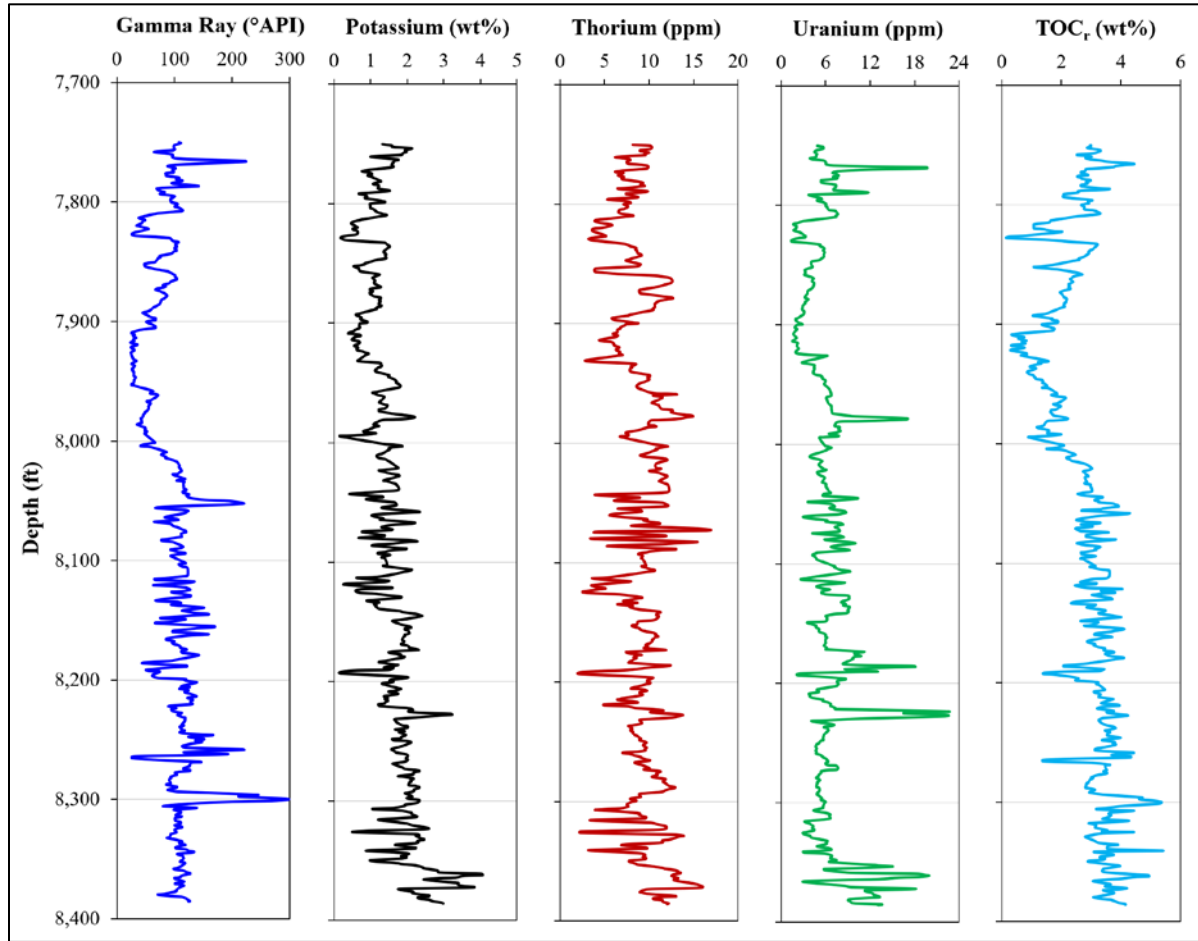


Figure 4: The input log data of the bulk GR, potassium, thorium, uranium logs as well as the TOC_r used to train the artificial neural networks model.

The performance of different combinations of design parameters of the ANN model was investigated through sensitivity analysis. The parameters considered during this optimization process include the number of iterations, the training function, the number of training layers, the number of training neurons per every training layer, as well as the transferring function. The number of iterations was optimized between 1 to 2000 and the iteration gave the lowest training error and prevented model memorization was considered as the optimum. Inserted *for* loops constructed using MATLAB software were considered to investigate the performance of all combinations of the other ANN model design parameters.

Different values of the design factors were considered for the sensitivity analysis, the use of the training function of Levenberg-Marquardt backpropagation function, Bayesian regularization backpropagation function (trainbr), gradient descent backpropagation function, and others were considered. The use of the transferring functions of the logarithmic sigmoid, pure-linear function, function, and tan-sigmoid (tansig) function was also studied. The use of 1 to 3 learning layers and 5 to 50 neurons on each layer was also investigated.

Out of this sensitivity analysis, the parameters summarized in Table 2 represent the combination of the optimum design parameters for the ANN model which is also presented schematically in Figure 7.

Table 2. The design parameters of the optimized ANN model.

Parameter	Value
Number of iterations	494
Training layers	Single
Neurons per layer	27
Training function	trainbr
Transferring function	tansig

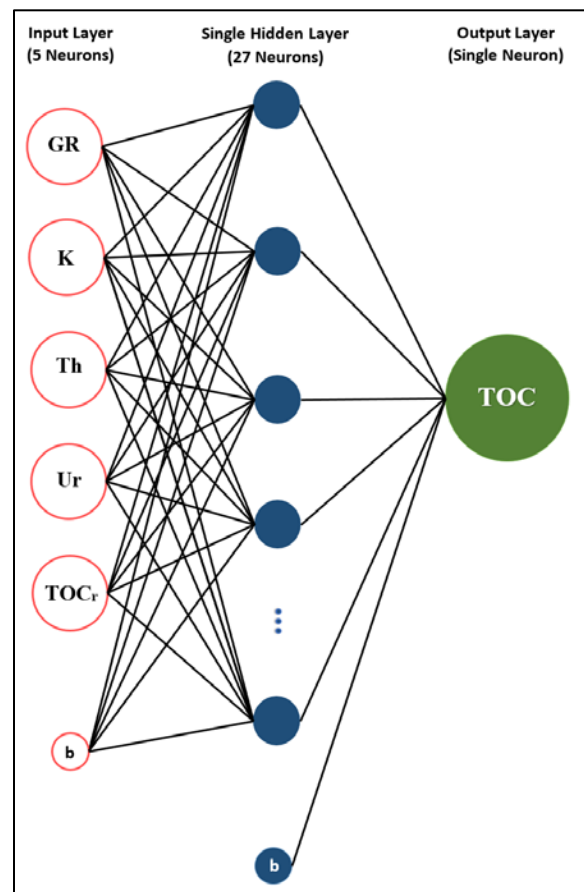


Figure 5: The schematic representation of the optimized ANN model for prediction of the TOC, GR is the gamma-ray, K, Th, and Ur represent the potassium, thorium, and uranium, respectively, and TOC_r is the linear regression-based TOC as calculated from Eq. (6).

Testing and Validating the Optimized Artificial Neural Networks Model

To test the accuracy of the optimized ANN model, 226 datasets from Well-B were used. Then it was validated on 73 datasets from Well-C. The accuracy of the optimized model was compared to the Schmoker model, $\Delta\log R$ method, and [Zhao et al. \(2017\)](#) correlation.

Results and Discussion

Training the Artificial Neural Networks Model

750 datasets of the bulk GR and SGR logs of the potassium, uranium, and thorium from Well-A, in addition to the newly developed parameter called TOC_r were considered for optimizing the ANN model in evaluating the TOC. The actual and estimated TOC of the training data are compared in Figure 6. The high accuracy of the ANN in evaluating the TOC for the training data is confirmed in Figure 6. As shown in this figure, the TOC was estimated with an AAPE of 8.5% and an R of 0.97.

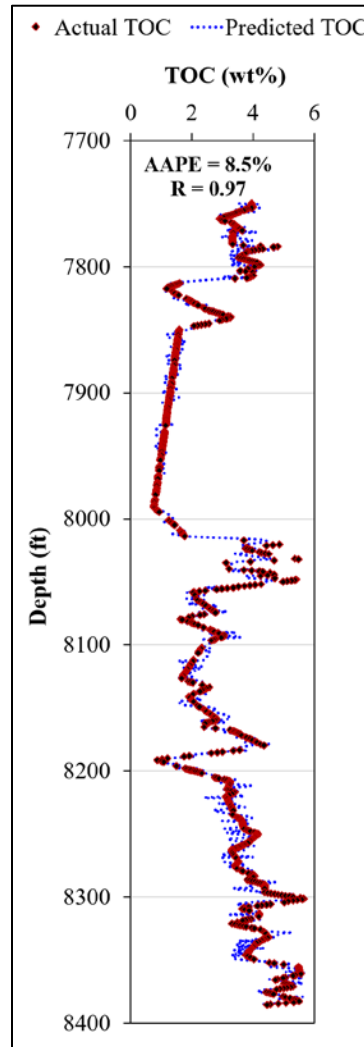


Figure 6: The actual and predicted TOC for training data of Well-A.

Testing the Optimized Artificial Neural Networks Model

The optimized ANN model was tested for TOC estimation using unseen 226 data points of Well-B with the results shown in Figure 9. As confirmed by the plots of this figure, the TOC estimated using the optimized ANN model is in excellent matching with actual TOC, where the TOC was predicted with AAPE and R of 11.5% and 0.95, respectively.

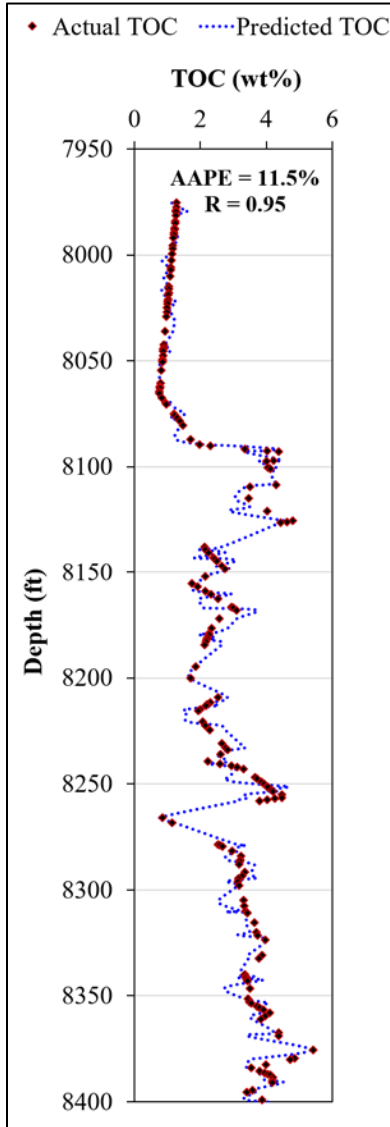


Figure 7: The actual and predicted TOC for testing data of Well-B.

Validating the Artificial Neural Networks Model for TOC Estimation

The previous results indicate the high accuracy of the ANN model optimized in this study in estimating the TOC in Devonian shale. In this section, this optimized model will then be validated on 73 data points from a third well (Well-C), which is located in the vicinity of the training and testing wells, the datasets of Well-C cover a depth interval of 140.5 ft. The prediction accuracy of the optimized ANN model was compared with three of the available models for TOC prediction, namely the Schmoker model, $\Delta\log R$ method, and Zhao et al. (2017) correlation.

The accuracy of the optimized ANN model and the available empirical correlations in predicting the TOC in Well-C is compared in Figure 10. The results in this figure, confirm the high accuracy of the optimized ANN model which

outperformed all other models in predicting the TOC with AAPE of 11.9% and a high R of 0.95, while TOC was predicted with AAPE and R of 20.2% and 0.84, respectively, using Zhao et al. (2017) correlation. $\Delta\log R$ method and Schmoker correlation calculated the TOC with AAPEs of 24.6% and 48.6%, respectively. Visual comparison of all plots of Figure 10 also confirmed the high accuracy of the optimized ANN model compared to the other correlations.

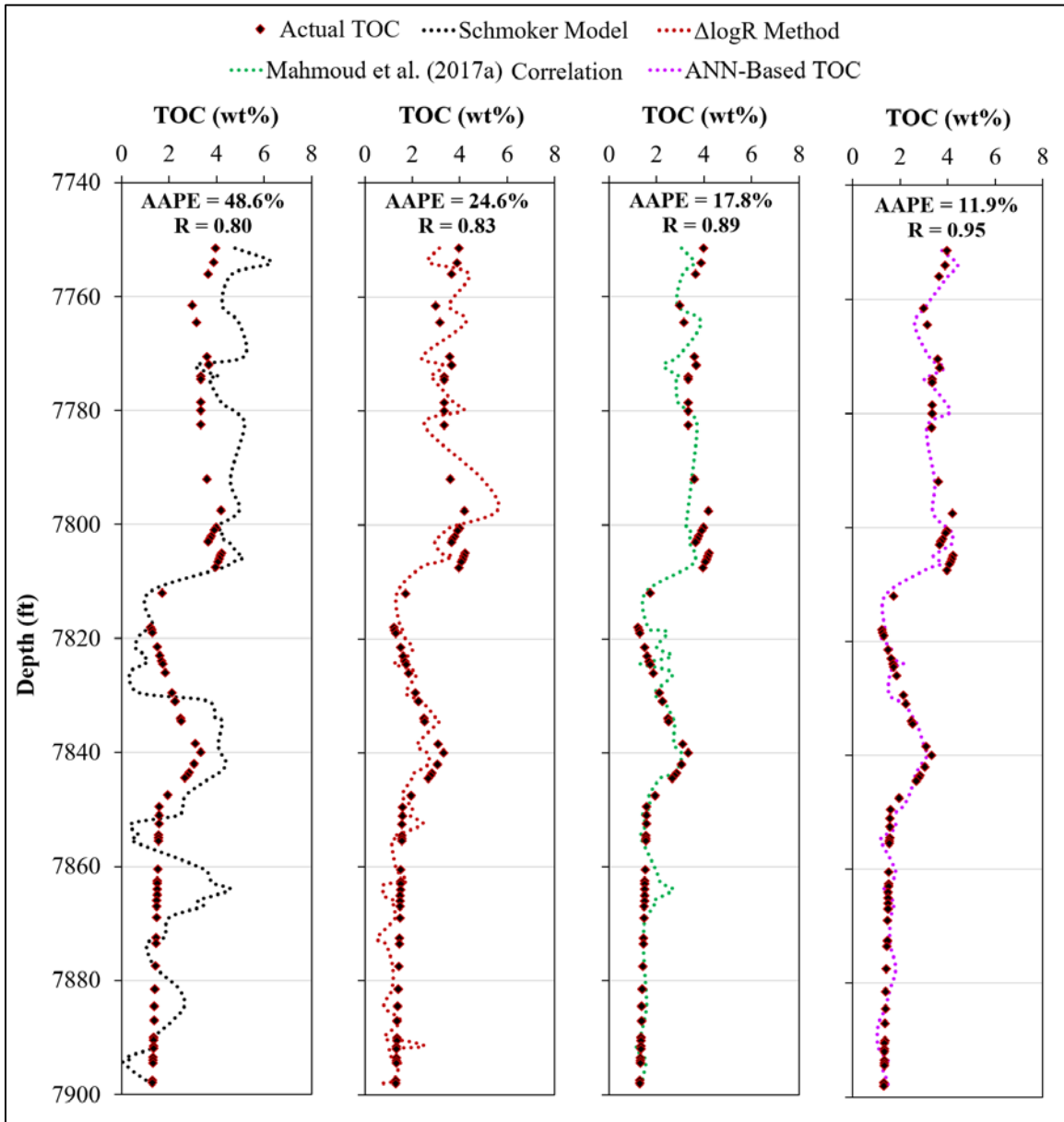


Figure 8: Prediction accuracy of the Schmoker model, $\Delta\log R$ method, [Zhao et al. \(2017\)](#) correlation, and the optimized ANN model, for the 73 validation data points of Well-C.

The results of this work confirmed the high accuracy of the optimized ANN model in evaluating the TOC in Devonian shale. Although the optimized ANN model predicted the TOC from only the bulk and SGR logs, it outperformed the available empirical equations which estimated the TOC base on RHOB log only (Schomoker model), or a combination of formation resistivity, sonic transit time, and LOM ($\Delta\log R$ method), or bulk GR, formation resistivity, and sonic transit time, or RHOB logs ([Zhao et al. \(2017\)](#)).

Conclusions

In this study, the ANN algorithm was optimized to predict the TOC in Devonian Duvernay shale from only the bulk GR and SGR logs of uranium, thorium, and potassium as well as a newly developed term that accounts for the TOC estimated from regression analysis (TOC_r). The following are concluded out of this study:

- The ANN model was able to predict the TOC for the training data with an AAPE of 8.5%.
- For the testing data, TOC was predicted with an AAPE of 11.5% only, using the optimized ANN model.
- The optimized ANN model was also validated on 73 data points and it estimated the TOC with AAPE of 11.9%.
- The optimized ANN model outperformed the available correlations in estimating the TOC.

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