

Received March 20, 2019, accepted April 12, 2019, date of publication April 22, 2019, date of current version April 29, 2019.

Digital Object Identifier 10.1109/ACCESS.2019.2912214

An Improved Theoretical Nonelectric Water Saturation Method for Organic Shale Reservoirs

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This work was supported in part by the Yangtze University Excellent Doctoral and Master's Degree Thesis Cultivation Program, in part by the National Natural Science Foundation of China under Grant 41404084 and Grant 41504094, in part by the Natural Science Foundation of Hubei Province under Grant 2013CFB396, in part by the Open Fund of Key Laboratory of Exploration Technologies for Oil and Gas Resources (Yangtze University), Ministry of Education under Grant K2015-06, Grant K2016-09, and Grant K2017-01, K2018-11, in part by the Youth Innovation Team, Key Laboratory of Exploration Technologies for Oil and Gas Resources (Yangtze University), Ministry of Education under Grant Nos.PI2018-03, in part by the National Science and Technology Major Project under Grant 2017ZX05032003-005, in part by the China National Petroleum Corporation major projects under Grant 2013E-38-09, and in part by the Yangtze University ESI Discipline Enhancement Program.

ABSTRACT The saturation of a shale gas reservoir is used to characterize the fluid content within the pores and to calculate the free gas content and reserves of the reservoir. Thus, accurately evaluating the saturation of a shale gas reservoir is of great significance. However, little research has been performed to quantitatively evaluate the saturation relative to other parameters used for evaluating the gas content. Moreover, because the conductive mechanism of shale gas reservoirs is very complex, the existing electric saturation model is insufficient. In this paper, based on the results of our analysis, we postulate that the organic pores in shale gas reservoirs are full of gas; furthermore, clastic pores also contain some gas. Thus, an improved model based on the original petrophysical model and the theory of shale density characteristics is proposed, and a calculation scheme based on the saturation model of shale gas reservoirs is deduced. The simulation results indicate that the improved model is less sensitive than the original model to changes in the total organic carbon content (TOC), and the water saturation calculated when the TOC is equal to 0 can be less than 100%, which is more consistent with the actual geological conditions of shale gas reservoirs. Because the saturation model incorporates an exceedingly large number of parameters, we propose the use of a genetic algorithm to automatically optimize those parameters. An evaluation of the Longmaxi formation-Wufeng formation shale gas reservoir in the Yongchuan block of the southern Sichuan Basin reveals that the optimized parameters are consistent with the geological conditions. The prediction accuracy of the proposed method is also higher than that of the original method, especially for the Wufeng formation, for which the number of samples is very small. Moreover, the absolute error is reduced by nearly 10%, which reflects a high accuracy. The proposed model can enhance accuracy through further improving the determination of shale gas reservoir characteristics and thus has the potential to be improved further. This method can also partially resolve problems by evaluating the saturation of shale gas reservoirs and hence could be helpful for core and well logging evaluations of the saturation, especially in overmature shales.

INDEX TERMS Saturation, nonelectric, organic shale, petrophysics, organic pore, clastic pore.

I. INTRODUCTION

Shale reservoirs represent a very broad class of reservoirs that contain highly abundant reserves. Because shales serve

The associate editor coordinating the review of this manuscript and approving it for publication was Bora Onat.

as source rock reservoirs, the occurrence of fluid in a shale gas reservoir is much more complex than that in a conventional reservoir [1]. Natural gas exists as free gas within pore spaces, adsorbed gas in liquid and solid states within organic pore spaces, and dissolved gas within water [2]. Thus, a high free gas content is beneficial for the development of shale

gas reservoirs. The extraction of different types of gases ranges in difficulty; hence, it is very important to evaluate the various phases of gas present [3]–[4]. In this regard, relevant research has shown that one of the most fundamental parameters for accurately calculating the gas volume of various phase states is the saturation parameter [5]–[8].

Water saturation (S_w) refers to the ratio of the water pore volume to the rock pore volume; together with porosity and permeability, water saturation constitutes a basic reservoir parameter and is essential for calculating the amount of reserves [9]–[10]. For a purely gas layer (without oil), the gas saturation is equal to $1 - S_w$, and thus, only one parameter must be calculated accurately for a shale gas reservoir. Evaluating the saturation accurately is even more important in a shale gas reservoir than in a conventional reservoir because the saturation is also used to calculate the free gas content and adsorbed gas content. In other words, either directly or indirectly, the saturation determines all the gas-bearing parameters of a shale gas reservoir. Consequently, the saturation represents the most basic parameter for a shale gas reservoir. However, its importance can be obscured by the introduction of additional parameters to evaluate the gas content. Therefore, accurate saturation calculations for shale gas reservoirs using existing model calculations are highly important, albeit difficult.

Although many studies have been performed on saturation models based on the rock resistivity characteristics of sandstone and carbonate reservoirs, few researchers have applied similar research to shale reservoirs. Through a study on the traditional water saturation model, Amiri et al. predicted that the use of a correction factor to reduce the water saturation was incorrect [11]–[12]. Ali et al. proposed a correction model for the Archie formula based on a compensation for the kerogen-clay conductivity [13]. Moreover, Zhang et al. proposed another correction model for the Archie formula based on the total organic carbon content (TOC) [14]–[19]. In essence, the models used to calculate the saturation utilizing the resistivity characteristics of shale gas reservoirs have not been systematically studied. To complicate matters arising from an insufficient focus on the saturation parameter, the pores of shale gas reservoirs exist mainly at the micro- to nano-scale [20]; hence, as a consequence of their complex pore structures [21], diverse pore types [22], diverse fluid occurrence states [23], large wettability changes [24] and diverse matrix mineral compositions [25], shale gas reservoirs are highly complex. These characteristics also greatly affect the conductivity, making it difficult to obtain resistivity saturation models for shale gas reservoirs.

Alternatively, some scholars have employed nonelectric methods to calculate the shale saturation. For instance, Wang et al. proposed a method for calculating the gas saturation using the elastic modulus [26], while Gui et al. presented an approach using the fluid bulk compressibility [27]. Furthermore, Tan et al. proposed a technique to calculate various types of porosities and performed saturation calculations using the nuclear magnetic resonance (NMR) T2

spectrum [28]. All of the abovementioned methods have achieved success to some degree; unfortunately, because they lacked theoretical bases, they also possessed notable limitations. Accordingly, Alfred et al. developed a method to calculate the shale rock saturation using density characteristics to ascertain the differences between organic and inorganic pores in shale gas reservoirs [29]. Their method, which treats rocks within a shale gas reservoir unconventionally, has achieved good results when evaluating the saturation of shale reservoirs. However, this method is currently the only available approach for calculating the saturation of shale reservoirs based on theoretical models. Moreover, this model was proposed many years ago when the geological understanding of shale gas was inadequate; as a result, this model does not consider the fluid state in inorganic pores. In addition, their approach employs empirically based assumptions, and thus, the model parameters can be determined only through experience.

Thus, we believe that an accurate theoretical model is urgently needed to evaluate shale gas reservoirs and calculate the reservoir saturation. In this paper, the fluid occurrence in different pore types is analyzed, and the unreasonable hypotheses of previous models are corrected. Correspondingly, an improved theoretical model for calculating the saturation through a detailed theoretical derivation is presented, and the use of optimization theory is proposed to quantitatively solve the parameters within the model and evaluate the saturation. Based on an evaluation of actual data from shale gas reservoirs, the saturation of which is difficult to calculate using resistivity data, we conclude that the new model boasts a higher precision, reliability and accuracy and is both more reasonable and more suitable for providing continuous quantitative and accurate evaluations of the saturation of shale gas reservoirs.

II. ANALYSIS OF PORE TYPES AND THE NATURAL GAS CONTAINED THEREIN

The microstorage space classification scheme of shale gas reservoirs is diverse, as it includes comprehensive classifications based on the pore size, the pore production structure and the pore genesis type. Slatt et al. established a three-dimensional morphological model of pores in organic matter and proposed that pore types in shale include clay pores, organic pores, dung pellet pores, granular pores, and microfracture channel pores [30]. Loucks et al. postulated that pores can be classified into 3 basic types, namely, intergranular pores, intragranular pores and organic pores [31]. Yu subsequently developed a comprehensive classification scheme of pore production structures in shale gas reservoirs [32]. Based on the work of Slatt, He et al. constructed a systematic and complete classification scheme of shale reservoirs according to the pore genesis type [33].

Shale rocks boast a far greater number of pore types than any other type of rock. This variety of pore types complicates the migration of hydrocarbons through shales after the generation of oil and gas, leading to the complexity that is

characteristic of shale reservoirs. Therefore, even if the saturation of a shale reservoir is evaluated using the nonelectric method, the differences in fluid occurrences in different types of pore spaces must still be clarified. Nevertheless, although many classifications of pores within shale gas reservoirs have been developed, no shale gas reservoir pore classification scheme considers the occurrence characteristics of fluids. Accordingly, we classify pore types into organic pores, clastic pores (intragranular pores, intergranular pores, cracks, etc.) and clay pores according to their genesis and wettability and analyze the various corresponding porosity types.

Organic pores, which refer to generally well-developed pores in the interiors of organic particles within shale, are widely developed within shales and constitute one of the most important characteristics of source rocks [34]–[35]. With maturation, the organic matter in shale begins to transform and produce organic pores that contain oil and gas. Although the organic matter often decreases with increasing maturity, the number of organic pores accounting for the total volume of organic matter grows rapidly. These organic pores represent the only sources of oil and gas in shale reservoirs [36]. Furthermore, as organic pores are produced during diagenesis, such pores are likely to contain a mixture of oil and gas without water. During the short-term migration that occurs later in the maturation of shale, the volume of organic pores gradually expands following fluid generation; thus, the pressure inside these pores significantly increases. Subsequently, oil and gas are squeezed into other pore spaces [37]. Therefore, organic pores are most certainly composed of oil and gas.

The genesis of mineral clastic pores is related mainly to the type, content and dissolution of granular minerals. According to the differences in their genesis and in the minerals formed, mineral clastic pores can include intergranular pores formed by the dissolution of shale matrix minerals such as quartz and feldspar, intergranular pores formed by mineral cleavage cracks, and intercrystalline pores formed by pyrite. Relevant studies have also indirectly indicated that mineral clastic pores, especially inner and intergranular pores, exhibit a mixed wettability and can aid in the migration of fluids, nearly guaranteeing that oil and gas will exist in the regions above hydrocarbon pores [38]–[39]. During actual shale gas exploitation, formation water will typically fail to flow outward, indicating that moveable fluids in clastic pore spaces are replaced by hydrocarbons with an increase in the organic pore pressure [40]–[41]. In 2018, Hu et al. conducted tracer migration experiments and reported both that shale presents a unique "double channel" migration mechanism in three-dimensional space and that clastic pores exhibit spotted dog-type mixed wettability characteristics [42]. The above studies all indicated that mineral clastic pores usually contain oil and gas and may even occupy all moveable spaces within clastic pores; thus, these types of pores must be considered during evaluations of the shale reservoir saturation.

Clay minerals constitute one of the most important mineral components of shale rocks. The clay content in a shale can

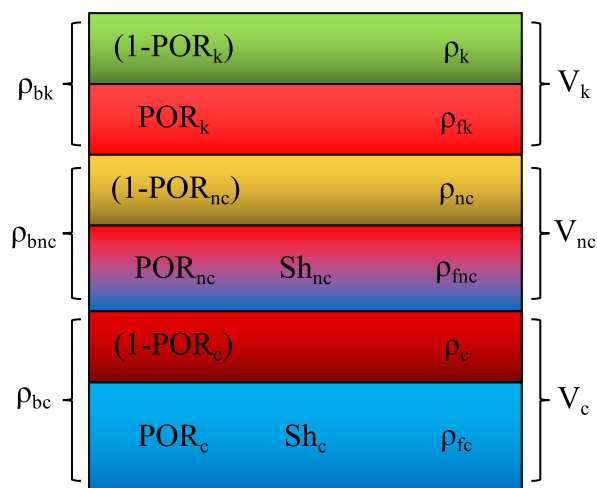


FIGURE 1. Shale rock volumetric model produced by the combination of three pore systems.

range from 16.8% to 70.1%, and the clay minerals are usually dominated by illite. Most articles have reported that clay pores exhibit strongly hydrophilic characteristics and that the wettability of clay pores is attributable to water; hence, clay mineral pores are considered to be filled with water in our petrophysical model.

III. THEORY AND METHOD

After a brief analysis of the gas-bearing properties of various organic shale pores, the fluid occurrence characteristics of different pore types are clarified. Through this clarification, we construct a new, more suitable petrophysical model that is different from the shale petrophysical model proposed by Alfred et al. Accordingly, we analyze this difference through a simulation later in this paper. The basic premise of the model of Alfred et al. is twofold: first, organic pores in organic shales are rich in hydrocarbons; second, not all inorganic pores should be classified collectively because they contain different types of pores, different pore sizes, and different wettabilities. Based on the results of our analysis, we believe that inorganic mineral clastic pores contain a certain hydrocarbons and may even be occupied by oil and gas, leaving only bound water within the pores. In addition, the fluids within clay mineral pores, which are assumed to be filled with water, must be discussed. Based on the above information, a new petrophysical model is proposed.

The proposed model is defined as having three pore systems: an organic domain containing organic matter and organic pores, a clastic mineral domain containing mineral clastic pores and non-clay minerals, and a clay mineral domain containing clay mineral pores and clay minerals. The hypothesized model is shown in Fig. 1.

In Fig. 1, ρ_k is the density of organic matter, ρ_{fk} is the density of the fluid in the pores of organic matter, ρ_{nc} is the density of non-clay minerals, ρ_{fnc} is the density of the fluid in the pores of non-clay minerals, ρ_c is the density of clay minerals, ρ_{fc} is the density of the fluid in the pores

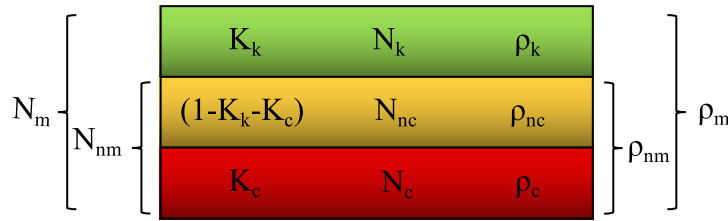


FIGURE 2. Shale matrix rock physics model.

of clay minerals, ρ_{bk} is the density of the entire organic matter domain, ρ_{bnc} is the density of the entire clastic mineral domain, ρ_{bc} is the density of the entire clay mineral domain, POR_k denotes the proportion of organic pores in organic matter, POR_{nc} denotes the proportion of non-clay pores in clastic minerals, POR_c denotes the proportion of clay pores in clay minerals, V_k signifies the volume of the entire organic domain, V_{nc} signifies the volume of the entire clastic mineral domain, V_c signifies the volume of the entire clay mineral domain, and the sum of the volumes of the 3 abovementioned domains is 1. In each pore domain, red represents saturated oil and gas, blue represents saturated water, and red and blue together represent both oil and gas (excluding oil in a shale gas reservoir) as well as water in the pores. We use this generalized petrophysical model for further derivation and to obtain a saturation model based on the proposed petrophysical model.

A. MATRIX VOLUMETRIC MODEL

We extract and reorganize the matrix component of the shale petrophysical model to obtain the matrix volumetric model of shale. The corresponding matrix volumetric model is shown in Fig. 2.

1) ORGANIC MATTER VOLUME CHARACTERIZATION

Based on Fig. 2, the following equations can be obtained (1):

$$\begin{cases} K_k = K_k \rho_k + K_c \rho_c + (1 - K_k - K_c) \rho_{nc} \\ \rho_{nm} = K_c \rho_c + (1 - K_c) \rho_{nc} \end{cases} \quad (1)$$

Here, ρ_m is the density of the entire matrix, K_k denotes the proportion of organic matter in the matrix, ρ_k is the density of organic matter, K_c denotes the proportion of clay minerals in the matrix, ρ_k is the density of organic matter, ρ_c is the density of clay minerals, and ρ_{nm} is the density of non-clay minerals. Taking these differences into consideration and substituting the second formula in equation (1) into the first formula, the following formula is derived:

$$K_k = (\rho_m - \rho_{nm}) / (\rho_k - \rho_{nc}) \quad (2)$$

Subsequently, ρ_{nm} in equation (2) is replaced with the second formula in equation (1):

$$K_k = (\rho_{nc} - \rho_m + K_c (\rho_c - \rho_{nc})) / (\rho_{nc} - \rho_k) \quad (3)$$

Then, the second formula in equation (1) is transformed:

$$K_c = (\rho_{nc} - \rho_{nm}) / (\rho_{nc} - \rho_c) \quad (4)$$

Thus, through the proposed shale matrix petrophysical model, the proportions of organic matter and clay in the matrix can be obtained. An accurate representation of the proportion of organic matter is helpful for deriving the saturation in the following section.

2) CONVERSION OF THE TOTAL ORGANIC CARBON CONTENT

The TOC is a very common parameter used to characterize the relative size of organic matter [43]–[44]. Coring experiments and logging methods can be used to effectively determine the TOCs of shale reservoirs. Therefore, the TOC is introduced here as a parameter in our model. Then, assuming that the influence of asphalt does not need to be considered (i.e., a low asphalt content is negligible), the volume of organic matter can be represented as follows:

$$K_k = TOC \rho_m / C_k \rho_k \quad (5)$$

where C_k is the proportion of the organic carbon content in the organic matter (commonly between 0.8 and 0.95) and ρ_k is the density of organic matter. The density of organic matter, which is related to the maturity, is often difficult to accurately determine experimentally.

By combining equations (2) and (5), ρ_m is eliminated from the system, and the result is as follows:

$$K_k = TOC (K_c \rho_c + (1 - K_c) \rho_{nc}) (C_k \rho_k - TOC \rho_k + TOC \rho_{nc}) \quad (6)$$

The above formula shows that the ratio of organic matter in the matrix is related to the ratio of clay minerals in the matrix, the ratio of the organic carbon content in the organic matter, the TOC, and the densities of various minerals in the matrix. After determining the above parameters, the ratio of organic matter in the matrix K_k can be calculated accurately. For a drill core, the organic matter density can be determined experimentally by investigating the specific density of the organic matter; furthermore, the TOC can be accurately obtained by experimental measurements of the TOC (i.e., the carbon content of organic matter that is either dissolved in or suspended on water), and the densities of various minerals in the matrix can be determined by X-ray diffraction (XRD) and whole-rock experiments. Consequently, the volume of organic matter K_k within the shale core can be determined.

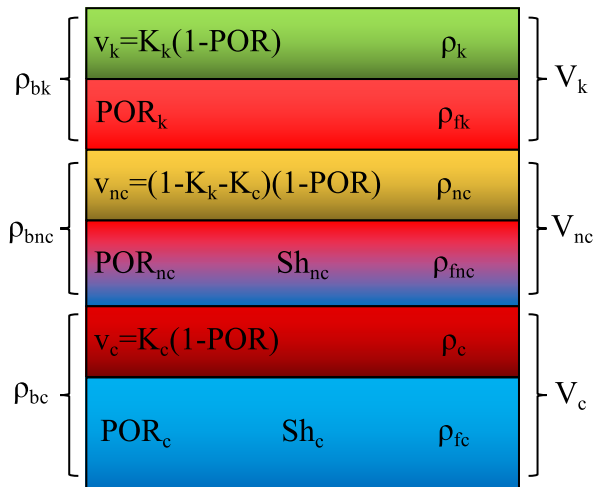


FIGURE 3. Shale rock volumetric model resulting from the combination of three pore systems (after derivation).

B. SHALE ROCK VOLUMETRIC MODEL

After characterizing both the volume of organic matter in the matrix and the volume of clay minerals, we constructed an entire shale rock volumetric model to determine the total density ρ_b and total porosity (POR) of the rock. After the introduction of K_k and K_c into the model, the characterization of the matrix elements in the volumetric model of the entire rock changes (Fig. 3).

Fig. 3, which modifies primarily the matrix characterization, presents the petrophysical model derived from the shale matrix petrophysical model. Such changes will be explained in the subsequent deduction. First, for the petrophysical model, we have the following:

$$V_k + V_c + V_{nc} = 1 \tag{7}$$

$$v_k = K_k (1 - POR) \tag{8}$$

$$v_{nc} = (1 - K_k - K_c) (1 - POR) \tag{9}$$

$$v_c = K_c (1 - POR) \tag{10}$$

According to the matrix model results, the following can be obtained:

$$\begin{cases} V_k = v_k + POR_k V_k = K_k (1 - POR) / (1 - POR_k) \\ V_c = v_c + POR_c V_c = K_c (1 - POR) / (1 - POR_c) \\ V_{nc} = 1 - V_k - V_c \end{cases} \tag{11}$$

After characterizing the volume of each part using equations (9) and (11), a formula for calculating the porosity can be deduced according to equation (11), (12) as shown at the bottom of this page, where POR denotes the total porosity. Then, the bulk density of the entire system can be characterized. The volumetric model of the entire matrix should be composed of three domains, including the matrix and fluid components. The bulk density of the entire rock system can be represented by equation (13):

$$\rho_b = V_k \rho_{bk} + V_c \rho_{bc} + (1 - V_k - V_c) \rho_{bnk} \tag{13}$$

Based on the detailed explanation provided in our previous paper, the pore spaces in the proposed model are occupied by a combination of oil, gas and water. Therefore, the corresponding density of each domain is characterized as (14), as shown at the bottom of this page.

Equation (14) is derived from the proposed petrophysical model and is consistent with the discussion provided in Section II. Unlike the petrophysical model in [25], there are more factors to consider here. Combining equations (13) and (14), we can calculate the bulk density. By setting each parameter as a constant and changing the relative sizes of organic pores, clastic pores, and clay pores, the effects of various porosity changes on the final total porosity and system bulk density can be observed.

First, we determine the effects of variations in the organic porosity. The proportion of organic pores in organic matter is set as 0.1, 0.2, 0.3, 0.4, and 0.5. The other parameters are set as follows: $POR_{nc} - 0.04$, $POR_c - 0.10$, $DEN_{nm} - 2.70 \text{ g/cm}^3$, $DEN_{nc} - 2.82 \text{ g/cm}^3$, $DEN_c - 2.55 \text{ g/cm}^3$, $DEN_k - 1.30 \text{ g/cm}^3$, $DEN_h - 0.25 \text{ g/cm}^3$, $DEN_w - 1.00 \text{ g/cm}^3$, $S_{nch} - 0.5$, and $C_k - 0.8$.

Second, we examine the effects of variations in the clastic porosity. The proportion of clastic pores is set as 0.02, 0.04, 0.06, 0.08, and 0.1. The other parameters are set as follows: $POR_k - 0.2$, $POR_c - 0.1$, $DEN_{nm} - 2.70 \text{ g/cm}^3$, $DEN_{nc} - 2.82 \text{ g/cm}^3$, $DEN_c - 2.55 \text{ g/cm}^3$, $DEN_k - 1.30 \text{ g/cm}^3$, $DEN_h - 0.25 \text{ g/cm}^3$, $DEN_w - 1.00 \text{ g/cm}^3$, $S_{nch} - 0.5$, and $C_k - 0.8$.

Finally, we ascertain the effects of variations in the clay porosity. The proportion of clay pores is set as 0.02, 0.04, 0.06, 0.08, and 0.1. The other parameters are set as follows: $POR_{nc} - 0.04$, $POR_c - 0.10$, $DEN_{nm} - 2.70 \text{ g/cm}^3$, $DEN_{nc} - 2.82 \text{ g/cm}^3$, $DEN_c - 2.55 \text{ g/cm}^3$, $DEN_k - 1.30 \text{ g/cm}^3$, $DEN_h - 0.25 \text{ g/cm}^3$, $DEN_w - 1.00 \text{ g/cm}^3$, $S_{nch} - 0.5$, and $C_k - 0.8$.

Figs. 4-6 show the simulation results of the petrophysical model proposed in this paper. First, under the

$$POR = 1 - (1 - POR_{nc}) (1 + (K_k / (1 - POR_k) + K_c / (1 - POR_c)) (1 - POR_{nc}) / (1 - K_c - K_k)) / (1 - K_c - K_k) \tag{12}$$

$$\begin{cases} \rho_{bk} = \rho_h POR_k + \rho (1 - POR_k) \\ \rho_{bnk} = \rho_h POR_{nc} S_{nch} \\ \quad + \rho + w POR_{nc} (1 - S_{nch}) + \rho_{nc} (1 - POR_{nc}) \\ \rho_{bc} = \rho_w POR_c + \rho_c (1 - POR_c) \end{cases} \tag{14}$$

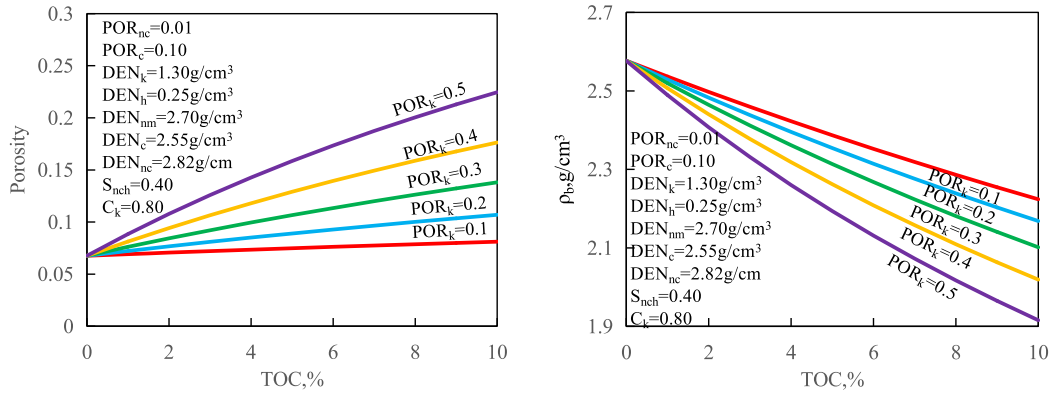


FIGURE 4. The porosity of porosity in organic matter to affect the parameters in the system.

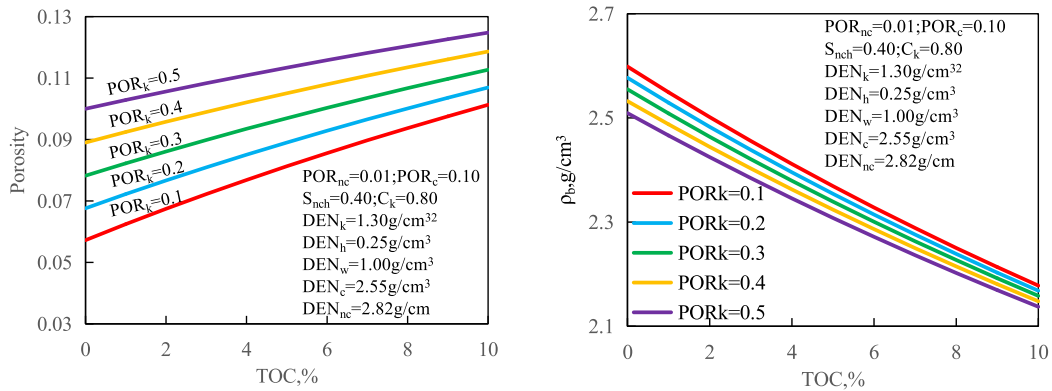


FIGURE 5. The porosity of clastic minerals to affect the parameters in the system.

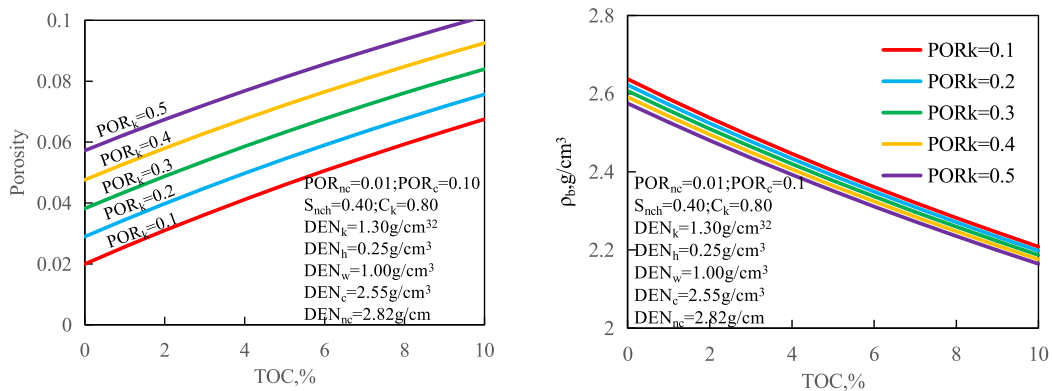


FIGURE 6. The porosity of clay minerals to affect the parameters in the system.

conditions that the porosities of organic matter, clastic minerals and clay minerals all remain unchanged, the porosity of the shale rock constantly increases with a continuous increase in the TOC, while the bulk density constantly decreases. As shown in Fig. 4, with the growth of organic pores in the organic matter, the growth rate of the total porosity constantly increases, indicating that the maturity of the shale reservoir also constitutes a key factor in conjunction with the TOC in determining the pore space size distribution within a shale reservoir [45]. A change in the organic porosity also leads to a decrease in the rock bulk density, and the rate at which the bulk density decreases begins to increase with an increase

in the proportion of organic pores. As shown in Fig. 5, the total porosity of the shale reservoir increases with an increasing clastic porosity; however, with an increasing TOC, the increase in the amplitude gradually slows down. This slowing is attributed to the decreasing impact of the clastic porosity with a decrease in the relative clastic mineral content. However, in an actual shale reservoir, the clastic porosity is rather small, and thus, the influence of the total porosity is not as great as the organic porosity. In the case in which other parameters are determined, an increase in the clastic porosity will reduce the rate of increase of the total porosity. The effect of a change in the clastic porosity on the bulk density is

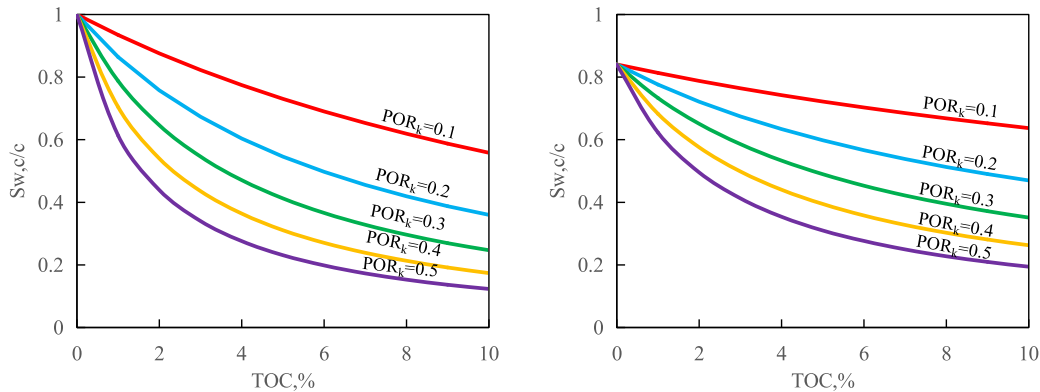


FIGURE 7. Differences in the results of two rock physics models for calculating saturation.

similar to the effect on the total porosity. As seen in Fig. 6, the difference in clay mineral porosity has no effect on the rate of increase of the total porosity, and its effect on the decrease in the bulk density is also minimal. Moreover, as shown in Figs. 4-6, an improvement in the number of organic pores is most helpful for developing a shale reservoir. Therefore, for shale reservoirs, the development of organic pores constitutes the decisive factor with regard to reservoir quality.

C. SHALE ROCK VOLUMETRIC MODEL

The proposed petrophysical model is used to characterize the water saturation. In the constructed pore space of the model, only organic pores and elastic pores contain oil and gas, and thus, the water saturation can be represented as follows:

$$S_w = 1 - (POR_k V_k + POR_{nc} V_{nc} S_{nch}) / POR \quad (15)$$

where S_w denotes the water saturation. In other words, the water saturation can be calculated after establishing both the proportion of organic pores within the known organic matter and the proportion of clastic porosity within clastic minerals. In the shale petrophysical model proposed by Alfred et al., only organic pores contain oil and gas, and the corresponding water saturation formula is as follows:

$$S_w = 1 - POR_k V_k / POR \quad (16)$$

Equations (15) and (16) highlight the differences between the saturation calculations of the original model and the improved model. The saturation calculation model becomes even more complicated after considering the inclusion of hydrocarbons in the clastic pores. This result shows that the model of Alfred et al. is too simple to guarantee a sufficient saturation calculation accuracy. Similar to the saturation calculation model, the porosity calculations of these models are also different.

Due to the differences between the hypothetical petrophysical model and the model proposed in this paper, the porosity calculation formula is also different:

$$POR = 1 - (1 - POR_k) (TOC (\rho_{nk} - \rho_k) + C_k \rho_k) \times (\rho_{bnk} - \rho_b) / (TOC \rho_{nk} (\rho_{bnk} - \rho_{bk})) \quad (17)$$

where ρ_{nk} denotes the density of a mineral without organic matter and ρ_{bnk} denotes the density of a domain without organic matter. By comparing the saturation model proposed in this paper with the organic shale petrophysical model developed by Alfred et al., the influences of the organic porosity on the saturation parameters in both models can be determined. In the proposed model, the proportion of organic pores is set as 0.1, 0.2, 0.3, 0.4, and 0.5. The other parameters are set as follows: $POR_{nk} = POR_{nc} - 0.04$, $POR_{nk} = POR_{nm} - 2.70 \text{ g/cm}^3$, $DEN_{nc} = 2.82 \text{ g/cm}^3$, $DEN_c = 2.55 \text{ g/cm}^3$, $DEN_k = 1.30 \text{ g/cm}^3$, $DEN_h = 0.25 \text{ g/cm}^3$, $DEN_w = 1.00 \text{ g/cm}^3$, and $C_k = 0.8$.

In Fig. 7, the relationship between the water saturation model and the TOC based on the original petrophysical model is shown on the left, while the water saturation model based on the petrophysical model proposed in this paper is shown on the right. The test results demonstrate that the water saturation parameter in the new model should change more slowly with a change in the TOC. In theory, the TOC is 0, and there is no hydrocarbon source. However, under actual conditions, underground oil and gas exist and likely migrate over short distances through the clastic porosity (the longitudinal concentration difference may enable short migration distances up to 14 m [44]). Therefore, the vertical variation in the saturation of a shale reservoir is generally small, and no shale reservoir is completely full of water. Usually, as long as the shale gas formation being evaluated is close to a source rock with a higher TOC, it is difficult for the water saturation to approach 100%, even if the TOC is close to 0. Substantial quantities of block data can prove this phenomenon. Therefore, a TOC of 0 does not conform to the hypothesis constituting the organic shale petrophysical model proposed in this paper. Natural gas may be transported from adjacent, high-quality reservoirs over a short distance. In an actual evaluation, the predicted saturation result can be adjusted by adjusting the saturation with the clastic porosity. After considering the presence of fluids within the clastic porosity, changes in the saturation are gentler and more consistent with the characteristics of shale, namely, self-generation, self-storage and short-distance migration. Therefore, based on the characteristics of shale reservoirs, the proposed model can

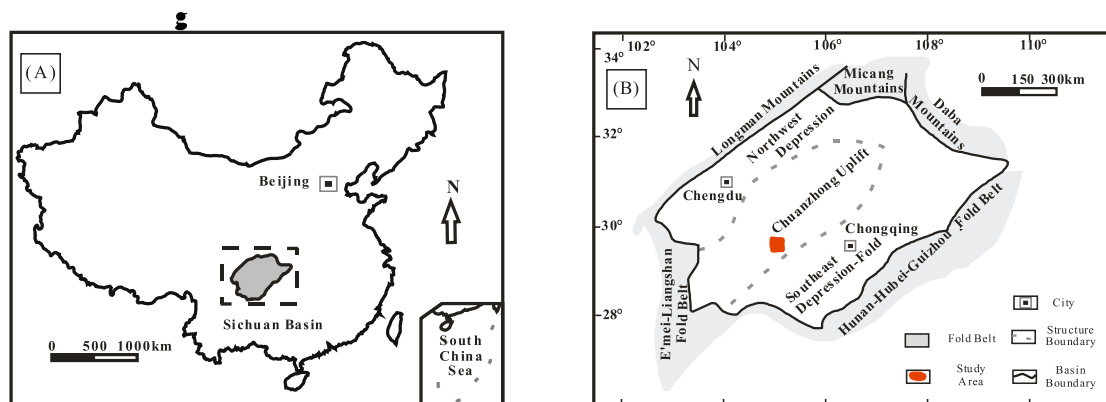


FIGURE 8. Yongchuan block location (red area in the figure).

better satisfy the needs for an evaluation of the shale reservoir saturation.

The compaction and diagenesis of clastic pores also determine the clastic pore size. Oil and gas can enter a shale and become stored through only larger pore sizes; similarly, smaller pore sizes can make it difficult for hydrocarbons to migrate over even short distances, leading to low hydrocarbon saturation within clastic pores. Thus, to select the hydrocarbon saturation in clastic porosity, the shale lithology must be considered. Generally, even if the differences in the mineral composition are not substantial, the shale rock lithology will vary due to differences in the stratigraphic age, diagenetic stage and mineral type. For example, the dissimilarity in the mineral composition between a siliceous shale and a carbonaceous shale may not be remarkable, but the clastic pores in a siliceous shale will certainly be better preserved than those in a carbonaceous shale, and thus, the clastic porosity should be higher to enable hydrocarbon saturation [46].

IV. ACTUAL MODEL VALIDATION

After analyzing the spatial oil-gas properties of shale reservoirs based on geological data and deriving the proposed volumetric petrophysical shale model, an expression for the water saturation is obtained. In this section, data from the Yongchuan block in the Sichuan Basin are used for a trial evaluation of the water saturation to verify the model proposed in this paper.

A. DATA

The Yongchuan block in the southern Sichuan Basin is selected to verify the proposed model. The target strata of this block are the Upper Ordovician Wufeng formation and the Lower Silurian Longmaxi formation, which is a typical organic-rich clay shale reservoir [47]. The lithologies of the reservoir are silica shale, carbonaceous shale and black shale (the silica shale is generally developed in the Wufeng formation, whereas the carbon shale and black shale are developed mainly in the Longmaxi formation). The TOC range is 0-7.83% with an average value of 2.07%. The total porosity, which is measured using a gamma-ray imager (GRI),

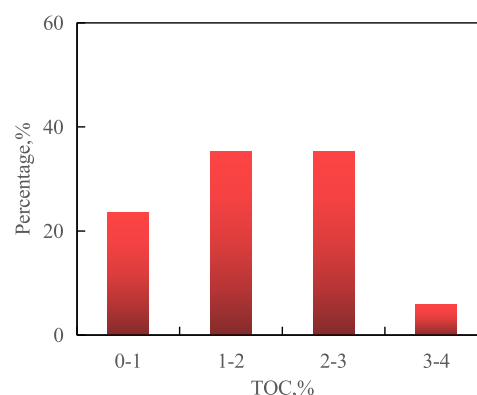


FIGURE 9. TOC distribution range of samples participating in all experiments.

ranges from 1.05% to 8% with an average of 4.02%. The water saturation ranges from 18.21% to 82.45% with an average of 57.51%; the saturation in the high-quality layer is 38.7%, which is lower than the average saturation of most conventional reservoirs. The vitrinite reflectance ranges from 1.83% to 2.43% with an average of 2.17%. The total gas content range is 0.49 m³/t–7.66 m³/t, and the average value is 3.92 m³/t. The entire area is similar to the Jiaoshiba block, which contains a continuous, overmature shale reservoir with a high reservoir quality. Nevertheless, due to the lack of developed faults, highly mature organic matter, high reservoir pressures and generally well-developed organic shale reservoirs in the Longmaxi formation and Wufeng formation within the Sichuan basin, an accurate calculation of the reservoir saturation is of great significance.

We take well A2 in the Yongchuan block as an example to test the saturation model. Numerous core plungers are employed to experimentally obtain the core TOC, mineral composition, clay type, true density and bulk density of the rock, GRI porosity and GRI water saturation. A CS-230 instrument was used to measure the TOC. The mineral composition and clay type were determined using an Ultima IV instrument, and the true density and bulk density of the rock were ascertained using an MDMDY-350 instrument. DJ-200 electronic balances and a PENTAPYC 5200e

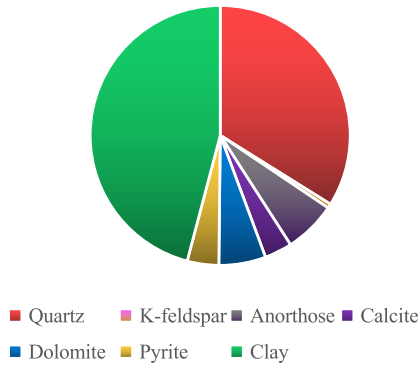


FIGURE 10. Average mineral composition distribution of samples participating in all experiments.

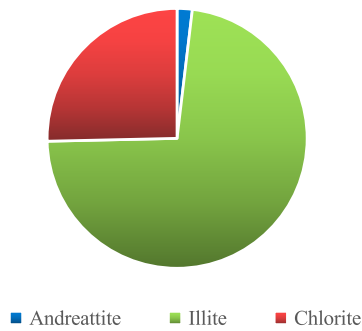


FIGURE 11. Distribution of clay minerals in samples from all experiments.

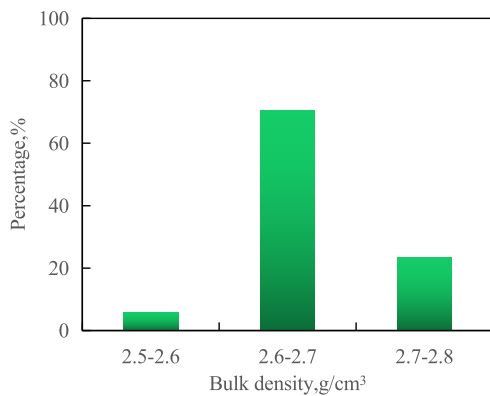


FIGURE 12. Bulk density distribution range of samples participating in all experiments.

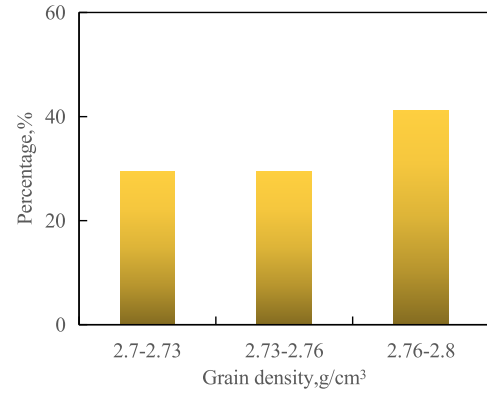


FIGURE 13. Grain density distribution range of samples participating in all experiments.

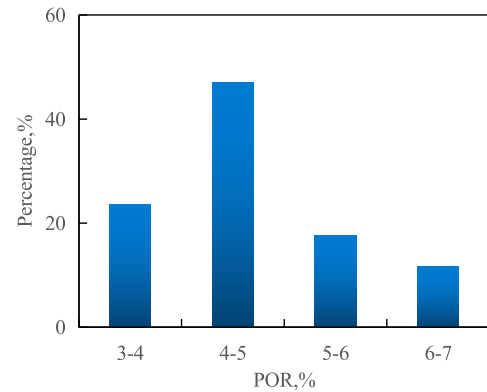


FIGURE 14. Porosity distribution range of samples participating in all experiments.

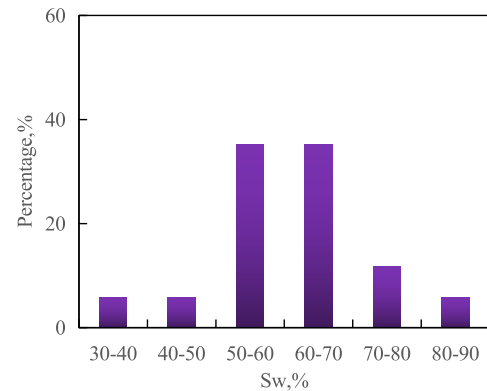


FIGURE 15. Water saturation distribution range of samples participating in all experiments.

pycnometer were used to determine the GRI porosity and GRI water saturation. A total of 127 cores participated in the TOC experiment, whereas 117 were involved to reveal the mineral composition. The number of cores involved in the experiment to determine the clay type was 109, 87 cores were used to measure the true density and bulk density of the rock, and 52 were taken to quantify the GRI porosity and GRI water saturation. Among them, a total of 16 cores were measured simultaneously for all of the above experiments. The large number of measured parameters makes it difficult to display them in the form of a table. Therefore, the ranges of the

reservoir parameters obtained from the samples participating in all experiments are shown in Figs. 9-15.

Figs. 11-18 show the ranges of the various parameters for the parallel samples. The TOC distribution is primarily 0-4% but ranges mainly from 1 to 3%. The block density ranges from 2.5 to 2.8 g/cm³ but varies mainly between 2.6 and 2.7 g/cm³. The grain density ranges from 2.5 to 2.8 g/cm³, and the porosity fluctuates between 3 and 7% but ranges primarily from 4 to 5%. The parallel samples have a widely distributed water saturation in the range of 30-90%, but it primarily varies between 50 and 70%. The clay and quartz min-

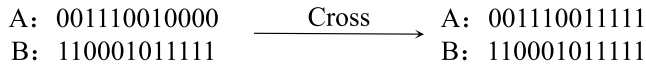


FIGURE 16. Crossover operation.

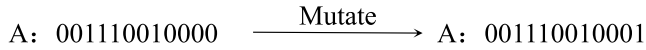


FIGURE 17. Mutation operation.

eral contents are the highest among the mineral components in the parallel samples; among the clay mineral components, the illite content is the highest. In general, the main reservoir parameters of the parallel samples are consistent with the average reservoir parameters of the studied block, indicating that the conclusions obtained from the above data are representative.

B. DETERMINING THE PARAMETERS OF THE PROPOSED SHALE PETROPHYSICAL MODEL BASED ON A GENETIC ALGORITHM

Genetic Algorithm (GA) is a computational model that simulates the natural evolution of Darwin’s biological evolution theory and the biological evolution process of genetics. It is a method to search for optimal solutions by simulating natural evolutionary processes. The three most important operations in the genetic algorithm are selection operation, crossover operation, and mutation operation. Among them, the selection operation of the population can eliminate the inferior solution, and the fundamental purpose of the crossover process and the mutation process is to increase the diversity of the alternative solutions.

1) SELECTION OPERATION

This operation refers to the selection of individuals from the previous generation population with a certain probability of entering the next generation population. The better the individual fitness is, the greater the probability of being selected for the next population generation. The selection operation is the most fundamental guarantee for obtaining the optimal parameters, and it also represents the fundamental manifestation of the survival of the fittest philosophy within a genetic algorithm; in other words, the best individual is ultimately retained through many iterations.

2) CROSSOVER OPERATION

This operation combines two individuals in the encoded population to produce new individuals by exchanging one or more chromosomal locations. The purpose of the crossover operation is to increase the diversity of the population to avoid falling into local minima. The schematic is shown in Fig. 16.

3) MUTATION OPERATION

This operation refers to the selection of an individual in a population and the selection of a point in the chromosome to conduct a mutation to create a new individual. The mutation operation is illustrated in Fig. 17.

We use the abovementioned genetic algorithm while taking equation (15) as the optimized model and determine the density of organic matter, porosity of organic pores, porosity of clastic pores, hydrocarbon saturation in clastic pores and conversion rate of organic carbon. Our inputs include the total core porosity, core TOC, volumetric density of various parts of the core (calculated from the results of core mineral composition measurements), and core water saturation.

Since the coefficients of the equation that must be determined are derived from equation (15), the corresponding objective function is:

$$ObjFunction = \min |S_w(target) - S_w(predicted)| \quad (18)$$

where $S_w(target)$ is the actual saturation value, which can be obtained experimentally, and $S_w(predicted)$ is the predicted saturation value, which is the result calculated by the optimized parameters. The optimization algorithm ensures that the parameters corresponding to the optimal water saturation are the best for continuous optimization. This method can obtain the best parameter results for a particular reservoir, significantly improving the prediction. For other shale reservoirs, although we still recommend the determination of specific parameters, the parameters determined in this fashion retain a certain referential significance, and the parameters can be used to evaluate the saturation.

Before optimizing the parameters, it is necessary to first determine the optimal ranges of those parameters, thereby reducing the difficulty of the optimization and yielding an excellent accuracy. The density of organic matter usually ranges from 1.1 g/cm³ to 2.0 g/cm³, and the density of organic matter increases with increasing thermal maturity. The organic porosity does not typically exceed 50%. Due to the compactness of shale gas reservoirs, the total porosity of shale gas is usually less than 10%, while the organic porosity usually exceeds 10%. Thus, the clastic porosity is usually no greater than 10%. The water saturation of clastic pores should be greater than that of bound water. In addition, the proportion of the organic carbon content in organic matter is generally considered to fall between 0.85 and 0.9. Therefore, the corresponding overall ranges are set as follows: $DEN_k = 1.1 - 2.0\text{g/cm}^3$, $POR_k = 0.1 - 0.5$, $POR_{nc} = 0.01 - 0.1$, $S_{nch} = 0.3 - 0.7$, and $C_k = 0.8 - 0.95$.

The optimal parameters of the Longmaxi formation and Wufeng formation are determined separately. Meanwhile, to facilitate a comparison, we also apply the formula for calculating the water saturation obtained from the original petrophysical model for optimization, and we employed the acquired parameters to calculate the corresponding saturation. The parameters calculated using the new method and the original method are listed as follows. For the Longmaxi formation using the new method, $POR_k = 0.2481$, $DEN_k = 1.93\text{ g/cm}^3$, $POR_{nc} = 0.0306$, $S_{nch} = 0.4961$, and $C_k = 0.9324$. For the Longmaxi formation using the original method, $POR_k = 0.2061$, $DEN_k = 1.02\text{ g/cm}^3$, and $C_k = 0.8$. For the Wufeng formation using the new method,

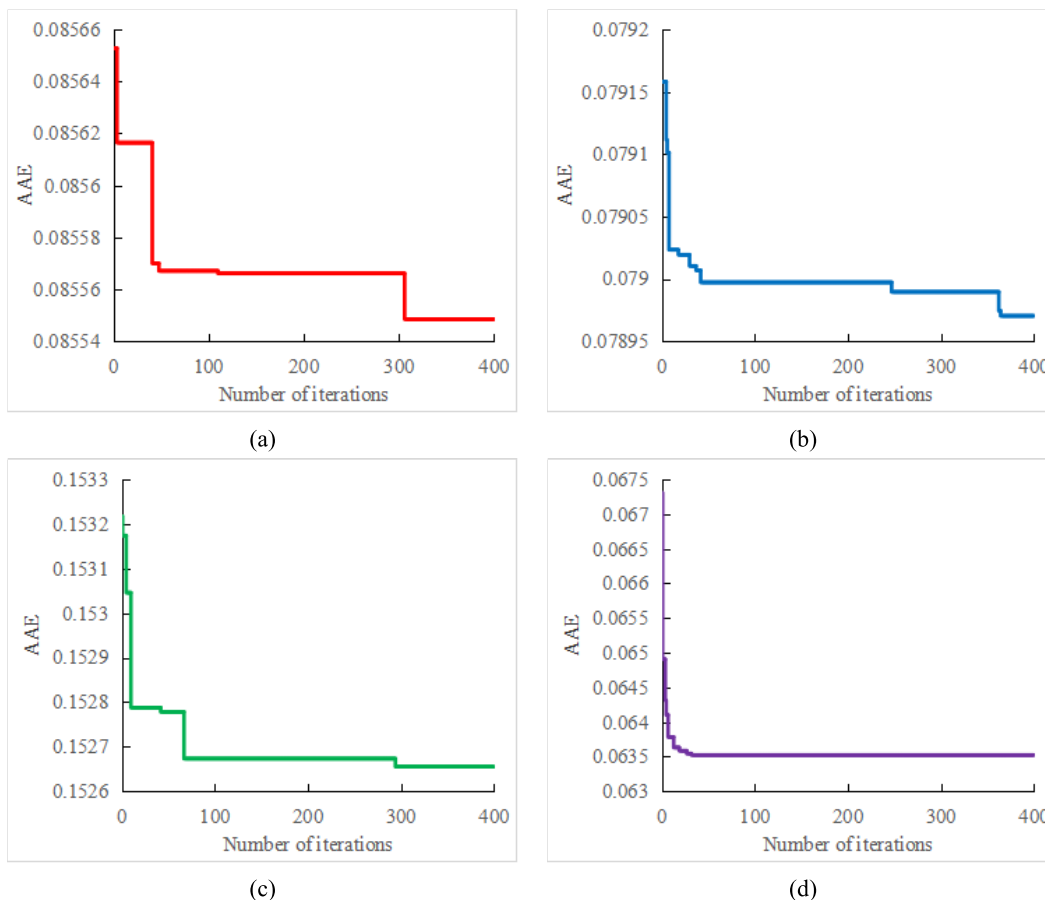


FIGURE 18. Using genetic algorithm to optimize the parameters of research block saturation model (a. original model to optimize the parameters of Longmaxi formation; b. new model to optimize the parameters of Longmaxi Formation; c. original model optimizes the parameters of the Wufeng formation; b. new model to optimize the parameters of Wufeng formation).

$POR_k = 0.1472$, $DEN_k = 1.928 \text{ g/cm}^3$, $POR_{nc} = 0.0383$, $S_{nch} = 0.5387$, and $C_k = 0.9036$. Finally, for the Wufeng formation using the original method, $POR_k = 0.1804$, $DEN_k = 1.035 \text{ g/cm}^3$, and $C_k = 0.8$. The optimization results obtained by the corresponding methods are shown in Fig. 18, where the ordinate refers to the average absolute error (AAE) of the calculated saturation. The calculated saturation results for the Longmaxi formation and Wufeng formation are shown in Fig. 19.

We combined Fig. 18 and Fig. 19 to perform a comparative analysis of the obtained results. First, based on the optimization curve for the Longmaxi formation, it is easier to optimize the new model than the original model under the same parameter settings in the genetic algorithm. When the number of iterations reaches 5, the proposed model begins to enter a stage characterized by a gently decreasing error, whereas the original model enters a stage with a gentle error after reaching 25 iterations. This result shows that it is easier to optimize the parameters of the new model and that the proposed model is more correct. In addition, based on the AAE values obtained from the final optimization, the AAE

of the calculated saturation with the optimal parameters of the new model is lower than that of the original model, indicating that the former is more reliable. Regarding the optimization results of the Wufeng formation, the optimization of the new model is obviously less difficult, and the saturation optimization error is much smaller than that of the original model. From the perspective of the optimization process, the new model is more in accordance with the actual situation of a shale reservoir. Based on the parameters obtained by the optimization, the densities of organic matter determined by the original method for the Longmaxi and Wufeng formation are 1.02 g/cm^3 and 1.035 g/cm^3 , respectively, which obviously do not agree with the conclusions of related research. These findings demonstrate that the reliability of the original model is questionable. As shown in Fig. 23, the prediction results of the new model are better than those of the original model, especially for the Wufeng formation.

Next, to ascertain the differences between the Wufeng and Longmaxi formations ascertained via the original method and the new method, field emission scanning electron microscopy

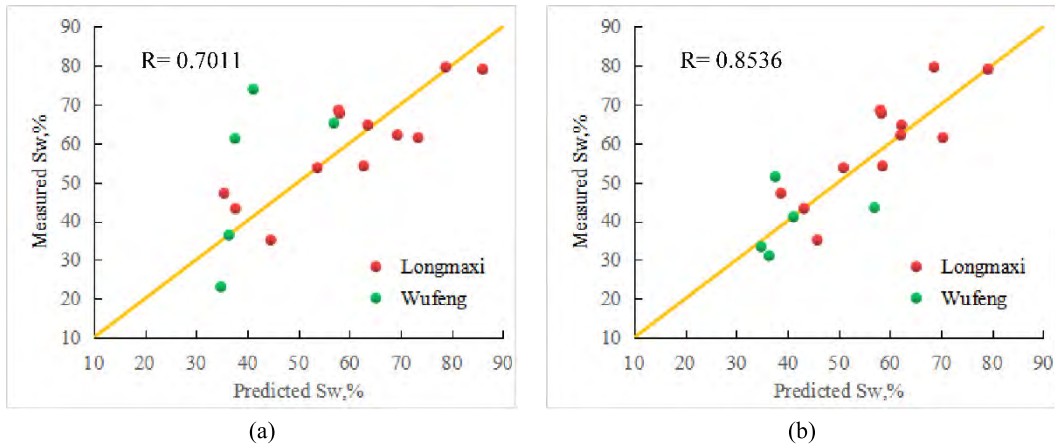


FIGURE 19. Prediction results of optimization parameters. (a) Original model. (b) New model.

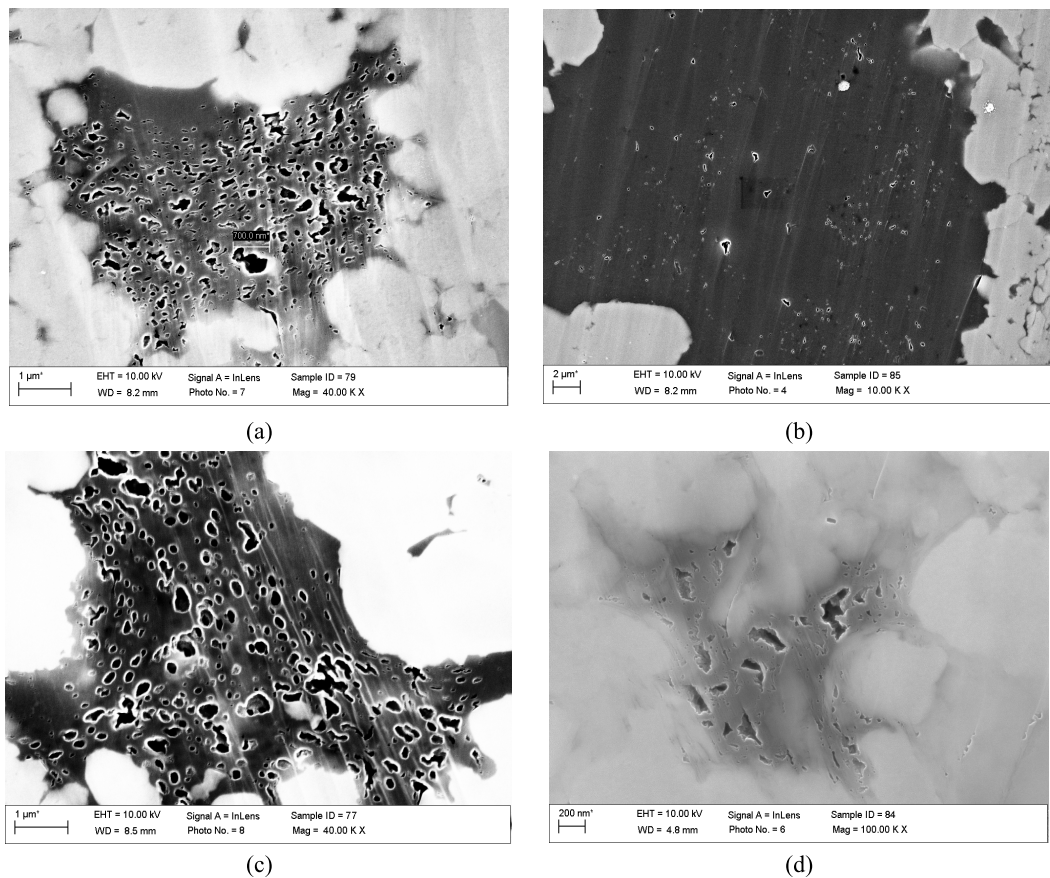


FIGURE 20. FE-SEM results of shale gas reservoirs in Longmaxi Formation and Wufeng Formation (a. A2 well, 4089.63m, Longmaxi Formation, massive organic matter, showing organic pore diameter up to several hundred nanometers; b. A2 well, 4094.68m, Wufeng formation, large organic matter, showing less development of organic pores, and the shape is prismatic; c. A2 well, 4087.84m, Longmaxi Formation, massive organic matter, a large number of organic pores are visible, the pore size is hundreds of nanometers, and the connectivity is good; d. A2 well, 4093.33m, Wufeng Formation, massive organic matter, organic pores visible in organic matter, pore size from tens of nanometers to 200 nanometers).

results (Fig. 20) of the Longmaxi and Wufeng formations in the studied block are selected for analysis.

Fig. 20 (a) and Fig. 20 (b) clearly demonstrate that the Longmaxi and Wufeng formations exhibit substantial differences in the organic pore quantity, pore size, and plane porosity difference. Furthermore, the degree to which organic pores

are developed in the Longmaxi formation is obviously better than that in the Wufeng formation, proving that the proposed model correctly reveals the remarkable difference in the proportion of organic pores between the Longmaxi and Wufeng formations. In addition, Fig. 20 (c) and Fig. 20 (d) show that the morphologies of the organic pores in the Longmaxi

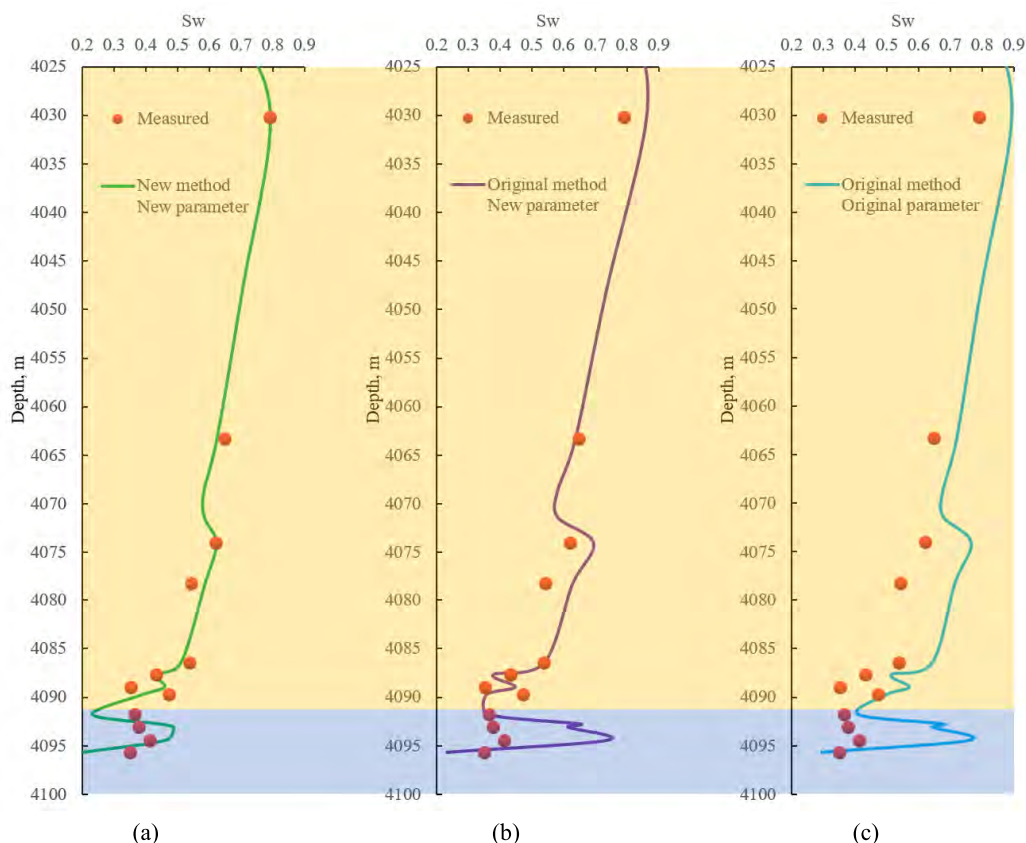


FIGURE 21. Prediction results of optimization parameters (a. new model,new parameter; b. original model,new parameter; c. original model,original parameter).

formation and Wufeng formation are very inconsistent; the organic pores of the Longmaxi formation are mainly circular, whereas those of the Wufeng formation are mainly irregularly angular in shape. Relevant studies have shown that the Wufeng formation was subjected to obvious tectonic compression and slippage along bedding planes, which caused a drop in the overburden that resulted in changes to the shale pore morphology and even pore closure within the Wufeng formation. This tectonism constitutes the main reason for the reduction in organic porosity within the Wufeng formation despite the small difference in the maturity [48]–[49]. After organic pores are squeezed, the gas within those organic pores will overflow into other types of adjacent pores. Without this mechanism, we cannot elucidate why the stages of maturity of the Wufeng formation and Longmaxi formation are the same; nevertheless, this explanation obviously shows that the organic pores were compressed and that surplus free gas entered the clastic pores. This reasoning is also consistent with the estimated increase in the gas saturation in the clastic pores of the Wufeng formation within our optimization results, demonstrating that the proposed model is consistent with the current geological understanding of the Longmaxi and Wufeng formations. Therefore, the content of free gas in the Wufeng formation is higher than that in the Longmaxi formation. In addition, the siliceous minerals in the Wufeng formation are mostly biogenetic, and their existence

is conducive for the maintenance of micropores in shale. Moreover, the porosity of clastic pores in the Wufeng formation should be larger than that of clastic pores in the Longmaxi formation, which is also consistent with the optimization results of the genetic algorithm. Therefore, it is necessary to consider the presence of hydrocarbons in clastic pores when calculating the saturation of shale reservoirs with a high maturity, especially when the pores have been subjected to tectonic compression [50].

The core results are shown in units of depth (see Fig. 21). Among them, the yellow area represents the Longmaxi formation, and the purple area represents the Wufeng formation. As observed in Fig. 21, the calculated water saturation using the original method is significantly larger because the selection of those parameters is based on experience, and the original parameters in this paper are estimated through the literature [29]. Employing the original method with the original parameters generally results in a higher water saturation, especially for the 4020 m–4040 m depth section, the 4070 m–4090 m depth section and the Wufeng formation depth section. Superior to other methods, the proposed method is more consistent with the trend of the core and does not erroneously estimate the saturation. This result indicates that the proposed saturation model based on the fluid occurrence characteristics of the shale pore system is successful. Related studies have shown that the highest-quality interval in

the entire Longmaxi formation-Wufeng formation reservoir section usually extends from the bottom of the Longmaxi formation to the Wufeng formation. In contrast, the accuracy of the calculated saturation using the original method is low, and it is also easy to miss potential high-quality reservoirs. It is obviously difficult to calculate the exact saturation value (especially for the Wufeng formation) without considering the presence of hydrocarbons in clastic pores. However, from the longitudinal variations revealed by the core water saturation calculations, the saturation results obtained by both the original method and the new method are not consistent with the core trend, indicating that the proposed model still has room for improvement. In general, the advantage of the new method over methods that calculate the saturation based on the resistivity (i.e., research on the conductive mechanism of shale is in its infancy) is that the proposed petrophysical model does not need to consider the combination of pores with the pore structure or other parameters [51]–[52]. In other words, the proposed method is simple and practical, and it can assist with the exploration and development of shale gas reservoirs.

V. DISCUSSION

The saturation parameter of a shale gas reservoir not only reflects the fluid content in pores, which is consistent with a conventional reservoir, but also aids in accurately calculating the free gas content, which is very meaningful for shale gas reservoirs. However, it is difficult to apply conventional electric saturation models to shale gas reservoirs as a result of their complexity. In 2012, a saturation calculation method based on the density curve that improved the reliability of the saturation calculation was proposed; however, at that time, the existing geological understanding of shale gas reservoirs was insufficient, and thus, it was simply assumed that only organic pores in shale gas reservoirs contain gas. In contrast, this paper considers that clastic pores (especially intergranular pores and inner granular pores) in addition to organic pores are also characterized by a mixed wettability and serve as channels for fluid seepage. Moreover, natural gas also exists in clastic pores. Based on this understanding, in this paper, we propose a new kind of shale petrophysical model and derive a new theoretical saturation model in detail. By comparing the differences between the developed method and the original technique, the simulation results show that the proposed model is less affected by the TOC because organic pores do not constitute the only reservoir space.

Since all of the parameters in the proposed method are microscopic, it is difficult to accurately determine those parameters without conducting specific experiments. Instead of simply selecting approximate values, as is the case in the original method, we propose the use of a genetic algorithm to determine the optimal model parameters. Accordingly, the optimal model parameters of a shale gas reservoir in the southern Sichuan Basin are determined. It is believed that the optimal parameters, including the organic matter density, determined by the new model are consistent with

the geological characteristics of shale gas reservoirs. The saturation of well A2 is also calculated. The results show that the method proposed in this paper can calculate the saturation of shale gas reservoirs more accurately than can the original method; furthermore, the ability of the new model to estimate the tectonic compression of a shale gas reservoir is superior to that of the original model. Thus, the proposed model, which expands the methodology utilized to evaluate the saturation of a shale gas reservoir by incorporating a nonelectric method and improves the corresponding interpretation accuracy, is more helpful than the original model for evaluating the saturation of a shale gas reservoir. For other shale gas reservoirs, we recommend a reasonable determination of the range of parameters in combination with actual geological conditions. For example, for a less mature reservoir, the corresponding organic pores have a smaller organic porosity, and so on.

Currently, some components of the hypothesized model must be further studied. At present, our research regarding the new model is ongoing. First, does gas exist in clay pores? Clay pores usually exhibit water wettability, but it is still possible for clay pores with large pore sizes to contain oil and gas. Second, will hydrocarbon fluids in an adsorbed state have an impact on the calculation of the saturation (especially for reservoirs whose adsorbed gas content varies greatly along the vertical direction)? Both of these questions require further study in the future. Nevertheless, the proposed method for evaluating the saturation of shale rock based on nonelectric features has substantial research value.

VI. CONCLUSIONS

In this paper, we propose an improved nonelectric method for calculating the saturation within a shale gas reservoir. The improved model references the newer geological theory regarding shale reservoirs and improves the reliability and accuracy of the saturation model. From the research presented in this paper, we can obtain the following conclusions.

Based on an analysis of different shale gas pore types, we believe that clastic pores in addition to organic pores contain natural gas and serve as very effective seepage channels. Based on this conclusion, we propose a new petrophysical model based on shale density characteristics.

By deriving a petrophysical model, we obtain a new saturation evaluation model based on the density characteristics of shale reservoirs. After considering the presence of fluids in clastic pores, the proposed model can better meet the requirements of evaluating the reservoir saturation. Considering that the proposed model contains an excessive number of parameters, making it difficult to practically evaluate the saturation of a shale reservoir, the use of a genetic algorithm is proposed to automatically optimize the model parameters. Based on data from the Longmaxi and Wufeng formations in the Yongchuan block in the southern Sichuan Basin, the optimization results show that the new model is more correct than the original approach and that the determined parameters are more reasonable. The results of a final evaluation also

indicate that the accuracy of the new model proposed in this paper is higher than that of the original model. The results of a core calculation are more consistent with the core measurements and are less affected by the TOC; hence, the new technique can aid in evaluating the saturation of a shale reservoir. The above results indicate that it is necessary to make targeted improvements to the theoretical model for the geological features of shale; nevertheless, we believe that this approach can provide guidance for subsequent research regarding evaluations of the saturation of shale gas reservoirs.

ACKNOWLEDGMENT

The authors would like to express their deep thanks to all the editors of the IEEE-Access, for their enthusiasm, patience, and tireless efforts. Finally, they are very grateful to experienced anonymous reviewers for their constructive advice on how to make the paper significantly.

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