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Well log prediction of total organic carbon: A comprehensive review

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ABSTRACT

Source rocks are fundamental elements for petroleum systems, and Total Organic Carbon (TOC) is one of the most important geochemical parameters in source rock property evaluation. The TOC determination methods using laboratory tests are expensive and limited, therefore prediction of TOC using geophysical well logs are vital for source rock characterization. Though there are various proposed TOC quantitation method, however, there still remains large uncertainty in delineation and quantitation of TOC using well log data due to the complex non-linear relationships between TOC and well log information, as well as the inherent limitations of various methods for TOC prediction. To fill the gaps between TOC and well logs, and eliminate uncertainties existing in empirical methods such as ΔlgR method, the geological, geophysical and geochemical data are integrated. History of source rock evaluation using well logs is reviewed, and sensitive well log parameters for source rocks are selected. The TOC content is correlated with well log series to unravel the well log responses of source rock intervals, and the organic matter rich intervals have high Uranium (U) concentrations and gamma ray (GR) readings, high sonic transit time (AC) and compensated neutron log (CNL), high resistivity, but low density readings. Then the various methods used for TOC quantitation are summarized in terms of their principles, interpretation process, and advantage and limitations. The Schmoker method is not applicable in shales, and borehole regularity will affect the linear regression relationship between TOC and bulk density. The Passey's ΔlgR method is widely used, however, the baseline selection will reduce the accuracy, and ΔlgR method is not applicable in highly mature or deep burial source rocks. The multiple regression analysis is hard to extend in other source rocks. The spectral GR method can hardly be used for lacustrine source rock analysis. The high acquisition costs of Nuclear Magnetic Resonance (NMR) and spectral mineral composition log (Schlumberger's Litho-Scanner logs) limit their extension in source rock evaluation. Artificial intelligence methods such as Back propagation (BP) neural network, Extreme Gradient Boosting (XGBOOST) can be used to predict TOC content via conventional logs, and the results are compared with the geochemical-measured TOC and ΔlgR method. The optimization of various methods for TOC prediction should fully consider their advantage and limitations. Additionally, comprehensive assessment of source rock should determine TOC, quality, and maturity of source rocks. This comprehensive review provides systematic and novel insights in applications of well logs in source rock evaluation, and has potential to fill gaps between geologists, geochemists and petrophysicists.

1. Introduction

Source rocks are fundamental to petroleum systems: no source rocks, no hydrocarbons (Tissot and Welte, 1984; Hunt, 1996; Bolandi et al., 2015). Source rocks are sedimentary rock units containing enough organic matters in the form of kerogen to generate and expel hydrocarbons via biogenic or thermal processes (Tissot and Welte, 1984; Khoshnoodkia et al., 2011; Sêco et al., 2019). Recognition and delineation of hydrocarbon source rocks are key aspects for petroleum system evaluation (Bolandi et al., 2015; Sahoo et al., 2021). Source rocks, which are the precursors of oil and gas, will generate and expel hydrocarbon under favorable conditions, and the expelled hydrocarbons may migrate to reservoir rocks, and they provide a seal rock for accumulation of fluids (Bolandi et al., 2017). Absence of source rock analysis is one of the main

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risks in hydrocarbon exploration (Bolandi et al., 2015; Sêco et al., 2019).

The source rock properties (kerogen type, relative abundance and thermal maturity), which are vital basis for evaluating hydrocarbon quality and production potential, can be evaluated by laboratory organic geochemical analysis (Mulashani et al., 2021; Feng et al., 2023). The Rock-Eval analysis will provide insights into the geochemical parameters of source rocks (Vandenbroucke and Largeau, 2007; Mahmoud et al., 2017; Mulashani et al., 2021; Gama and Schwark, 2023). However, the geochemical analysis data, which are conducted on core or drilling cuttings, are very limited, and they cannot represent the whole interval (Khoshnoodkia et al., 2011; Wang et al., 2019; Gama and Schwark, 2023). Consequently, the geophysical well logs, which continuously record the geophysical properties, are needed for source rock property evaluation (Tan et al., 2015; Handhal et al., 2020; Bai and Tan, 2021; Lai et al., 2022a; Lohr and Merrill, 2024). As a matter of fact, organic matters have distinctive responses on logging curves, and evaluation and prediction of source rocks using well logs is feasible (Rui et al., 2020). An integrated analysis of geochemical data and well logs are needed to map the distribution and quantify the organic richness source rocks (Meyer and Nederlof, 1984; Zheng et al., 2021; Sahoo et al., 2021; Chan et al., 2022; Venancio et al., 2022; Gama and Schwark, 2023; Lai et al., 2024a).

In view of source rock evaluation, TOC is one of the most important parameter, and TOC quantification using geochemical analysis, especially by geophysical well logs, is a fundamental step in source rock evaluation (Bolandi et al., 2017; Qian et al., 2019; Handhal et al., 2020). TOC is the amount of organic carbon in rocks, and it is a measure of the organic richness in source rocks (both kerogen and bitumen) (Langford and Blanc-Valleron, 1990; Wang et al., 2019; Handhal et al., 2020; Venancio et al., 2022). For many years, scholars have attempted to relate geochemical parameters to well log information, and many methods are proposed to recognize source rock intervals and predict TOC content (Schmoker, 1979; Passey et al., 1990; Khoshnoodkia et al., 2011; Huang and Williamson, 1996; Kamali and Mirshady, 2004; Kadkhodaie-Ilkhchi et al., 2009; Mahmoud et al., 2017; Wang et al., 2019; Handhal et al., 2020; Lai et al., 2022a; Gordon et al., 2022). However, the complex non-linear relationships between geochemical parameters (TOC, free hydrocarbon S1, and pyrolysed hydrocarbon S2) and well log information, make it difficult to accurately predict TOC content using well logs (Wood, 2020; Gordon et al., 2022). In addition, the advantages and disadvantages of various methods should be considered to improve the TOC prediction accuracy (Zhu et al., 2020; Lai et al., 2022a). There still remains large uncertainty in the delineation and quantitation of source rocks using well data calibration with core data.

The main objectives of this study are to help geologists, geochemists and petrophysicist to predict TOC content using geophysical well logs, without the need to measure TOC in the laboratory. By reviewing the history of source rock evaluation using well logs, the well log series sensitive for source rocks are selected. By correlating TOC content with well log, the well log responses of source rock intervals are unraveled using typical source rocks in China (the Cretaceous Qingshankou Formation in Songliao Basin, the Permian Lucaogou Formation in Junnggar Basin, the Upper Triassic Yanchang Formation in Ordos Basin) (Fig. 1). Then the principles, dealing process, and advantage and limitations of

Fig. 1. Map showing the petroliferous sedimentary basin (Junngar, Ordos and Songliao Basin) in China (Zhang et al., 2022).

various methods used for TOC quantitation are summarized, and they include the Schmoker method, the ΔlgR method, spectral GR method and multiple regression analysis method. In addition, the utility of Nuclear Magnetic Resonance (NMR) and Schlumberger's Litho-Scanner logs in source rock evaluation are also reviewed. The Artificial Intelligent (AI) methods are also integrated to model the relationship between TOC and well logs. Lastly, the seismic prediction of source rocks is mentioned, and the existing problems as well as future prospects of well log evaluation and prediction methods are reviewed. The ultimate goal of this study is to predict TOC content with high accuracy using conventional and advanced well logs, and hope beginners and interested readers can use for future work.

2. Organic geochemical experiments

Quality (kerogen types), quantity (abundance) and maturity (thermal maturity) are three fundamentally geochemical indexes using for source rock property evaluation (Zhao et al., 2019; Lai et al., 2022a; Gordon et al., 2022). Laboratory organic geochemical analysis, which are performed on outcrops, drilled cores and drilling cuttings, are the most reliable method for quantifying source rock property (Mulashani et al., 2021).

The Rock-Eval analysis is designed to obtain the geochemical parameters of source rocks (Khoshnoodkia et al., 2011; Handhal et al., 2020; Balumi et al., 2022; Nyakilla et al., 2022). Rick-Eval pyrsolisis experiments are performed to obtain source rock parameters such as TOC (wt%), volatile or free hydrocarbon (S1, mg-HC/g-rock), hydrocarbon released by cracking of kerogen and heavy hydrocarbons (S2, mg-HC/g-rock), temperature at the highest yield of S2 (Tmax, °C), as well as CO_2 evolved from thermal cracking of kerogen (S3, $mgCO_2/g$ Rock) (Lafargue et al., 1998; Sfidari et al., 2012; Handhal et al., 2020; Hong et al., 2021; Nyakilla et al., 2022).

In addition, there are several indirectly derived parameters from measured parameters by normalizing generated hydrocarbons to TOC, and they include (1) hydrogen index: (S2/TOC) × 100 [mg HC/g TOC]; (2) oxygen index: (S3/TOC) × 100 [mg CO_2/g TOC] and (3) production index): S1/(S1 + S2) (Lafargue et al., 1998; Bolandi et al., 2017; Hong et al., 2021; Souza et al., 2021; Nyakilla et al., 2022). The ratio of S1/(S1 + S2) can also be used for thermal maturity estimation (Borrok et al., 2019; Balumi et al., 2022).

The abundance of organic matters in rocks can be described by TOC, actually TOC effectively reflects the hydrocarbon generation potential to some extent, however, other factors also need to be considered such as lithology, Tmax, hydrogen index, oxygen index (Zheng et al., 2021; Zhang et al., 2023). TOC is commonly expressed in weight percentage (wt%) (Gama and Schwark, 2023), and TOC measure involves acidification (HCl) to remove carbonate minerals in rocks and then combustion of rock samples to generate CO_2 (Zheng et al., 2021). TOC is the sum of the pyrolyzable carbon and residual carbon. Analysis focusing on TOC alone fails to provide hydrocarbon generation potential, therefore other parameters such as S1, S2, Tmax should also be included in the analysis. Besides TOC values, the associated organic maturity indicators (vitrinite reflectance, Ro), can also be obtained in the laboratory analysis (organic petrography (reflected white and UV light)) (Khoshnoodkia et al., 2011; Zheng et al., 2021; Goodarzi et al., 2022; Gama and Schwark, 2023).

3. History of source rock evaluation using well logs

Geochemical analysis performed on geological samples provide direct insights into source rock property, however, core data have limitations including high cost, and low recovery rate (discontinuity) (Tan et al., 2015; Mahmoud et al., 2017; Mulashani et al., 2021; Gama and Schwark, 2023). In addition, the compensated drill cuttings are easily to be contaminated, and depth of drill cuttings are difficult to determine (Mulashani et al., 2021). Consequently, geochemical analyses conducted on core, drilling cuttings only provide discrete points of data, which cannot represent the whole interval (Khoshnoodkia et al., 2011; Zhao et al., 2016; Gama and Schwark, 2023). Geophysical well logs, which continuously record the geophysical properties (acoustic, electrical and nuclear logs such as density and neutron porosity) along borehole walls, have the advantages of high vertical resolution, and low cost (Lai et al., 2023a).

The wide difference in petrophysical properties between organic matter and host rock matrix has enabled source rock identification from wireline logs (Meyer and Nederlof, 1984; Passey et al., 1990; Lai et al., 2022a; Gama and Schwark, 2023). The source rock evaluation using well logs can be date back to the 1940s, when the high radioactivity of organic-rich source rocks was discovered by Beers (1945). The development history of well log characterization of source rocks is summarized into three distinct phases.

3.1. Qualitative recognition of source rocks by well logs

The distinctive petrophysical properties of organic matters (abundant in hydrogen (H) and carbon (C)) within source rocks are recognized by many authors (Wood, 2020). Beers (1945) points out the high GR readings associated with source rock intervals. Then the log parameters which are sensitive to source rocks are summarized as lower density and acoustic velocity, higher resistivity and neutron porosity (Fertl, 1979; Schmoker, 1979; Schmoker, 1981; Dellenbach et al., 1983; Autric and Dumesnil, 1985; Fertl et al., 1986; Mann and Müller, 1988; Fertl and Chilingar, 1988; Gama and Schwark, 2023).

In the 1970s to 1980s, density log curve is used to predict TOC (Schmoker, 1979), and GR log is integrated to predict TOC (Schmoker, 1981). Gamma-ray spectral (potassium, thorium and uranium) logs are used to estimate the TOC content (Fertl and Rieke, 1980). Acoustic (AC) log is also good indicator for TOC content prediction (Autric and Dumesnil, 1985). Additionally, AC and resistivity (RT) log curves are employed to reflect TOC variation (Dellenbach et al., 1983).

Simple linear regressions through bulk density logs as well as GR logs are introduced to semi-quantitatively predict TOC values (Schmoker, 1979, 1981, Schmoker and Hester, 1983; Fertl and Rieke, 1980; Dellenbach et al., 1983; Schmoker and Hester, 1983). In the 1980s, GR, sonic and resistivity logs are integrated and multivariate statistical methods are used to predict TOC using well logs (Dellenbach et al., 1983; Mendelson and Toksoz, 1985; Fertl and Chilingar, 1988). There are various methods proposed to quantitatively or semi-quantitatively characterize the source rock property in the 1970s to 1980s, however, these methods are not widely used in the academic and industrial fields now due to low accuracy and complex processes.

3.2. Quantitative evaluation of source rocks using well logs

Besides qualitative recognition of source rocks, accurate methods to quantitatively predict organic matter content and source rock properties using well logs are of great importance (Passey et al., 1990; Zhao et al., 2017; Silva et al., 2017; Sêco et al., 2019; Wood, 2020; Zhu et al., 2020; Zheng et al., 2021; Ochoa et al., 2022; Maroufi and Zahmatkesh, 2023).

Passey et al. (1990) devised a ΔlgR method, which integrates porosity logs (AC, DEN and CNL) and deep resistivity (RT) log, to calculate TOC content. The ΔlgR method properly scaled porosity logs and resistivity logs, and the two overlaid log curves can separate source rock and non-source rock intervals (Passey et al., 1990). Up to now, the Passey's ΔlgR method is still used for well log based TOC evaluation by many scholars (Zhao et al., 2017; Sêco et al., 2019; Zhu et al., 2020; Mulashani et al., 2021; Zeng et al., 2021; Ochoa et al., 2022; Lai et al., 2022a; Gama and Schwark, 2023), and additionally many modified ΔlgR methods are used to derive TOC content using well logs (Zhao et al., 2016). The ΔlgR and modified ΔlgR method provide accurate TOC content, however, they are not applicable for high mature source rocks (Lai et al., 2024a).

In the 1990s, statistical analysis and Artificial Intelligence (AI) techniques are gradually introduced to formulate well log data to TOC (Huang and Williamson, 1996; Suykens and Vandewalle, 1999). Carpentier et al. (1991) uses sonic and resistivity cross-plot to estimate TOC content. In addition, some modified ΔlgR methods are proposed to derive TOC using well logs. Schwarzkopf (1992) estimates TOC values to assume that source and non-source rocks have same porosity and matrix density, and non-source rock has an organically lean trend.

3.3. Comprehensive prediction of source rocks via well logs

In the new century (since 2000), unconventional oil and gas resources became research hotspots due to increasing energy demand and technological advances (Zhu et al., 2019; Lai et al., 2022a). Consequently, source rock property evaluation of unconventional hydrocarbon resources via well logs is crucial since they are characterized by self-sourced and self-retained, i.e., source rocks also act as reservoir rocks (Zhu et al., 2019; Lai et al., 2022a; Ochoa et al., 2022).

The ΔlgR and neuro-fuzzy methods are integrated together to predict the TOC-rich intervals (Kamali and Mirshady, 2004). Jacobi et al. (2008) introduces a method to derive TOC using the porosity difference calculated by DEN logs and derived from NMR logs. In addition, more and more data-driven AI methods are introduced to predict TOC content, with the aim to reduce uncertainty and improve accuracy (Kadkhodaie-Ilkhchi et al., 2009; Tan et al., 2015; Mahmoud et al., 2017; Zhu et al., 2020; Ganguli et al., 2022).

With the advent of unconventional resources, full-scale geophysical well logs and new petrophysical workflows using single or multiple well log series (including advanced well logs, Litho-Scanner and NMR logs) for source rock evaluation have been proposed (Wood, 2020; Ochoa et al., 2022; Lai et al., 2022a).

4. Well log responses of source rocks

A full range of conventional geophysical log suites comprise gamma-ray (GR), GR spectrometry logs (K, Th, U), photoelectric log (Pe), caliper (CAL), spontaneous potential (SP), acoustic log (AC, DT), neutron porosity (CNL, NPHI and TNPH), bulk density (DEN, RHOB, ZDEN) and resistivity logs (Wang et al., 2019; Aziz et al., 2020; Ganguli et al., 2022; Lai et al., 2022a; Huang et al., 2023). Elemental Capture Spectroscopy (ECS) logs, Schlumberger's Litho-Scanner logs, Nuclear Magnetic Resonance (NMR) and image logs are classified as advanced logs (Lai et al., 2022a; Zhang et al., 2023). Standardization of well log data has been performed before data processing and TOC prediction. Histogram is used for standardization of GR, AC, DEN and CNL from various wells to confirm that the data from different wells are comparable.

Source rocks are rock units abundant in kerogens, which are prone to generate and expel hydrocarbons with increasing thermal maturity through biogenic or thermal processes (Tissot and Welte, 1984; Sêco et al., 2019). Immature source rocks only contain rock matrix, organic matters (kerogen) and formation water in the pore spaces, while mature source rocks consist of rock matrix, solid organic matter, and hydrocarbon in the pore-fracture systems (Passey et al., 1990; Kenomore et al., 2017; Zhang et al., 2023). In contrast, the non-source rocks (reservoir rocks) include rock matrix and formation water or hydrocarbon within the matrix (Kenomore et al., 2017; Zhang et al., 2023). Consequently, the presences of organic matters within source rocks and the associated expelled hydrocarbons will result in the distinctly different petrophysical properties compared with organic-poor rocks (Xu et al., 2017; Wang et al., 2019; Lai et al., 2022a; Zhang et al., 2023). Hydrocarbon source rocks can be identified and evaluated through the comprehensive analysis of above well log suits (Schmoker, 1980; Meyer and Nederlof, 1984; Passey et al., 1990; Sfidari et al., 2012; Wang et al., 2019; Handhal et al., 2020; Zhang et al., 2022; Maroufi and Zahmatkesh, 2023; Lai et al., 2024a).

The source rocks used in this article include the Cretaceous Qingshankou Formation in Songliao Basin, the Permian Lucaogou Formation in Junngar Basin, the Upper Triassic Yanchang Formation in Ordos Basin (Fig. 2). The Permian Lucaogou Formation (P_2l) in the Junggar Basin is lacustrine mixed fine-grained sedimentary rock, which was deposited in a saline lacustrine environment (Lai et al., 2022b; Pang et al., 2022). The lithologies mainly include mudstone, dolomitic mudstone, dolostones and siltstone (Lai et al., 2023c) (Fig. 2). The source rocks of Lucaogou Formation are thermally low-mature to mature (Ro, 0.8 %–1.0 %), and they have a huge shale oil reserves (Fig. 2).

The Yanchang Formation can be subdivided into ten members (Chang 1 to Chang 10 from top to bottom) according to sedimentary cycles or lithological association. Among them, the Chang 7 member was formed at the most expansive stage and are therefore rich in organic matters, and the lithologies mainly include oil shale and black mudstone together with thin beds of siltstone, and the clay, organic matter and silt lamina can be observed (Fig. 2) (Lai et al., 2016). Abundant oils have been produced from Chang 7 member of Yanchang Formation (Lai et al., 2023c).

The Qingshankou Formation, which was formed in semi-deep to deep lakes, are rich in organic matter, and also contains abundant shale oil resources. Clay minerals are common in Qingshankou Formation, and in some cases, shell fossils can be observed (Fig. 2) (Pang et al., 2023).

4.1. Conventional well log series

4.1.1. Natural gamma-ray and spectral gamma ray

The gamma ray logging tool measures natural radioactivity emitted from potassium (K), thorium (Th), and uranium (U), which are dominated in clay minerals within shales and mudrocks (Khoshnoodkia et al., 2011; Abarghani et al., 2019; Lai et al., 2019). The GR logs are records of a formation's radioactivity, while spectral gamma-ray logging provides individual K, Th and U content respectively (Zhao et al., 2016; Bolandi et al., 2017; Shalaby et al., 2019; Handhal et al., 2020; Gama and Schwark, 2023).

The organic matters in source rocks have high hydrogen content, and often exhibit abnormally adsorption capacity, and therefore uranium elements will be enriched in source rocks (Fertl, 1979; Zhao et al., 2016; Bolandi et al., 2017; Abarghani et al., 2019; Godfray and Seetharamaiah, 2019; Handhal et al., 2020; Lia et al., 2023d). Consequently, source rocks have abnormally high GR readings due to high concentrations of radioactive elements including K, Th and U, especially high uranium concentrations (Bolandi et al., 2017; Handhal et al., 2020).

As is evident in Fig. 3, the maximum gamma ray readings of source rock intervals are approaching 700 API units (Fig. 3). The highest gamma-ray responses are the most recognizable petrophysical features of source rocks in the Upper Triassic Yanchang Formation in Ordos Basin, China (>300 API) (Fig. 3). There are controversies about whether TOC and GR logs are directly related (Passey et al., 1990; Wang et al., 2019). There is a general trend that GR readings increasing with TOC content, however, the correlation factor is moderate ($R^2 = 0.62$, and the data point are scattered), in addition, photoelectric factor (Pe) log is also weakly positively correlated with TOC content (Fig. 4A-4B). Pe log is sensitive to variation in lithology and mineralogical composition (Lai et al., 2015).

4.1.2. Sonic interval transit time

Three derived-porosity logs (AC, DEN and CNL) are comprehensive reflections of inorganic rock matrix minerals, kerogen and porosity (Zhao et al., 2016; Lai et al., 2020). Among them, the sonic transit time is the reciprocal of compressional wave velocity, and reflects lithology, porosity and fluid types as well as presences of kerogen (Sfidari et al., 2012; Bolandi et al., 2017; Handhal et al., 2020). Kerogen and even bitumen is recognized as acoustically slow (Harris et al., 2019). Sonic transit interval time of organic matters (about 524.9 μs/m) is much larger than that of rock matrix, therefore source rock intervals have high AC (compressional) values (Fig. 3) (Wang et al., 2019; Harris et al.,

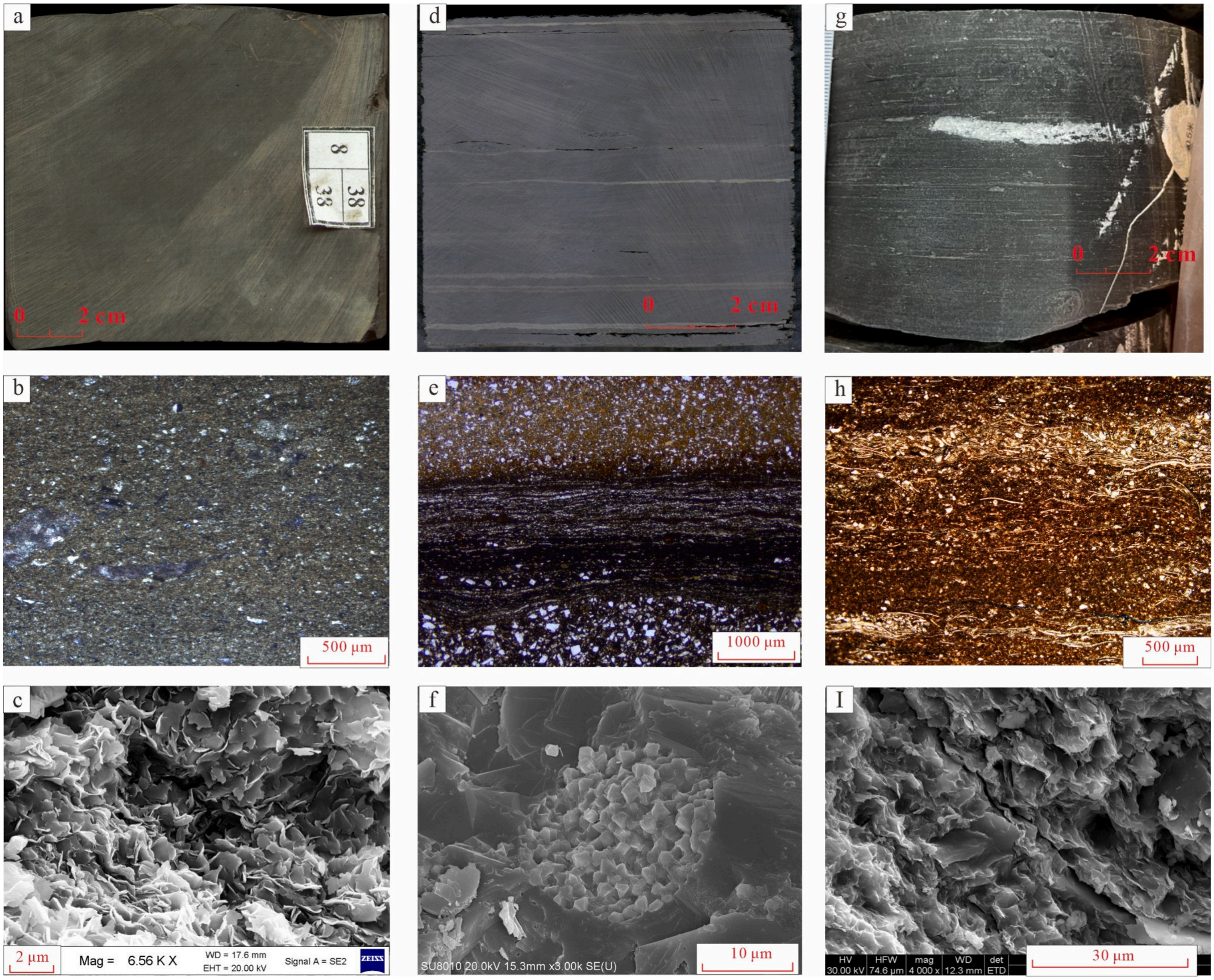

Fig. 2. Core photos, thin sections and SEM image showing the various source rocks in China (Lai et al., 2022a,b, 2023b, 2023c).
a. Dolomitic mudstones, Lucaogou Formation in Junngar Basin, Well Ji 10,025, 3536.19 m (Lai et al., 2023c).
b. Dolomitic mudstones, Lucaogou Formation in Junngar Basin, Well Ji 10,025, 3525.3.
c. Micropores in clay minerals, Lucaogou Formation in Junngar Basin, Well Ji 10,014.
d. Shaley siltstone, Yanchang Formation in Ordos Basin, Well Cheng 96, 2056.59–2056.72 m.
e. Clay, organic matter and silt lamina, Yanchang Formation in Ordos Basin, Well Le 85, 1589.89 m.
f. Pyrite, Yanchang Formation in Ordos Basin, Cai 30, 1970.05 m.
g. Laminated shales, Qingshankou Formation in Songliao Basin, Well Guye 33.
h. Shales abundant in shell fossils, Qingshankou Formation in Songliao Basin, Well Guye 2HC.
i. Abundant clay minerals, Qingshankou Formation in Songliao Basin, Well Guye 2HC, 2378.58 m.

2019; Lai et al., 2022a). The AC value actually increases with TOC content (Fig. 4C). However, moderate R^2 values are observed in the linear regression analysis between TOC and AC values (Fig. 4C).

With the increasing burial depth, the degree of formation compaction will be increased, and therefore deeply buried source rocks may have lower AC readings than the immature source rocks (Wang et al., 2019; Handhal et al., 2020). In addition, the effects of lithology, porosity, fracture as well as gas-bearing layers on AC logs are greater than the DEN logs (Ali et al., 2022). Therefore, the single AC log curve can't actually reflect the variations of source rocks alone (Passey et al., 1990).

4.1.3. *Compensated neutron porosity*

The compensated neutron log measures porosity of the logged formation based on the concentration of hydrogen atoms, as measured by incoming neutrons from a chemical radioactive source in logged formation (Bolandi et al., 2017). The organic matter-rich source rocks are characterized by high hydrogen index, and high neutron logging value will be encountered in source rock intervals (Sfidari et al., 2012; Wang et al., 2019). As a result, very high CNL log readings (>45 %) are detected in the source rock intervals (Fig. 3). In addition, positive relationships will be observed between the neutron log values and TOC content, however, neutron porosity is easily affected by gas effects (Fig. 4D) (Bolandi et al., 2017; Wang et al., 2019; Shalaby et al., 2019).

Large variations between helium-measured porosity and neutron porosity values will be detected in the source rock intervals since kerogen and bitumen belong to rock volume, but have high hydrogen index (Harris et al., 2019). The advantage of neutron logging tool is its sensitivity to low amounts of organic carbon (Passey et al., 1990; Khoshnoodkia et al., 2011). In shale gas play, "neutron mining" effect

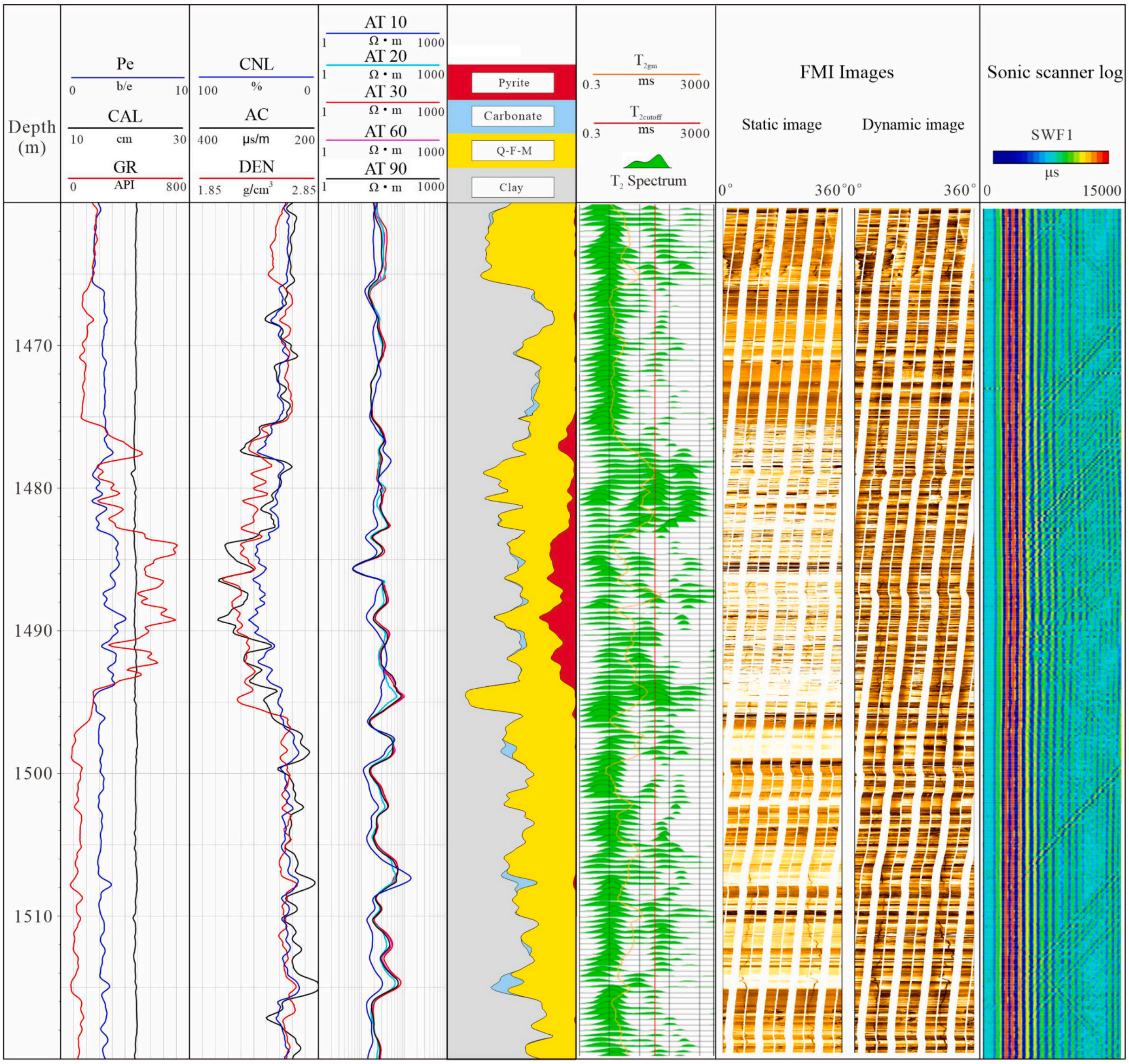

Fig. 3. Conventional and advanced well log responses of source rocks (1480–1495 m) in Upper Triassic Yanchang Formation Member 7 in Ordos Basin (Well Zheng 53).

(decreased neutron logging value) should be taken into consideration (Hui et al., 2023).

4.1.4. *Bulk density*

Density logs (DEN, RHOB) measure the bulk density of the logged formation, and bulk density is mainly influenced by matrix mineral density, porosity and fluids (Bolandi et al., 2017; Lai et al., 2018; Shalaby et al., 2019; Handhal et al., 2020). Organic matter-rich shales have only bulk density of about 1.1 to 1.4 g/cm^3, and bitumen density (0.8–1.2 g/cm^3) is lower than that of kerogen (Harris et al., 2019). In contrast, the bulk density of non-organic shales is close to 2.7 g/cm^3, additionally reservoir rocks (2.65 g/cm^3 for sandstone, or 2.71 g/cm^3 for carbonate rocks) also have a much higher bulk density than organic matter-rich shales (Shalaby et al., 2019; Wang et al., 2019; Wood, 2020).

As a result, the presence of organic matter tends to decrease the bulk density of the source rock intervals (Shalaby et al., 2019). The bulk density is significantly decreased to 2.2 g/cm^3 or lower in source rock intervals in the Upper Triassic Yanchang Formation in Ordos Basin (Fig. 3). In addition, the density log is negatively correlated with TOC content, and the bulk density is almost less than 2.3 g/cm^3 when TOC content is higher than 5.0 % (Fig. 4E). DEN log produces the higher R^2 value in Fig. 4E, which indicates a strong correlation between DEN log and TOC content.

Therefore many scholars proposed the method to predict TOC content using density logs (Schmoker, 1979; Khoshnoodkia et al., 2011; Kim et al., 2017; Harris et al., 2019; Handhal et al., 2020; Ali et al., 2022). However, bulk density log is sensitive to the borehole regularity, and borehole collapse, which are common in mudrock intervals, will affect the linear relationships between TOC and bulk density. The TOC prediction should not rely on single-well log data.

4.1.5. *Resistivity*

Resistivity logs (induction logs, laterlog logs, etc) measure the formation electrical conductivity (Handhal et al., 2020; Zheng et al., 2021). Resistivity is affected by lithology, pore fluids (water or hydrocarbon) as well as specially conductive (pyrite) or resistive (carbonate) mineral components (Zhao et al., 2016; Zheng et al., 2021; Lai et al., 2021). Non-organic mudstone intervals will exhibit low resistivity due to the conductivity of mudstones (both the rock skeleton clay minerals and the pore saline water are conductive) (Wang et al., 2019). Hydrocarbon and organic-rich source rocks are associated with high resistivity values since the organic matters are nonconductive (Nixon, 1973; Meissner,

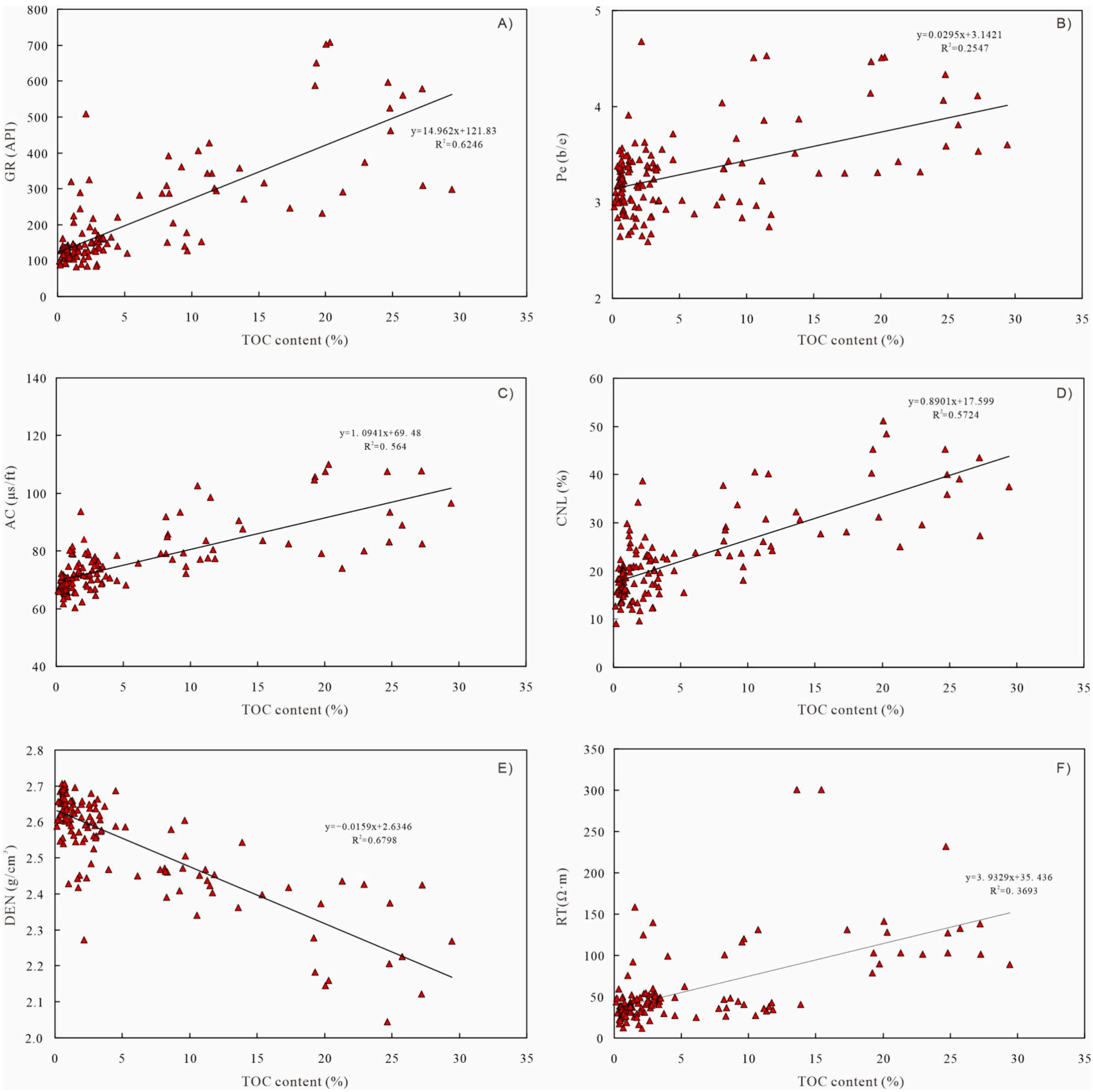

Fig. 4. Crossplots of logging curves versus TOC content of source rocks in Upper Triassic Yanchang Formation Member 7 in Ordos Basin.

1976), and additionally the resistivity will be dramatically increased in mature source rocks due to the expelled hydrocarbons (Khoshnoodkia et al., 2011; Bolandi et al., 2017; Shalaby et al., 2019). Resistivity logs are very sensitive to the organic matters (Gama and Schwark, 2023).

The high and fluctuated resistivity curves of source rock intervals in the Upper Triassic Yanchang Formation in Ordos Basin support the high resistivity responses (Fig. 3). Apparently, data points in the crossplots of resistivity and TOC are more scattered (Fig. 4F). The resistivity responses of source rocks will be affected by its inherent TOC content as well as the presences or pyrites (Bolandi et al., 2017).

4.2. Advanced well log suits

Source rock intervals can be identified by distinguishable responses of gamma rays, porosity and resistivity logs (Tan et al., 2015; Godfray and Seetharamaiah, 2019). The rich hydrogen index, high radioactivity and low electrical conductivity of kerogen result in high GR, high CNL and high resistivity values (Feng et al., 2023). Additionally, the acoustically slow and loose physical properties of kerogen contribute to a high sonic transit time and low bulk density (Tan et al., 2015; Zhao et al., 2016; Godfray and Seetharamaiah, 2019; Handhal et al., 2020; Feng et al., 2023; Maroufi and Zahmatkesh, 2023; Lai et al., 2024a).

Besides conventional well logs, advanced well log suits, which include Elemental Capture Spectroscopy (ECS) logs or LithoScanner logs, image logs, Nuclear Magnetic Resonance (NMR) logs, can also be used for recognition of source rock intervals (Fig. 3).

The image logs are bright yellow to white due to the high resistivity of source rocks (Fig. 3). The image log patterns of source rock intervals are very frequently alternated due to the abundant millimeter-scale laminae in shales (Fig. 3). In addition, dark spots can be recognized, which imply the presences of conductive pyrites in the 1480–1490 m (Fig. 3) (Lai et al., 2022a). In addition, there are interesting fractures in the 1460–1470s interval (Fig. 3).

The ECS logs, which provide the relative content of clay, quartz-feldspar-mica, carbonate and pyrites, have distinguishable responses to the source rock intervals. Highest pyrite content is encountered in the source rock intervals, which the content of quartz-feldspar-mica and carbonate is low (Fig. 3) (Lai et al., 2022a).

The long transverse relaxation (T_2) time of NMR logs, wide and multi-modal T_2 spectrum as well as the tail distributions may indicate the residual hydrocarbons within the source rock intervals (Fig. 3) (Lai et al., 2022a).

The array acoustic logs show no distinguishable responses in the source rock intervals, however, the "V" shape interferometric fringes may imply the attenuation (loss of energy) of sonic waves in source rock intervals (Fig. 3) (Lai et al., 2022a).

5. TOC prediction using conventional well logs

TOC is a basic and critical parameter for hydrocarbon potential evaluation (Tan et al., 2015; Wang et al., 2018; Bai and Tan, 2021). High TOC content often means a high productivity and a high rate of organic carbon burial (Wu et al., 2017). However, TOC is the physical property that cannot be directly measured by geophysical logging methods (Qian et al., 2019). Different well log series have varied responses to TOC variations, which lay the foundation for TOC characterization via well logs (Passey et al., 1990; Wang et al., 2016; Xu et al., 2017; Wood, 2020). Therefore, compared with the expensive and time-consuming core laboratory analysis results, geophysical well log predicted TOC can provide continuous results through the borehole (Tan et al., 2015; Wang et al., 2018). Up to now, there are many geophysical models (resistivity log, sonic, density or GR spectrum logs based, etc) proposed to determine TOC content from borehole geophysical data (Schwarzkopf, 1992; Mahmoud et al., 2017; Wang et al., 2018; Ali et al., 2022; Lee and Lumley, 2023; Lai et al., 2024a).

5.1. Schmoker method

Schmoker's methods are proposed in the 1980s to calculate TOC mainly using bulk density logs (Schmoker, 1979; Schmoker, 1981; Schmoker and Hester, 1983). The total density of formation is the comprehensive reflection of matrix (~2.65 g/cm^3), pores, pyrite (~5.0 g/cm^3), and organic matters (~1.0 to 1.5 g/cm^3) (Schmoker, 1979; Mahmoud et al., 2017). Then the content of organic matters can be estimated by regression analysis using density logs.

The relationships between TOC content (weight) and logged bulk density of formation can be written as:

$$TOC = (\rho_b - \rho)/1.378 \tag{1}$$

In Eq.1, ρ_b is the formation density without organic matter (g/cm^3), ρ is the logged formation density (g/cm^3) (Schmoker, 1979; Mahmoud et al., 2017).

Schmoker and Hester (1983) further proposed that TOC has a positive linear correlation with reciprocal of bulk density (Eq.2) (Schmoker and Hester, 1983; Yu et al., 2017):

$$TOC = \left(A \times \frac{1}{\rho}\right) - B \tag{2}$$

In Eq.2, ρ is the logged formation density (g/cm^3), while A and B are constants (Schmoker and Hester, 1983; Yu et al., 2017):

In the previous decades, Schmoker and ΔlgR models are two frequently adopted conventional techniques to estimate TOC content using well logs (Mulashani et al., 2021). The Schmoker methods assume that any change in the bulk density is due to presence or absence of organic kerogen (Mahmoud et al., 2017). However, the borehole regularity will affect the logged bulk density values. Additionally, the presences of pyrites will destroy the linear regression relationship between TOC and bulk density. Therefore, Schmoker's methods are not widely used now, especially in the era of unconventional hydrocarbon resources (Lai et al., 2022a; Lee and Lumley, 2023).

5.2. Passey's ΔlgR method

Passey et al. (1990) proposed the method of overlaying RT and porosity logs (AC, DEN, CNL), known as the ΔlgR method (Eq.3; Eq.4), to predict TOC content. Up to now, Passey's ΔlgR method is widely used for TOC prediction via well logs in carbonates and clastic rocks (Mahmoud et al., 2017; Zhu et al., 2020; Cappuccio et al., 2021; Lai et al., 2022a).

$$\Delta logR = log(R/R_{Baseline}) + 0.02(\Delta t - \Delta t_{Baseline}) \tag{3}$$

$$TOC = \Delta logR \times 10^{(2.297-0.1688LOM)} \tag{4}$$

In the above equations, R is deep resistivity (RT) log (Ω·m), and Δt (AC) is the sonic transit time (μs/ft. or μs/m); R_{Baseline} and $\Delta t_{\text{Baseline}}$ are the base lines of RT and AC (50 μs/ft. AC log is scaled to one logarithm resistivity cycle, likewise, 100 μs/ft. equals two logarithmic resistivity cycles); LOM is local Level of Organic Metamorphism, which is associated with thermal maturity, and it can be estimated according to the vitrinite reflectance method. LOM = 7 means the beginning of source rock, while LOM = 12 refers to the high mature of source rocks (Hood et al., 1975; Passey et al., 1990; Sfidari et al., 2012; Iqbal et al., 2018; Shalaby et al., 2019; Tenaglia et al., 2020; Ochoa et al., 2022; Lai et al., 2022a).

The two log curves will overlap with each other in organic-lean intervals, while they will be significantly separated in organic-rich intervals, and the quantitative separation between the two logs is used to define ΔlgR (Passey et al., 1990; Ali et al., 2022; Gama and Schwark, 2023). The separation in the organic-rich rocks is due to the effect of the low density and low velocity of kerogen and the high resistivity (Mahmoud et al., 2017). After the porosity and resistivity curves are superimposed, a baseline is obtained within a fine-grained, non-source interval (Passey et al., 1990; Ali et al., 2022). If AC log curve is not available, then density or neutron log can be used instead (Khoshnoodkia et al., 2011; Mahmoud et al., 2017; Shalaby et al., 2019; Tenaglia et al., 2020; Lai et al., 2022a).

By superimposing the deep resistivity log over DEN, one logarithmic resistivity cycle equals 0.4 g/cm^3 (1 Ω·m corresponds to 0.4 g/cm^3). When using CNL logs (CNL against LLD), 1 Ω·m may be equal to 0.25 *v*/v. The equations to determine ΔlgR using DEN and CNL log, which is then used to calculate *TOC*, can be written as (Eq.5, Eq.6).

$$\Delta logR = log(R/R_{Baseline}) + 4.0(\varphi_n - \varphi_{nBaseline}) \tag{5}$$

$$\Delta logR = log(R/R_{Baseline}) + 2.5(\rho_b - \rho_{bBaseline}) \tag{6}$$

R_{baseline} is the baseline value for the resistivity curve related to the DEN baseline value; ρ_{b} is bulk density values from DEN curve, and ρ_{baseline} is the DEN baseline value. In addition, $\text{CNL}_{\text{baseline}}$ is the neutron porosity baseline value related to resistivity curve. (Passey et al., 1990; Mahmoud et al., 2017; Li et al., 2020).

The ΔlgR method (the baseline is selected as 4.5 Ω·m and 73 μs/ft) is used to predict the TOC content of the Cretaceous Qingshankou Formation shales in the Gulong Sag of Songliao Basin in East China, and the good fits between predicted TOC and core-measured TOC proves the accuracy of ΔlgR method (Fig. 5). However, there are some data points offset the fitting lines with a R^2 of 0.56, indicating ΔlgR method may need modified to improve accuracy (Fig. 6A).

The ΔlgR method is still widely used for TOC prediction due to its convenience and versatility (Li et al., 2020). Passey's ΔlgR method has

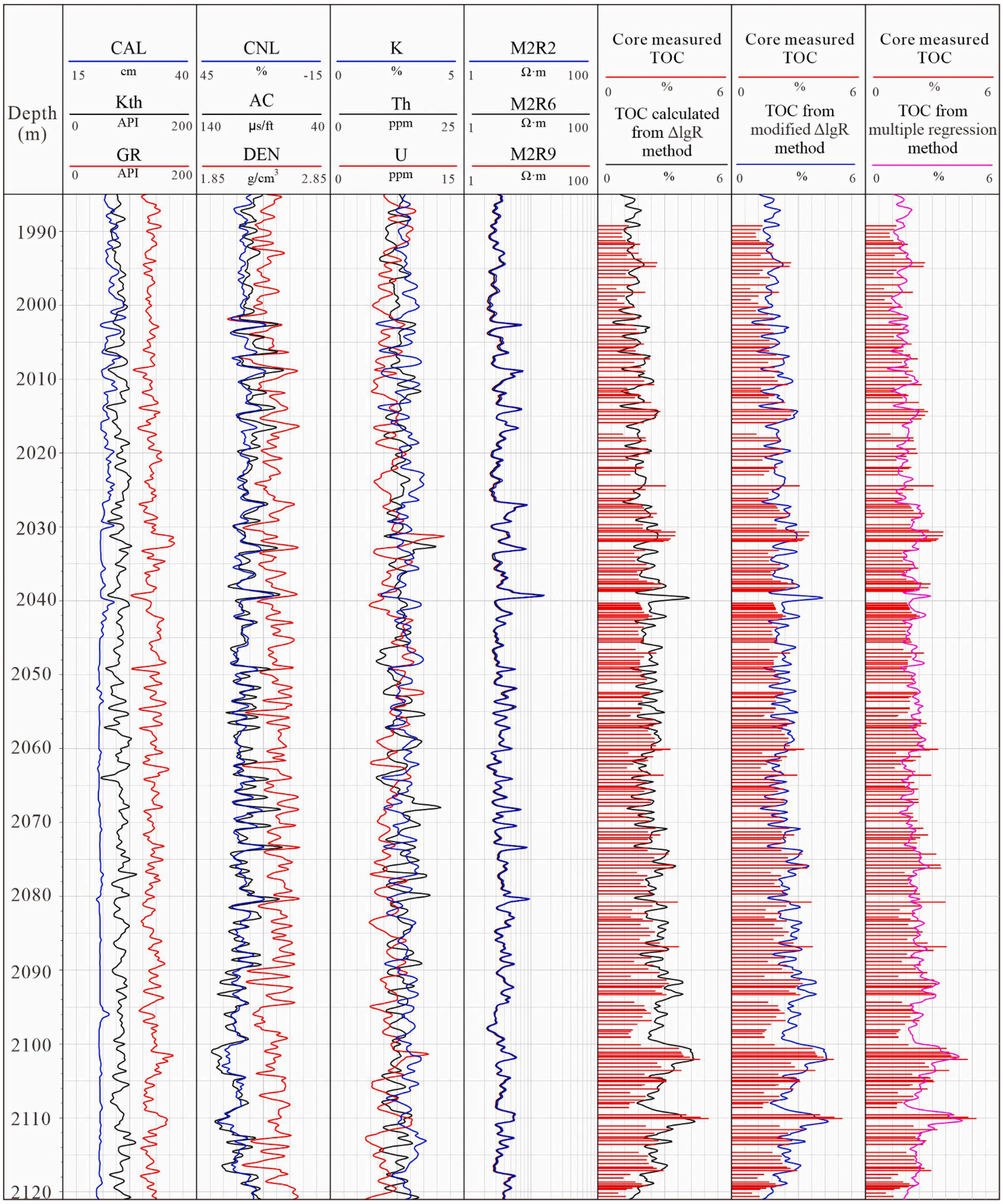

Fig. 5. The prediction of TOC content in the Cretaceous Qingshankou Formation in the Gulong Sag, Songliao Basin, using ΔlgR method, ΔlgR method with variable baseline value and multiple regression analysis method.

more widely selected parameters than Schmoker method (Yu et al., 2017). This method is a qualitative approach to predict TOC with high accuracy (Ochoa et al., 2022; Lai et al., 2022a).

Though widely applied in industrial and academic fields, two major drawbacks exist in the ΔlgR technique: (1) the constant slope of 0.02 between the porosity and logarithmic resistivity logs is too ideal; (2) the assumption of homogeneous rock composition and texture (Mahmoud et al., 2017; Iqbal et al., 2018; Wang et al., 2019; Zhu et al., 2019). Therefore, the ΔlgR method is not extended in the shale play and frequently interbedded sandstone and mudstone strata (Mahmoud et al., 2017; Zeng et al., 2021). In addition, artificial factors such as baseline selection, will reduce the accuracy of ΔlgR method (Li et al., 2020; Mulashani et al., 2021; Zhang et al., 2022). The presences of pyrite (low resistivity and high density), poor borehole conditions and low porosity intervals should be considered (Kenomore et al., 2017; Sohail et al., 2020).

5.3. *Modified ΔlgR method*

Many scholars try to overcome the limitations of ΔlgR, and proposed modified ΔlgR methods (Wood, 2020; Zheng et al., 2021). There are many ΔlgR based methods to derive TOC content using well logs, and these methods are widely used in various basins worldwide (Zhao et al., 2016). The common revisions on the ΔlgR method include (1) use a changeable slope but not 0.02 in Eq.3; (2) changing baseline in different formation; (3) integrate additional logs to improve TOC prediction accuracy; (4) replacing LOM with thermal indicator Tmax or Ro (Wang et al., 2016; Zhao et al., 2017; Mahmoud et al., 2017; Wood, 2020).

For instance, an improved ΔlgR method, which selected baseline and optimized coefficient D automatically according to minimum error between log predicted value and core-measured value, is proposed to evaluate TOC and S1 (Li et al., 2020).

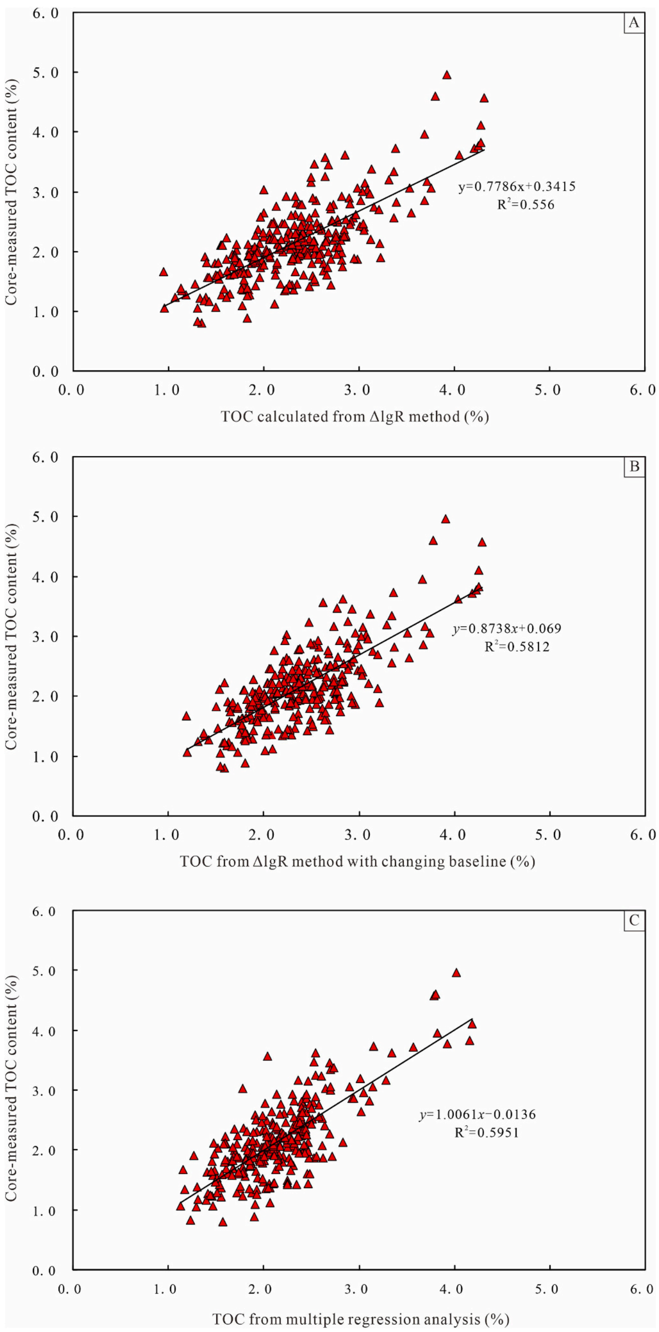

Fig. 6. Crossplots of core-measured TOC content versus TOC predicted from well logs in the Cretaceous Qingshankou Formation in the Gulong Sag, Songliao Basin of East China.
A. core-measured TOC content versus TOC predicted from ΔlgR method.
B. core-measured TOC content versus TOC predicted from ΔlgR method with changing baseline value.
C. Core-measured TOC content versus TOC predicted from multiple regression analysis method.

$$\Delta logR = D \times log(R/R_{\text{Baseline}}) + (1-D)(\Delta t - \Delta t_{\text{Baseline}}) \quad (7)$$

$$TOC = A \times \Delta logR + B \quad (8)$$

where $\Delta t_{baseline}$ (μs/ft) and $R_{baseline}$ (Ω·m) are baseline values of AC and RT log. D is proportionality coefficient representing the relative proportion of resistivity curve in ΔlgR. A and B are model coefficients, constant (Li et al., 2020).

The shortcomings of the ΔlgR are the variable log-baseline in various logged formations and different wells (Wang et al., 2019; Mulashani et al., 2021; Zhang et al., 2022), therefore, the commonly used modified ΔlgR method is the changing baseline ΔlgR method. As the varying baselines of different formations, changing baselines are selected to improve prediction accuracy (Zheng et al., 2021).

The modified ΔlgR method (changing baseline, the baseline of Member 1 of Qingshankou Formation is selected as 3.5 Ω·m and 75 μs/ft., while the baseline of Member 2 of Qingshankou Formation is selected as 5.0 Ω·m and 71 μs/ft) is used to predict TOC content of the Cretaceous Qingshankou Formation in the Gulong Sag of Songliao Basin in East China, and the predicted TOC values fit well with core-measured TOC (Fig. 5). In addition, correlation coefficient is improved than ΔlgR method, and R^2 is improved from 0.56 to 0.58 (Fig. 6B).

5.4. Natural gamma ray spectrum

As previously discussed, TOC content is strongly correlated to natural gamma ray spectrum (especially uranium, U) in source rocks (Harris et al., 2019). Therefore, spectral gamma ray logs (K (%), U (ppm), and Th (ppm), and their ratios) can be used for TOC prediction through regression analysis (Sérgio et al., 2018; Wood, 2020; Lai et al., 2022a; Gama and Schwark, 2023).

The linear or non-linear relationship between TOC and U curve can be established by regression analysis (Tenaglia et al., 2020). In addition, TOC content can be correlated with U/Th ratio, and higher U/Th relates to higher TOC content (Wood, 2020). Actually decreased TOC content will be encountered with increasing Th/U ratio (Gama and Schwark, 2023).

Regression analysis is performed between spectral GR logs (K, Th, U and U/Th) and core measured TOC content in the Cretaceous Qingshankou Formation in the Gulong Sag of Songliao Basin, however, it is found that there are no curve can be used in TOC prediction (with very low R^2 values) (Fig. 7).

Actually, the Cretaceous Qingshankou Formation in the Gulong Sag of Songliao Basin in East China is deposited in a lacustrine environment (Pang et al., 2023), and TOC content shows very poor correlation relationships with spectral gamma ray logs, maybe it is the abundant of clay minerals affect the relationship between TOC and gamma ray spectrum, consequently, the application of spectral gamma ray logs in lacustrine source rock analysis is difficult (Fig. 7).

The disadvantage of this method is that the unavailability of spectral gamma ray logs (Wood, 2020), and in addition, for marine source rocks, spectral gamma ray logs are useful indicators of high hydrocarbon amounts because of uranium enrichment. However, U enrichment is not common in lacustrine source rocks, and GR readings mainly indicate overall clay contents (Zheng et al., 2021).

5.5. Multiple regression analysis

Almost all the geophysical well log series are sensitive to the presence of organic matter (Passey et al., 1990; Handhal et al., 2020; Lai et al., 2022a; Gordon et al., 2022). However, a single log curve may also be influenced by downhole conditions, lithology, and pore fluids (Gordon et al., 2022; Lai et al., 2023a). In addition, the complex relationships between TOC and well logs make it difficult to evaluate TOC using a single log curve (Zhang et al., 2022). Consequently, multiple log curves, which include a wide range of log series (GR, AC, CNL, DEN and RT, etc), are needed for source rock prediction (Khoshnoodkia et al., 2011; Godfray and Seetharamaiah, 2019; Gordon et al., 2022). Mendelson and Toksoz (1985) proposed the multi-variate regression analysis method to predict TOC from combination of wireline log curves.

Taking TOC as the dependent variable, while the logging parameters as independent variables, a multiple regression equation can be regressed (Eq.9). As is shown in Eq.9, the *TOC* is positively correlated with GR, AC and RT while negatively correlated with density (Feng et al., 2023). The log prediction model of TOC of Permian Lucaogou

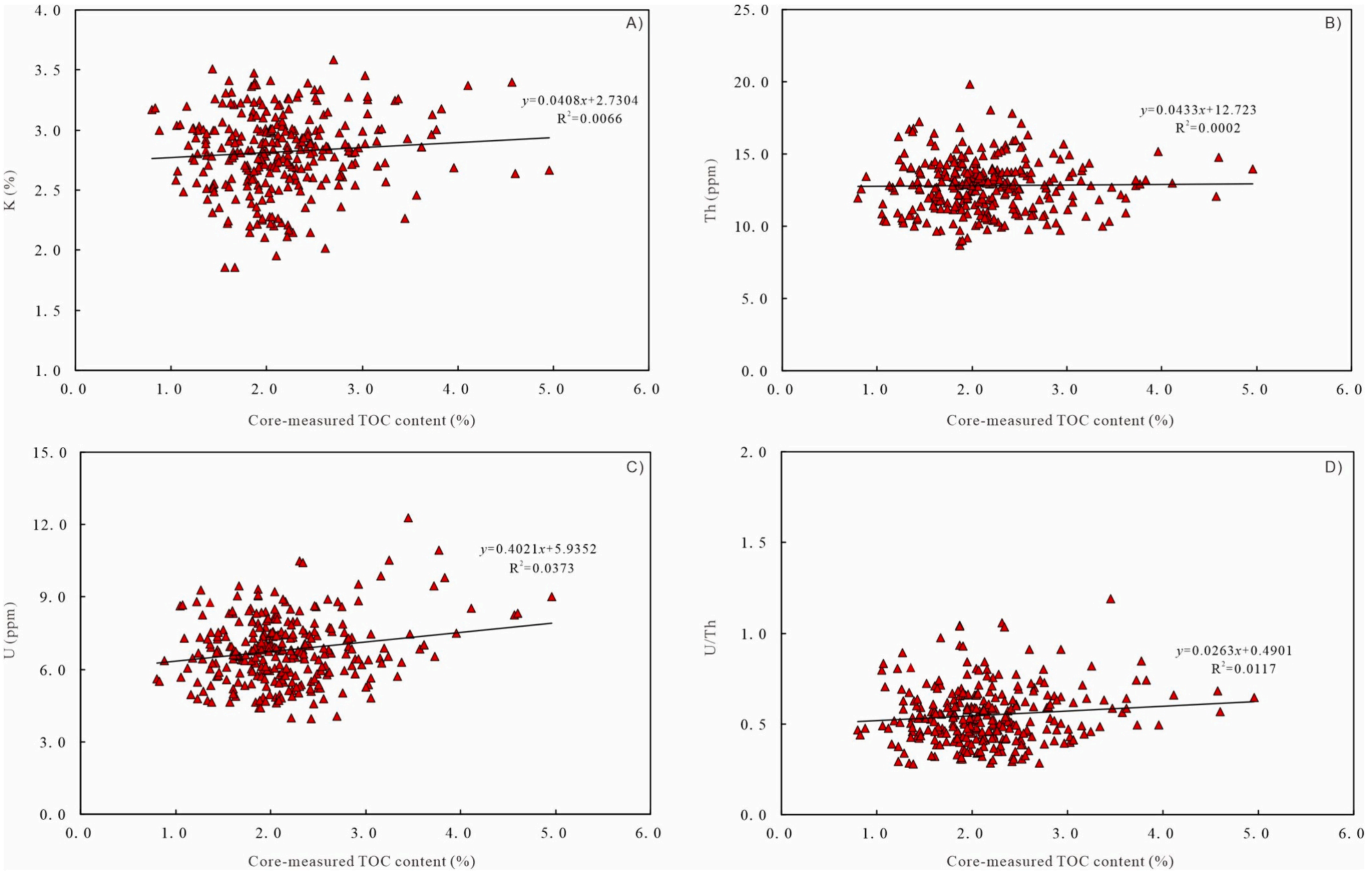

Fig. 7. Crossplots of spectral gamma ray versus core-measured TOC content in the Cretaceous Qingshankou Formation in the Gulong Sag, Songliao Basin of East China.
A. K content versus core-measured TOC content.
B. Th content versus core-measured TOC content.
C. U content versus core-measured TOC content.
D. U/Th ratios versus core-measured TOC content.

Formation in Jimusar Sag of Junngar Basin in West China, is established by multiple regression analysis method (Fig. 8), and the results show a good correlation ($R^2 = 0.69$) with core measured TOC values (Fig. 9). The predicted TOC curve is infinitely close to the core measured TOC content (Fig. 9), indicating that the results are reliable. Actually, the accuracy of multi-parameter fitting model is higher than the single variable model (Zhang et al., 2023; Feng et al., 2023). The multiple linear regression method considers many explanatory parameters as inputs, therefore it can give a relatively accurate output result (Hui et al., 2023).

$$TOC = -0.52*DEN + 0.034*AC + 0.0074*GR + 2.85*log(RT) - 1.99 \tag{9}$$

Multiple regression analysis is also performed on the Cretaceous Qingshankou Formation in the Gulong Sag of Songliao Basin in East China, and the regression formula can be written as (Eq.10). As a result, the prediction results of TOC are in good accordance with core measured TOC values (Fig. 5), and the correlation coefficients ($R^2 = 0.59$) are a little higher than the ΔlgR and modified ΔlgR methods (Fig. 6C), indicating that multiple regression analysis can be better to predict TOC in the Gulong Sag.

$$TOC = -0.052*CNL + 0.033*AC + 0.0074*GR + 4.04*log(RT) - 5.78 \tag{10}$$

The disadvantage of this method is that the established correlations only work well for one location, but cannot be reliably applied universally (Aziz et al., 2020; Wood, 2020; Lai et al., 2022a).

6. TOC prediction using advanced well logs

6.1. NMR logs

Advanced well log series, which include image logs, NMR logs and array sonic logs, have advantages in the fields of structural analysis, sedimentary interpretation, in situ stress analysis, fracture characterization as well as geological and geomechanical evaluation of unconventional reservoirs (Iqbal et al., 2018; Yarmohammadi et al., 2020; Mukhametdinova et al., 2021; Lai et al., 2022a). In addition, the advanced logs also help evaluation and prediction of source rock properties (Jacobi et al., 2008; Zhao et al., 2016; Zhu et al., 2020; Lai et al., 2022a; Lai et al., 2024a).

The method to calculate TOC using NMR logs is proposed by Jacobi et al. (2008), and the differences between NMR log derived porosity and DEN log calculated porosity can be used to estimate TOC content (Zhao et al., 2016; Zhu et al., 2020). NMR logs, which are only sensitive for the presences of pore fluids (hydrogen), will give a total porosity without the contribution from rock matrix (Golsanami et al., 2014; Wang et al., 2020). Therefore, the NMR log derived porosity mainly reflects the hydrogens from pore water and hydrocarbon, and the contribution from kerogen to NMR logs are treated as capillary pores. Bulk density logs are used to derive porosity according to model of bulk-volume rock, and the relationships between bulk density and porosity are mainly linear. Due to the distinctively low bulk density of kerogen, the bulk density log-calculated porosity also reflects the contribution of kerogen. Therefore, the calculated porosity from DEN and NMR logs are approximately

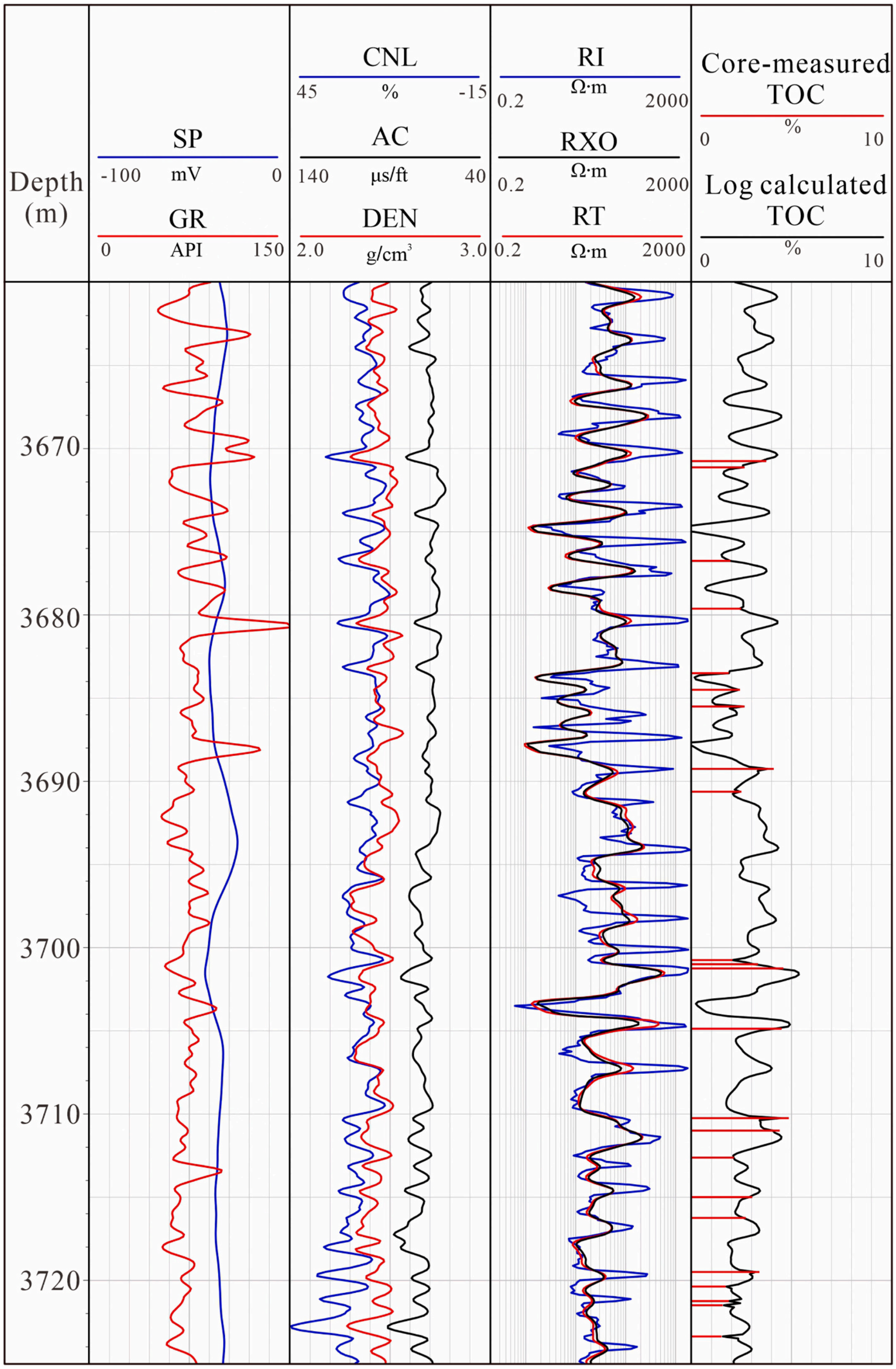

Fig. 8. The TOC content predicted from well logs using multivariate regression method of Lucaogou Formation in Jimusar Sag, Junggar Basin.

the same in nonsource rock intervals. In contrast, NMR porosity and density log porosity will be separated significantly in source rock intervals (Zhao et al., 2016).

Jacobi et al. (2008) method firstly differentiate source rocks and nonsource rocks reasonably, and in addition can be used to predict the TOC content (Fig. 10). In the Upper Triassic Yanchang Formation in Ordos Basin of China, density porosity is calculated in all the logged intervals through regression analysis between bulk density and core-analyzed porosity (Eq.11) (Fig. 10). Then NMR porosity is calculated using NMR T_2 spectrum (Kuang et al., 2020). The T_2 Signals less than 0.3 ms are mainly not the signals of fluids, and the short T_2 components are mainly related to the clay and capillary bound fluids. Lastly, the differences between NMR porosity and density porosity are overlapped to identify the source rock intervals, and the separations between the two curves are used to derive TOC content (Fig. 10).

$$Por = -45.529*DEN + 123.49 \tag{11}$$

The NMR T_2 spectrum has a continuous bimodal or multi-modal distribution with a wide range of amplitude (Fig. 10). In the highest TOC source rock intervals (2064–2074 m), the differences between NMR porosity and density porosity show good agreement with measured TOC content. However, in low TOC intervals (2030–2050 m), the measured TOC content is much lower than the predicted TOC. Generally, the TOC content has a relatively good relationship with the differences between the two porosities (density porosity minus NMR porosity) (Fig. 11). Therefore, the NMR log method, if validated by core-to-log calibration,

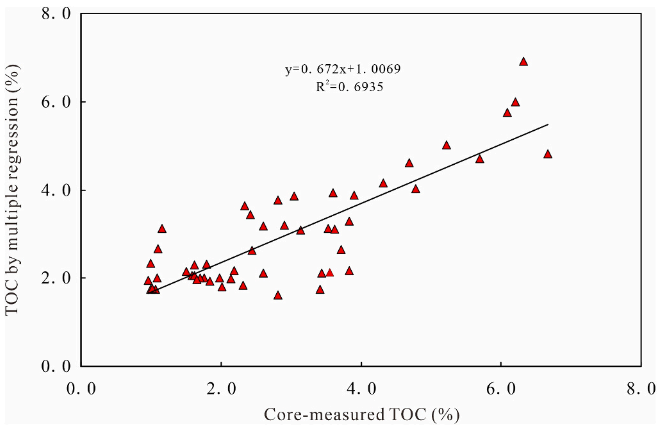

Fig. 9. Crossplot of core-measured TOC content versus TOC calculated using multivariate regression method of Lucaogou Formation in Jimusar Sag, Junggar Basin.

can provide a continuous TOC curve, especially in high TOC source rock intervals (Zhao et al., 2016; Feng et al., 2023). The disadvantage of this method is that NMR logs are not available in all wells due to high cost (Zhao et al., 2016). In addition, the presences of pyrites will affect the calculated NMR porosity, and gas effect will result in a low NMR porosity when the source rocks are saturated with gas, i.e., shale gas (Su et al., 2024).

6.2. Litho-Scanner logs

The Litho-Scanner logs provide element content of carbon (C), potassium (K), magnesium (Mg), aluminum (Al), silicon (Si), calcium (Ca) and sodium (Na), etc. (Guo et al., 2019). Then the mineralogy content, including total clay, quartz-feldspar-mica (Q-F-M), carbonate and pyrite can be obtained through data processing (Maliva et al., 2009; Collett et al., 2011; Lai et al., 2017) (Fig. 3). The Litho-Scanner log can provide the total carbon element content (TC), since the inorganic carbon (TIC) in the formation is mainly associated with carbonate rocks (calcite, $CaCO_3$, and dolomite $CaMg(CO_3)_2$, etc) (Lai et al., 2022a). Therefore the TOC content can be estimated using Litho-Scanner log by TC minus TIC (TC-TIC) (Fig. 10; Lai et al., 2024a). The Litho-Scanner log is also used for TOC prediction in Lucaogou Formation in Jimusar Sag of Junnggar Basin, and high inorganic carbon content is associated with the high carbonate content, while high TOC intervals are related to the high clay content (Fig. 12). Similar with NMR log, the disadvantages of Litho-Scanner log are mainly the high cost.

7. TOC prediction using artificial intelligence

Machine learning and artificial intelligence (AI) are now playing key roles in solid earth geoscience and earth system science (Bergen et al., 2019; Reichstein et al., 2019). The big geophysical well log data also require machine learning and artificial intelligence methods to dig and the decode the contained geological information. Relationships between TOC content and well logs in source rocks are complex, and the complicated and nonlinear relationships need the data-driven AI methods to be incorporated to predict TOC content using well logs (Sfidari et al., 2012; Tabatabaei et al., 2015; Wang et al., 2019; Wood, 2020; Lai et al., 2022a; Zhang et al., 2023; Lai et al., 2024b).

Therefore the traditional methods (multiple regression analysis, ΔlgR method, etc) to predict TOC content may face limitations of human error, complex operation and big workload (Wang et al., 2018; Zhang et al., 2023). Intelligent systems and machine learning methods are recently widely applied to analyze the complex relationships between TOC and geophysical well log variables (Mahmoud et al., 2017; Wang et al., 2019; Wood, 2020; Zhu et al., 2020; Ganguli et al., 2022; Lai et al., 2024a). Compared with simple or multivariate regression methods above, the AI methods involve multiple well log curves to unravel the complex nonlinear relationship, and they have advantages for TOC estimation (Zhang et al., 2022; Ganguli et al., 2022). The AI method will minimize the artificial error, improve accuracy and speed, especially for the big data matrix.

7.1. AI methods for TOC prediction

In the 1990s, attempts have been performed to predict TOC using machine learning method (Huang and Williamson, 1996). Nowadays, more and more data-driven intelligent methods are proposed to calculate TOC content using well logs. Artificial neural networks (ANN), support vector machine (SVM), and Gaussian process regression (GPR) are the most employed methods for TOC evaluation and prediction (Bolandi et al., 2017; Rui et al., 2020; Nyakilla et al., 2022).

The neuro-fuzzy methods are proposed to predict the TOC-rich intervals (Kamali and Mirshady, 2004). Ant colony optimization back propagation neural network is used to improve the TOC prediction accuracy using the combination of AC, DEN, RT and CNL logs (Kadkhodaie-Ilkhchi et al., 2009).

As an artificial neural network (ANN) method, the back propagation (BP) neural network method is employed by many scholars for TOC prediction (Sfidari et al., 2012; Tan et al., 2013; Mahmoud et al., 2017; Wang et al., 2019; Li et al., 2020; Zhang et al., 2023).

Support vector machine (SVM) method, which uses supervised kernel-based machine learning algorithm, can output a high accuracy TOC prediction result via well logs (Tan et al., 2015; Bolandi et al., 2017; Wang et al., 2018; Handhal et al., 2020; Wood, 2020). The SVR method is more suitable for predicting TOC content under small sample conditions (Rui et al., 2020).

Handhal et al. (2020) uses machine learning random forest (RF) model for TOC prediction using GR, AC, DEN, CNL, and RT logs. The advantage of RF method is that they can model non-linear relationships with high accuracy (Kim et al., 2021; Gordon et al., 2022). Shalaby et al. (2020) showed that the random forest model outperforms ANN and SVM method.

Zeng et al. (2021) uses the 3D surface fitting method, which fit discrete points in space onto a surface, to calculate TOC using GR, CNL, RILM and RILD logs.

7.2. ANN and BPANN method

ANN method provides a collection of connected artificial neurons modeling the neurons in a brain, and the brain-like tool has the ability to make a decision by a machine program (Mahmoud et al., 2017; Handhal et al., 2020). ANN is a neural network with an input layer, a hidden layer, and an output layer (Zheng et al., 2021). The processing of ANN includes training, validating, and testing (Bolandi et al., 2017). After training and validating with actual core data, TOC will be output by inputting log variables.

However, the complex relationships make it difficult for ANN machine learning methods to derive accurate predictions of TOC (Wang et al., 2019; Wood, 2020). In addition, ANN is easily stuck in the local optimum and suffers overfitting and low convergence speed (Wang et al., 2019; Mulashani et al., 2021). Convolutional Neural Network (CNN), which is a deep learning method, can thoroughly decode the multiple and multi-scale nonlinear relationships between input log curves and output TOC content (Zhang et al., 2022). The CNN method has better performance in TOC prediction than ANN method (Zhang et al., 2022).

In addition, back propagation artificial neural network (BPANN) is proposed to improve accuracy and reduce uncertainty (Bhatt and Helle, 2002; Khoshnoodkia et al., 2011). BPANN uses a training method sending input values forward through the network, and then computes differences between output results and the required outputs from

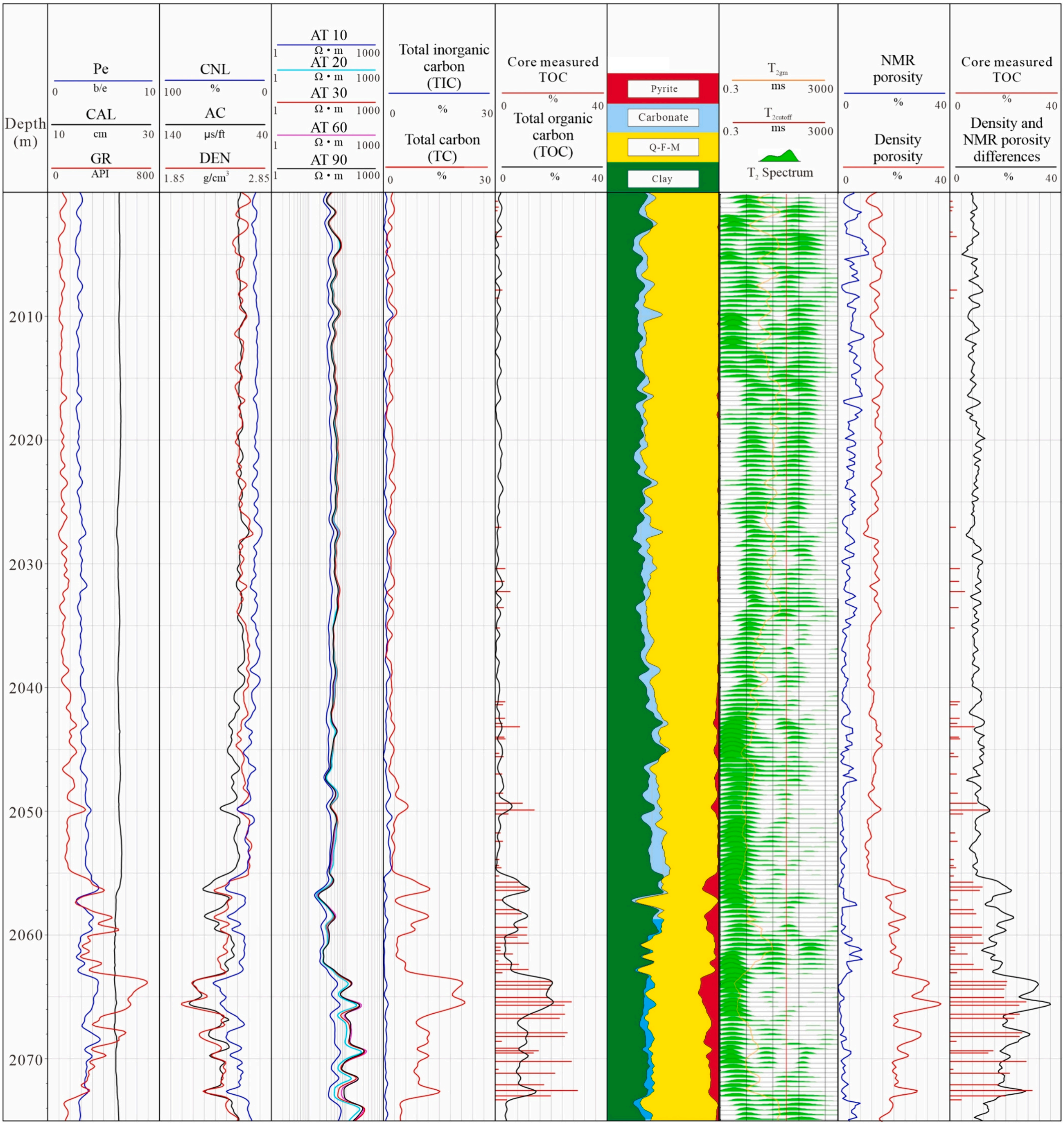

Fig. 10. TOC content predicted from LithoScanner log and NMR log together with density log in Yanchang Formation Member 7 of Ordos Basin, West China (Lai et al., 2024a).
Note the last track is the difference between NMR and density porosity.

training dataset (Bhatt and Helle, 2002; Khoshnoodkia et al., 2011). Then the error is propagated backward through the net, and a number of iterations work in order to improve accuracy. The training process stops when the output results are in accordance with the required values (Bhatt and Helle, 2002; Khoshnoodkia et al., 2011; Zhang et al., 2023). The data will be re-imported into the input layer if the output value is not as ideal as required (Zhang et al., 2023).

The utility of error back propagation algorithm makes the BPANN method widely used in data classification and prediction (Zeng et al., 2021). The geophysical well logs, which are sensitive for source rocks, are selected as input variables of the BP neural network, and they include AC, DEN, CNL, GR, U and RT logs. The Python platform is used for BPANN analysis. About 3/4 of the geochemical analysis data are used for training, while the remaining 1/4 is used for validation. The BPANN provides a more accurate result for TOC calculation than ΔlgR method for the Cretaceous Qingshankou Formation in the Gulong Sag, Songliao Basin of East China (Fig. 13). Crossplots also prove that the BPANN method can provide an accurate TOC predicted result with core-measured TOC content (Fig. 14; Lai et al., 2024a).

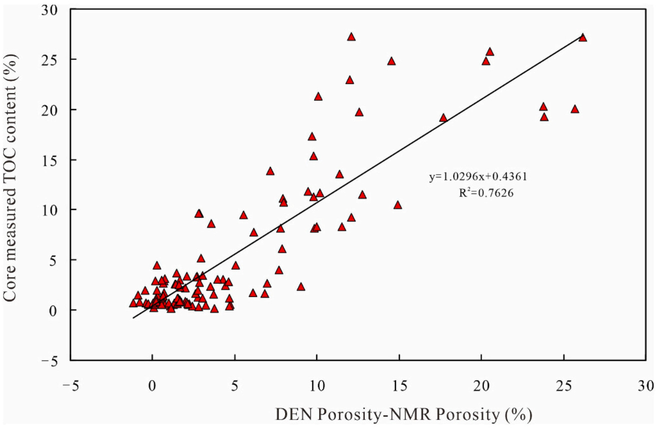

Fig. 11. Crossplot of core measured TOC content versus density and NMR porosity differences in Upper Triassic Yanchang Formation Member 7 in Ordos Basin, West China.

7.3. GBDT and XGBOOST model

Gradient Boosting Decision Trees (GBDT) is a decision tree ensemble learning algorithms (Friedman, 2001; Zhang et al., 2023). Extreme Gradient Boosting (XGBOOST), which is the improvement of GBDT, is powerful on pattern recognition with advantages of gradient boosting decision tree, classification tree and regularization (Gu et al., 2021). XGBoost, which is an excellent machine learning method, introduces regularization term and second-order expansion of Taylor's formula to improve training function, and therefore overfitting can be avoided, which training process can be improved (Fig. 15) (Gu et al., 2021; Pang et al., 2022). XGBoost algorithm has high prediction accuracy and strong generalization performance (Pan et al., 2022; Liu et al., 2023).

The sensitive well logs including CAL, SP, AC, DEN, CNL, GR, RT, Th, U and K logs are adopted for TOC prediction of the Cretaceous Qingshankou Formation in the Gulong Sag, Songliao Basin of East China. About 2/3 of the geochemical analysis data are used for training, while the remaining 1/3 is used for validation (Fig. 15). The XGBOOST provides a more accurate result for TOC calculation than ΔlgR method and BPANN method (Fig. 13). Crossplots also prove that the XGBOOST method output an accurate TOC result with core-measured TOC content

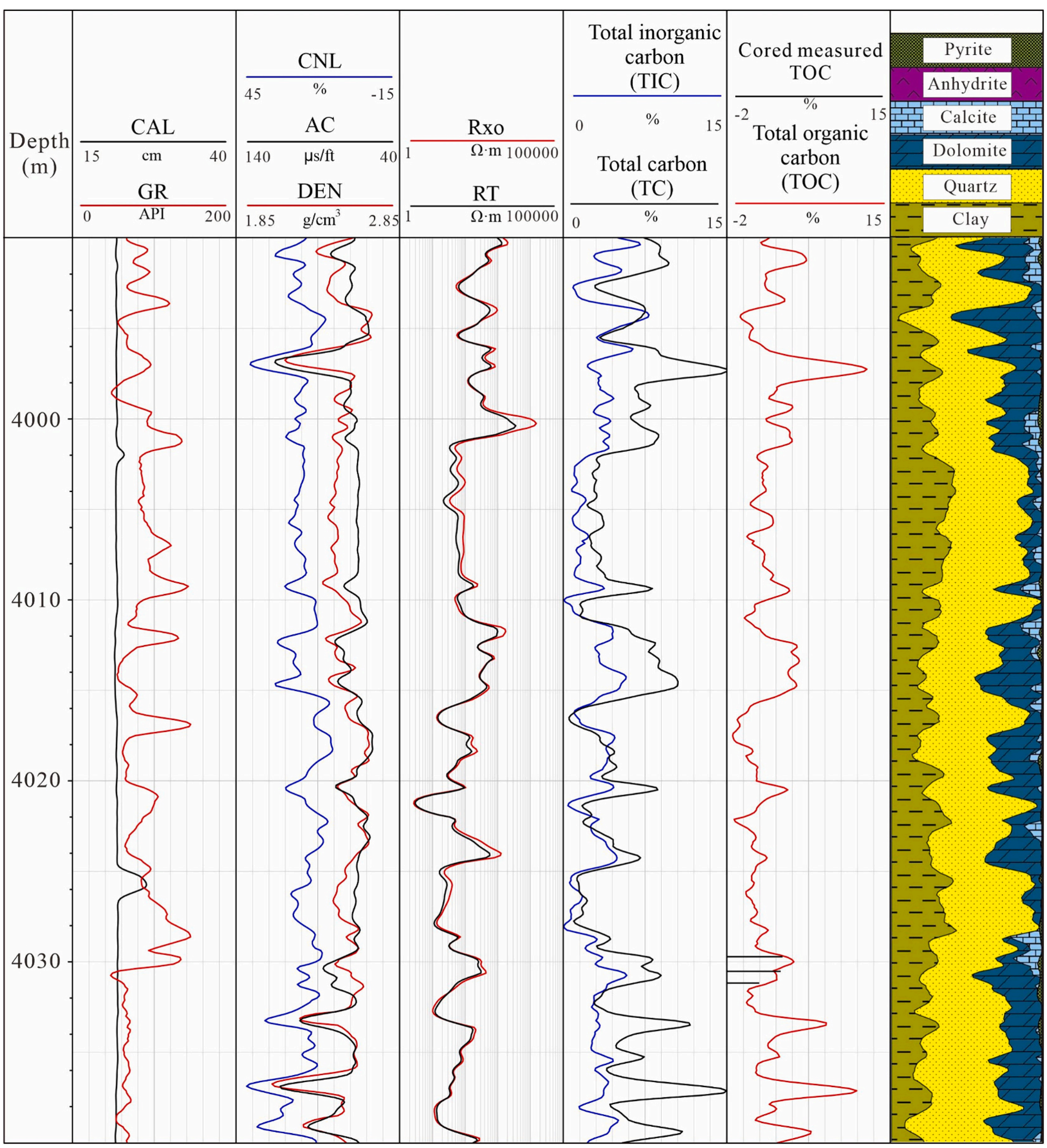

Fig. 12. TOC content predicted from LithoScanner log in Lucaogou Formation in Jimusar Sag, Junngar Basin.

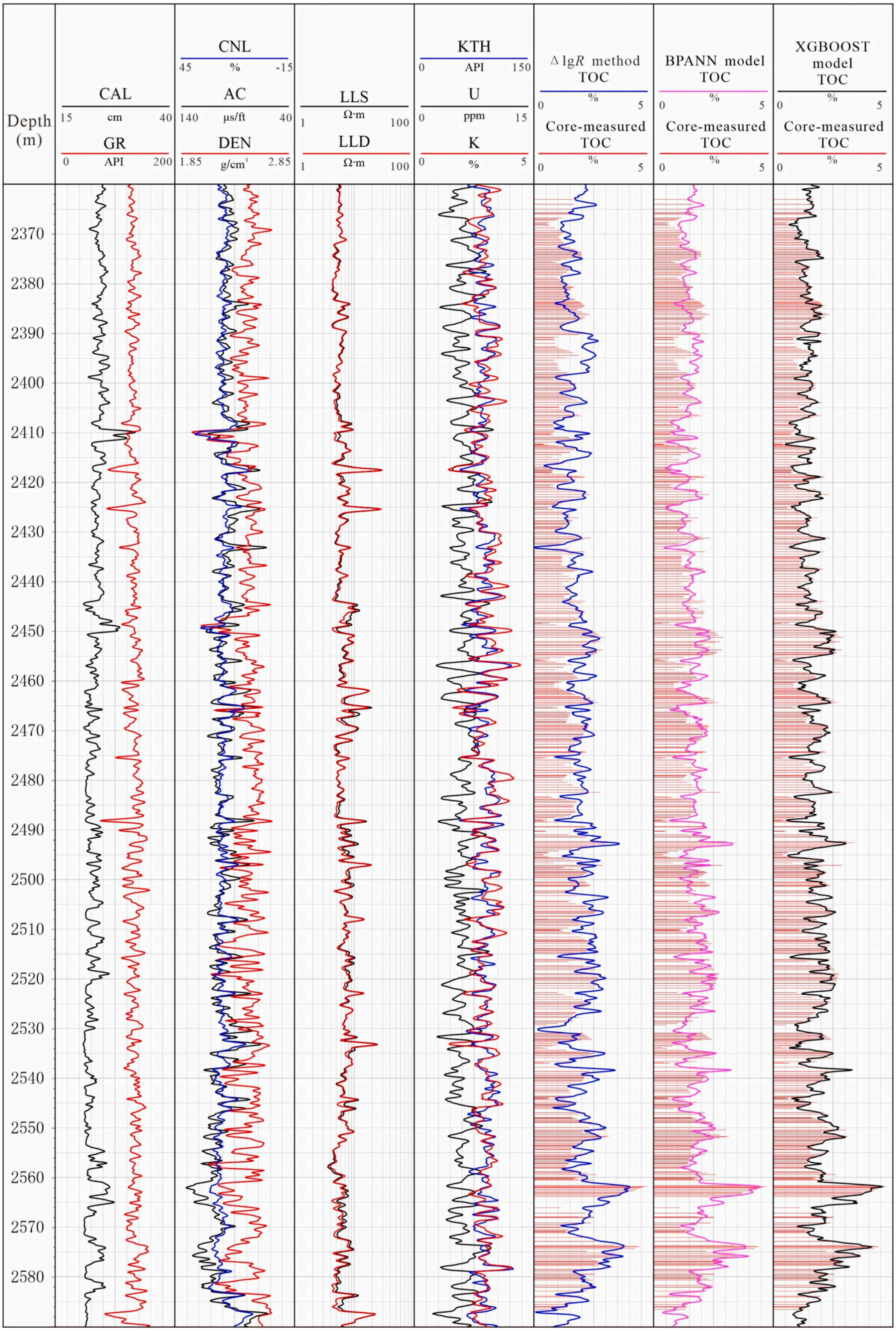

Fig. 13. The prediction of TOC content in the Cretaceous Qingshankou Formation in the Gulong Sag, Songliao Basin, using ΔlgR method, BP neural network and XGBOOST method.

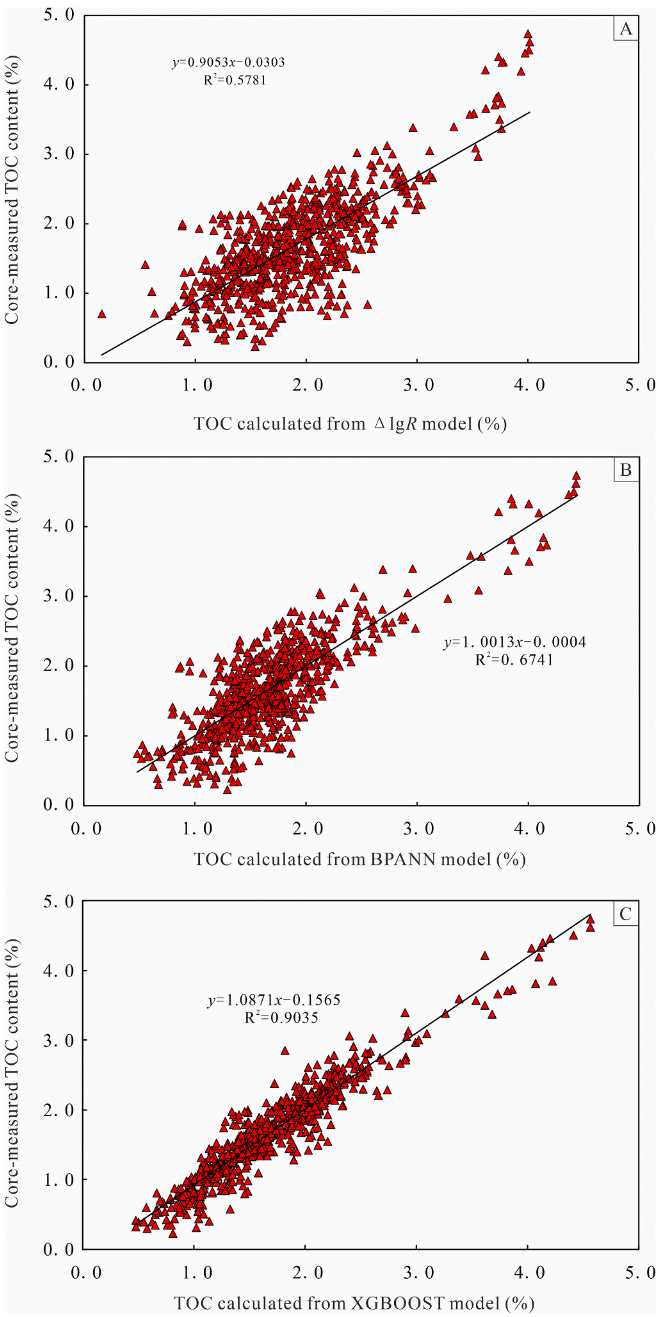

Fig. 14. Crossplots of core-measured TOC content versus TOC predicted from ΔlgR method, BP neural network and XGBOOST method in the Cretaceous Qingshankou Formation in the Gulong Sag, Songliao Basin of East China.
A. core-measured TOC content versus TOC predicted from ΔlgR method.
B. core-measured TOC content versus TOC predicted from BPANN method.
C. Core-measured TOC content versus TOC predicted from XGBOOST method.

with higher R^2 compared with BPANN method (Fig. 14; Lai et al., 2024a).

Consequently, the BPANN and XGBOOST models performed better than the conventional ΔlgR approach. The AI method can handle large datasets and output fast and cost-effective results (Gordon et al., 2022).

8. Seismic prediction

Organic matter-rich source rocks can be recognized by seismic data, and distribution and variations of organic matters can be characterized and mapped by seismic profile (Løseth et al., 2011). Sonic velocity, Vp/Vs, and acoustic impedance are the most sensitive elastic parameters for the source rocks (Chen et al., 2018; Harris et al., 2019; Sahoo et al., 2021). Intervals with high TOC content will exhibit lower velocities and densities (Paris and Stewart, 2020).

Relationship between TOC and Young's modulus (Alzate and Devegowda, 2013) as well as Vp/Vs (Xu and Payne, 2009) are used to predict TOC content (Qian et al., 2019). In addition, acoustic impedance, which can be estimated from density and sonic logs, or from seismic inversion, will reflect the source rock property (Vernik and Landis, 1996; Sahoo et al., 2021). However, in some cases, seismic prediction methods of source rocks will result in erroneous conclusions (Zeng et al., 2022).

9. Future prospects

9.1. Optimization of TOC prediction methods

As a matter of fact, TOC data of source rocks are sparsely distributed, and overcoming this difficulty may require large number of empirical relations and mathematical equations to predict TOC from well-log variables (Ganguli et al., 2022). As reviewed, all the mentioned techniques have advantages and limitations, and the optimization of various method depends on their correlation with core-measured TOC values (Table 1) (Sohail et al., 2020). Therefore, source rock evaluation in a new basin or a new formation, should tie petrophysical log responses to geochemical data analyzed from core, sidewall plugs, or cuttings, with the aim for petrophysical modeling (Ochoa et al., 2022).

There are many factors governing the accuracy of well log predicted TOC content.

(1) Core analysis errors.

Oil based drilling muds will contaminate the source rocks, resulting in increased TOC and HI values, but decreased Tmax (Silva et al., 2017). In some cases, the analyzed samples will be severely affected by drilling muds.

(2) Lithology variations of source rocks.

Coal, organic rich mudstones and carbonates can all act as source rocks. However, the same TOC content will result in a varied log responses if the lithologies of source rocks are different. Pyrites in source rocks will increase bulk density readings but reduce resistivity values. Conversely, coal will significantly reduce bulk density but increase resistivity values.

(3) Resolution variations between logs and core data.

Geophysical well log suits have a wide range of vertical resolution from millimeter scale to tens of meter scales, and the conventional well logs are characterized by meter or decimeter scale vertical resolution (Lai et al., 2022a; Gama and Schwark, 2023). In other words, the well log readings are the comprehensive reflection of a meter or decimeter scale depth ranges. Most of the conventional well log data have vertical resolution of decimeter scale to meter scale (Lai et al., 2023a). However, the geochemical analysis results are point to point data. The mismatching of well log and geochemical analysis results will give unreasonable prediction results providing the well log data are not calibrated with core analysis data (Gama and Schwark, 2023). The mismatching between core depth (drilling depth) and the well logging depth will result in significant errors (Zhu et al., 2020; Gama and Schwark, 2023).

(4) Borehole conditions.

Borehole collapse will cause the distinctly different responses on density logs, sonic log and resistivity logs (Lai et al., 2022a). Consequently, some well log readings, especially the bulk density and resistivity as well NMR logs, should eliminate the effects of borehole conditions. For instance, the borehole collapse (enlargement of CAL log) result in a decrease of DEN and resistivity logs (Fig. 10).

9.2. Free, pyrolyzing hydrocarbons (S1 + S2) and thermal maturity (Ro)

As in known, source rocks should be described in terms of volume, organic richness, and thermal maturity (Cappuccio et al., 2021).

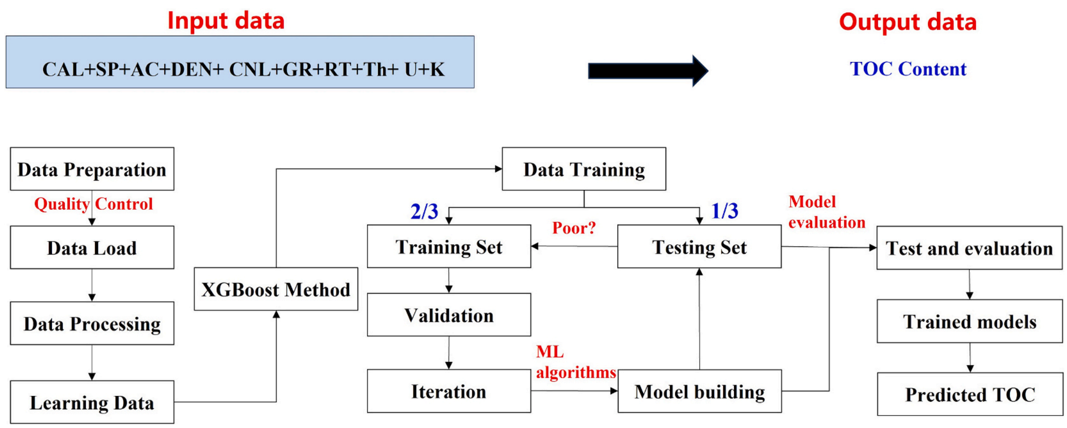

Fig. 15. Workflow processes to predict TOC content using XGBOOST methods using well log data.

Table 1
Advantages and limitations of various TOC prediction methods using geophysical well logs (Schmoker and Hester, 1983; Passey et al., 1990; Mahmoud et al., 2017; Wang et al., 2019; Handhal et al., 2020; Wood, 2020; Lai et al., 2023a; Zhang et al., 2023).

Method	Advantages	Limitations
Schmoker method	Simple and easy, only density log is used	Low accuracy
ΔlgR	Overlay of porosity and resistivity log will reduce the effect of porosity; Applicable in siliciclastic rocks and carbonate rocks	Requires advanced expertise in the basin to select the baseline; Prone to human error; Not applicable in shales and high maturity source rocks
Modified ΔlgR	Applicable in high maturity source rocks; No need to determine baseline	Complex process; hard to determine the fitting constant
GR spectrum	Easy process	Affected by abnormal high radioactive elements
Multiple regression analysis	High accuracy; sensitive log parameters are all incorporated	Not applicable in source rocks in other basins
NMR and density logs	High accuracy in high TOC intervals	Low acquisition of NMR logs; Hard to reflect the low TOC intervals
Litho Scanner log	No need to be correlated core analysis data	Low acquisition of Litho Scanner logs; Complex dealing processes
Artificial Intelligence	Reduce human uncertainty and workload; improve accuracy	Large number of samples are needed for training

Comprehensive assessment of source rock should determine TOC, quality (hydrogen Index), and thermal maturity (Ro, Tmax) of source rocks (Tissot and Welte, 1984; Gama and Schwark, 2023). Estimating the TOC is the first step for source rock property evaluation (Abarghani et al., 2019). TOC describes the amount of organic matter, while free hydrocarbon (S1) is the amount of free hydrocarbon before pyrolysis process, additionally pyrolyzing hydrocarbon (S2) represents the hydrocarbon formed during pyrolysis (Cappuccio et al., 2021; Mulashani et al., 2021). Also, hydrogen index (HI) and oxygen index (OI) are two critical parameters for hydrocarbon potential assessment (Souza et al., 2021; Gordon et al., 2022). Thermal maturity (Ro, Tmax) needs to be evaluated since it governs whether hydrocarbons have been produced or not (Abarghani et al., 2019). Therefore, source rock property characterization needs a comprehensive analysis of quality, quantity, and thermal maturity (Carvajal-Ortiz and Gentzis, 2015; Balumi et al., 2022; Gordon et al., 2022; Ali et al., 2022). However, the S1, S2 as well as thermal maturity estimations using well logs are still considered as challenges for the geologists and petrophyscists (Wang et al., 2019; Abarghani et al., 2019; Zhao et al., 2019).

Estimating thermal maturity and S1 + S2 from well logs has received less attention (Zhao et al., 2019). More attentions should be paid to how to evaluate and predict thermal maturity of source rocks using the full-range of geophysical well logs, especially for unconventional hydrocarbon resources (Abarghani et al., 2019; Harris et al., 2019; Zhao et al., 2019; Feng et al., 2023). The comprehensive assessment of source rocks by geological and geophyical methods, especially in the era of self-generated and self-stored unconventional hydrocarbon resources, will become more important.

10. Conclusions

Laboratory geochemical analysis performed on outcrops, cores and drilling cuttings are reliable methods for quantifying source rock property (quality, quantity and maturity). However, geochemical analysis data have limitations including high cost, and low recovery rate (discontinuity), and they cannot represent the whole interval. The full-scale geophysical well logs and petrophysical workflows using single or multiple well log series are needed for source rock evaluation.

The source rock evaluation using well logs can be date back to the 1940s, and three distinct phases can be summarized. In the 1970s to 1980s, it is in the qualitative recognition stage of source rocks using GR and density log. In the 1990s, the proposed ΔlgR method brings the well log evaluation of source rocks into quantitative stage. The stage of comprehensive prediction of source rocks via well logs is attributed to the improvements of well logs series and the revolution of unconventional hydrocarbon resources.

The presence of organic materials is distinct on well logs responses by lower density and sonic velocity, but higher resistivity, GR and hydrogen content compared with the rock matrix. The well logs sensitive for source rocks include GR, AC, CNL, DEN and RT. Also image logs will display bright bands due to high resistivity. Source rock intervals may have high content of pyrite and clay. The residual hydrocarbons within the source rock intervals will contribute to the long T_2 time, wide and multi-modal T_2 spectrum.

The accuracy of various methods for TOC prediction is testified by core-measured TOC content. Then the principles, interpretation process, advantages and limitations of various methods are discussed. The Schmoker method is not applicable in shales and irregular borehole condition will affect linear regression relationship between TOC and bulk density. The ΔlgR method integrate resistivity and porosity logs, and is widely used since it eliminates the effects of porosity variations, however, the baseline selection will reduce the accuracy, in addition, ΔlgR method is not applicable in highly mature or deep burial source rocks. The modified ΔlgR method improves accuracy but result in a complex process.

The regression model of multiple regression analysis is hard to extend in source rocks of different basins. The TOC content of lacustrine source rocks shows poor correlation relationships with spectral gamma ray logs. NMR and Litho-Scanner logs have advantages to provide accurate TOC results, however, the high acquisition costs of NMR and Litho-Scanner logs limit their application. Therefore optimization of various methods for TOC prediction by well logs should fully consider their advantage and limitations. The complicated non-linear function relationship between TOC content and well logs require the incorporation of machine learning and artificial intelligence methods to reduce human error and big workload. Back propagation (BP) neural network and Extreme Gradient Boosting (XGBOOST) will output accurate results compared with geochemical-measured TOC. However, large numbers of input data are needed for training for AI methods, and fewer lab-measured TOC data will output low accuracy TOC prediction results. Comprehensive assessment of source rock using well logs should determine TOC, S1, S2, Ro and Tmax of source rocks. The unconventional hydrocarbon resources provide a new opportunity and challenge for TOC prediction using well logs.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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