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WELL-LOG BASED TOC ESTIMATION USING LINEAR APPROXIMATION METHODS

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Abstract: Diverse measured physical parameters using open-hole wireline logging methods used for indicating source rock intervals and estimating total organic carbon (TOC) content are compared. Different methods (i.e., Passey, Schmoker, Uranium and Clay Indicator) for estimating TOC content in a data set of five wells from the Northern Sea (Norway) were tested, making it possible to delimit the organic-rich source rock intervals in the wells and estimate the TOC content for each well; results were compared with laboratory TOC data. It was shown that Passey's method is a robust tool to evaluate TOC content that is unlike other methods, since it considers more physical parameters for the petrophysical evaluation (e.g., resistivity, level of maturity, porosity), making it the most accurate method to evaluate TOC content. However, the other methods show good agreement with the measured TOC content.

Keywords: Total Organic Carbon Content, TOC, Passey, Schmoker, Clay Indicator, Unconventional reservoirs

1. INTRODUCTION

The increase in energy demand worldwide influenced by the increasing world population, domestic economies, and living standards has pushed the world oil and gas industry to consider the importance of exploration and exploitation of unconventional hydrocarbon deposits as conventional resource supplies diminish or become unavailable to multinational companies.

From an economical point of view, reservoir quality and completion quality are fundamental geological/petrophysical parameters that can determine high hydrocarbon production [1]. Since organic rich reservoir or source rock are characterized by low-to-ultralow permeability and low-to-moderate porosity, hydrocarbon reservoir must be stimulated to produce acceptable commercial quantities of hydrocarbon and such parameters assist to evaluate the economical viability.

Reservoir quality describes the hydrocarbon potential, amount of hydrocarbon in place, and hydrocarbon deliverability of the rock formation. These variables are a function of the key characterization parameters of organic rich reservoir, which include TOC, thermal maturity, organic matter, mineralogical composition, lithology, effective porosity, fluid saturations, permeability, and formation pressure [2].

An integrated multidisciplinary approach is needed to assay an optimal petroleum system analysis for the exploration stage since in practice data availability (cores, logs, seismic data, geochemistry, geological studies) is limited [1]. Thus, petrophysical analysis can help to evaluate the hydrocarbon potential.

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A critical indicator of hydrocarbon resource to be studied is TOC, which is very important when evaluating a potential organic shale gas reservoir [1]. TOC expresses the amount of organic carbon present in the formation, which has been shown to have a direct relationship with porosity and gas saturation [2].

Diverse well-log interpretation methods have been developed to assess accurate TOC estimation [3–7], from empirical relations to multivariate statistical analysis or inversion methods.

2. Well-log response to organic matter

2.1. Integral and Spectral Natural Gamma Ray Logs

Integral and Spectral Natural Gamma Ray tools measures the natural radioactivity in formations. The Integral and the Spectral Natural Gamma ray tools are composed of a scintillation spectrometer that can detect and measure the natural gamma rays. The Spectral Natural Gamma Ray tool records not only the number of gamma rays emitted by the formation but also the energy of each and processes the information into curves representing the amount of thorium (Th), potassium (K) and uranium (U) present in the formation.

The use of Integral and Spectral Natural Gamma ray logs for detection of potential source rocks has proved to be particularly useful as it has been observed that highly radioactive, black, organic-rich, and gaseous shales are potentially source rocks [8], making these logs especially helpful to distinguish between clay-rich strata and sandy or chalky layers, since it is common to have an abnormally high response in the natural gamma ray log due to the enrichment of uranium in shales, as a result of reductive environmental conditions during deposition [9].

2.2. Resistivity Logs

Numerous logging devices are offered for measuring the electrical resistivity of the formation (i.e., non-focused electric logs, focused conductivity-induction logs, etc.). Such logs have been used to distinguishing organic-rich intervals in the formation because the presence of organic matter and hydrocarbon can result in alteration of the formation resistivity [8]. Since these materials are usually nonconductive, a high increase in the resistivity of the formation is expected.

Also, clay content in shale gas intervals may be variable (30–70%), which may lower the resistivity of the rock as a function of the cation exchange capacity (CEC), which is the quantity of positively charged ions that a clay mineral can accommodate on its negatively charged surface [10], and which varies with the type of clay and mixed layers [9].

Some other factors may affect the resistivity readings in a log. The presence of different minerals in complex geological formation plays an important role in the formation evaluation. Commonly, pyrite in organic-rich intervals can produce a decrease in resistivity response if the volume is significant [2].

2.3. Density Log

Formation density log measures the electron formation density, which is directly related to the true bulk density. True bulk density depends on the composition of the rock matrix material, formation porosity, and density of the fluids filling the pore space.

Organic matter density-log-based interpretation in sedimentary rocks lies in the fact that the presence of organic matter (kerogen) reduces the density of the rock due to its relatively low density. Furthermore, kerogen matrix density is usually very low, meaning that kerogen volume is not estimated accurately and consequently porosity will be overestimated [9].

2.4. Sonic Log

The sonic log allows us to determine the porosity of the formation by means of the recorded transit times (Δt) of the acoustic waves, whose value is the inverse of the velocity of the P waves. The transit time is related to the capacity of the formations to transmit acoustic waves, which is related to the lithology present in the formation as well as the texture of the rock, which means the porosity and the types and distribution of fluids (i.e., water, gas, oil, kerogen, etc.) present in the pore space.

Kerogen and gas have high acoustic transit times. Fertl and Chilingar [8] mention that kerogen exhibits an interval transit time in the range of 150 to 185 μ sec/ft; thus, the sonic log can be calibrated to TOC content due to the high transit time of organic matter. In practice, the use of the sonic log for determining TOC is improved when it is combined with other logs [9].

2.5. Neutron Log

The neutron log is considered a radioactivity log, and a porosity log as well as the density log. The neutron and density logs differ in that the neutron register continuously emits high-energy neutrons through a radioactive source placed in the probe, while the density log measures the electron formation density. The neutrons interact with the hydrogen present in the fluids found in the pores of the rocks and the thermal neutron readings obtained are indirectly related to the porosity of the rocks.

The neutron log responds to the amount of hydrogen present in the formation, which is related to the fluids found in the pores of the rocks. In clean formations, where water, gas, or oil are found in the pores, the neutron record will measure the number of pores that are saturated with these fluids, that is, the porosity of the formation.

The compensated neutron log is one of the least used conventional records for the detection and evaluation of organic matter and the productive potential of oil and gas shales. Neutron records are affected by hydrogen in organic matter and hydrogen in the hydroxyl (OH-) in clays, in addition to the hydrogen in water and any liquid or gaseous hydrocarbons present in the formation [9].

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3. METHODOLOGY

Based on the response of organic matter in borehole logs several authors have proposed different techniques to identify and estimate the amount of TOC content in organic-rich shale formations. Employing some of these techniques, qualitative methodologies (*Figure 1*) and quantitative methodologies (*Figure 2*) were developed for identifying and estimating TOC content.

3.1. Delimitation of source rock intervals: Qualitative approach

The qualitative approach is based on a discriminant function proposed by Meyer and Nederlof [11], using the acoustic and resistivity logs as follows:

$$D = -6.906 + 3.186 \log_{10} \Delta t + 0.487 \log_{10} R_{75}, \qquad (1)$$

where Δt is in µs/ft and R_{75} is the resistivity corrected to a standard temperature of 75 °F (24 °C). Quantity *D* is interpreted qualitatively according to its sign, if *D* is positive, the formation is a probable source rock; if *D* is negative, the rock is probably barren; and if *D* is zero, the case is considered undetermined.



Figure 1

Discriminant Function workflow based on the method developed by Meyer and Nederlof [11]. Misclassifications due to thin-layer effects, heavy minerals presence, uncompacted soft formations, high density/velocity formations may occur, so careful evaluation should be conducted.

3.2. Quantification of TOC: Quantitative approach

The quantitative approach for estimating the TOC content uses linear approximation methods, for which a theoretical overview will be given in the following subchapters. These methods are based on the linear correlation that exists between the well log's response to content of organic matter in the formation. The general methodology is shown in *Figure 2* and it is explained along these lines: utilizing TOC from core samples, different regression analyses can be performed employing diverse well logs, and the combination of well logs in the form of derivate log indicators (e.g., clay indicator, delta log R) so the linear best fit parameters (i.e., slope and intercept) can be obtained and applied to calculate a TOC curve. The Pearson correlation coefficient between TOC content from core data and well log readings should be equal or over ± 0.7 for each regression analysis so that a continuous TOC log can be estimated. After that, a comparison between TOC from core data and the estimated TOC is done by obtaining the coefficient of determination and root-mean-square error to ensure the quality of the estimation.



Figure 2

Proposed quantitative methodology workflow for estimating TOC content

3.2.1. Uranium Spectral Gamma-Ray Response Method

Various studies [8, 12,13] have shown that gamma ray spectral logging data can be used for characterizing source-rock potential. This is due to the fact that generally most organic-rich sediments are deposited from areas of high organic productivity through reasonably calm waters, where the supply of bottom oxygen is minimal, leading to enrichment in uranium [13]. The characteristic uranium accumulation and high TOC values in organic- rich reservoirs has led to the idea that the use of radioactive elements as tracers can help to define the source rock in a formation and its TOC content.

Beers and Goodman [12] analyzed several hundred rock samples from Paleozoic black shales where a marked linear correlation between TOC (in percentage) and uranium content (in ppm) is exhibited, demonstrating that an empirical relationship between these variables can be established as follows:

$$TOC(U) = A \cdot w(U) + B, \qquad (2)$$

where w(U) is the well log-derived uranium content in ppm; A and B are regional empirical constants. An advantage of using spectral gamma ray logging information is that it allows continuous monitoring of the source rock potential of shale in both open and cased wellbores [13].

3.2.2. Density Log Method

Schmoker [3] was the first to propose an estimation of TOC using density logs in the Appalachian Devonian Shale, USA. He found that there was an inverse proportional relationship between TOC and formation rock density. In a later study Schmoker and Hester [14] suggest a more generalized equation for calculating organic-carbon content from density logs:

$$TOC(\rho_B) = A \frac{1}{\rho} - B \,. \tag{3}$$

Later, Decker et al. [15] tested such hypothesis in Michigan Basin, proving that TOC and bulk density are linearly related in such a way that TOC increases with decreasing shale density. This method is based on the fact that variations in organic content can cause significant changes in the bulk density of the formation, since organic matter has a density of about 1.0 g/cm³, while the shale mineral matrix has an average density of about 2.7 g/cm³. Therefore, the variation of organic matter abundance can be computed from formation density logs [3]. However, variations in density produced by other causes (i.e., mineralogy) must be taken into account; for instance, Decker et al. [15] observed that pyrite content highly affects TOC estimation.

3.2.3. Clay Indicator Method

Zhao et al. [6] proposed a new overlying method for estimation TOC from gamma ray log and porosity logs (i.e., neutron and density logs). This clay indicator method is based on the physical dependence and correlation between the apparent neutron porosity ϕ_{Na} and density porosity ϕ_{Da} , and was referred to by Zhao et al. [6] based on studies performed by Mao [16]. This physical dependence is used to calculate the clay indicator (I_{cl}):

$$I_{cl} = \phi_{Na} - \phi_{Da}. \tag{4}$$

The clay indicator index is the difference between the apparent neutron and density porosities, and it has been found that the clay indicator can be employed to estimate the clay volume in source rocks which contain non-significant amounts of gas, where the neutron log can be affected by the excavation effect.

Moreover, it has been observed that the clay indicator has a similar response to the gamma ray logs in non-source rocks, although the difference between the gamma ray log and the clay indicator index in source rocks intervals is larger than those for non-source. Thus, the gamma ray log and the clay indicator can be used, if displayed in the same track and properly scaled, to differenced intervals of source rock from organic-lean intervals.

The separation between the two curves is expressed as follows:

$$\Delta d = GR' - I'_{cl} \,, \tag{5}$$

where

$$GR' = \frac{GR - GR_{left}}{GR_{right} - GR_{left}},\tag{6}$$

and

$$I_{cl}' = \frac{I_{cl} - I_{cl_{left}}}{I_{cl_{right}} - I_{cl_{left}}},\tag{7}$$

where GR is the observed log value in API units, GR_{left} and GR_{right} are the left and right scale limits of the GR curve in API, and $I_{cl_{left}}$ and $I_{cl_{right}}$ are the left and right scale limits of the clay indicator curve.

According to the observations of Zhao et al. [6] there is strong correlation between Δd and the kerogen content, with the separation increasing as the kerogen increases. Therefore, a linear relationship has been established to estimate TOC

$$TOC(\Delta d) = A \cdot \Delta d + B, \tag{8}$$

where *A* and *B* are the slope and intercept. This method has been proposed for use where the Delta Log R method has proven to be unsuccessful because abnormal R_T values have been read. Also, it has the advantage that the gamma ray and clay indicator curves overlie each other in non-source reservoirs with oil or water. Moreover, this method is applicable to formations that present excess radioactivity source rocks with little or no K-feldspar.

3.2.4. Passey's Delta Log R method

Passey et al. [4] developed a technique known as Delta Log R. This method employs sonic travel time (Δ t), or other common porosity curves (i.e., bulk density and neutron porosity) and true formation resistivity (*R*) curves scaled such as a ratio of 50 µs/ft or 164 µs/m to one resistivity cycle. When both curves are overlaid on the same track organic-rich intervals can be recognized by separation and non-parallelism of the two curves; such separation forms the delta log R distance ($\Delta \log R$).

It has been observed that a linear relationship exists between $\Delta \log R$ and TOC content, which is also a function of level of organic maturity (LOM). By means of many tests and samples, Passey et al. [4] established a mathematical expression to calculate the TOC related to $\Delta \log R$ and LOM:

$$TOC = (\Delta \log R) \times 10^{(2.297 - 0.1688 \times LOM)}.$$
(9)

The $\Delta \log R$ is measured by the following equation for a sonic log

$$\Delta log R = log_{10}(R/R_{baseline}) + 0.02 \cdot (\Delta t - \Delta t_{baseline}), \tag{10}$$

where $R_{baseline}$ is the resistivity corresponding to the $\Delta t_{baseline}$ value when the curves are baselined in fine grained non-source, clay-rich rocks.

Passey's method is considered to be independent of porosity changes, because the sonic and resistivity curves are both functions of the porosity in a given lithology, so once a baseline is established in a given interval, a comparable magnitude variation in porosity will affect the responses of both curves [4]. That is to say, an increase in porosity will result in an increase in Δt values, but it also means an increase in the volume of conductive water, followed by a proportional decrease in resistivity readings. Hence, the amount of increased porosity results in deflections of similar magnitude in both porosity curves.

4. CASE STUDY: NORWEGIAN NORTHERN SEA

Five wells were analyzed to identify the source rock potential intervals and TOC estimation applying the previous methodology. The well-logs data set was provided by MOL Ltd. in the framework of internship practice at their Petrophysics Department in Szolnok, Hungary.

The five wells contain geochemical data from cores, corresponding to Total Organic Carbon (TOC). Caliper (CALI), Borehole Bit Size (BS), Natural Gamma Ray (GR), Deep Resistivity (RD), Sonic (DT), Density (RHOB) and Neutron-Porosity (NPHI) logs were recorded for each well, while Uranium Spectral Gamma Ray (U-SGR) was also recorded for Wells 1 and 3 (*Figure 3*).

4.1. Well-1

Because similar results were obtained in the other four wells, Well 1 is shown as a typical case applying the methodology proposed. The logs of measured data are shown in *Figure 3*. The depth is displayed in Track 1, starting from 60 m. The caliper and borehole bit size are given in the second track, while the natural gamma ray and uranium spectral gamma ray are shown in Track 3 with a GR baseline at 60 GAPI. In Track 4, sonic and deep resistivity logs. Density and neutron porosity logs are displayed in Track 5 and TOC data from cores are displayed in the last track.

Analyzing the data from logs, it can be noticed that there is an increased in uranium spectral gamma ray readings, from an average value of 0.91 ppm in the bottom part of the formation to values of tens of ppm at the top part. The density log shows in general complex behavior; however, a marked overall decrease in density towards the top of the formation can be seen, and this is followed by an increase in the sonic and neutron porosity log from an average porosity value of 73.1 μ s/ft to values around 110 μ s/ft for the latter, and from an average value of 0.13 v/v to values around 0.3 v/v for the former. The resistivity log shows a decrease in conductivity at the top of the formation. The behavior of the measured variables at the top of the formations agrees well with the high TOC values from the core, as was expected from the well log response due to organic matter enrichment.



Raw well log curves for Well 1

From the discriminant function (*Equation 1*), in *Figure 4* it can be seen that D is a positive value between 60 m and 87 m depth, indicating the boundaries of a possible organic-rich interval, confirmed by the TOC core data in Track 6 from *Figure 3*.

After the qualitative evaluation, the regression analysis to establish the linear models for estimating the TOC content was performed considering the physical relationships established in *Equations* (2), (3), and (8). It is important to mention that for estimating TOC using Passey's method it is necessary to know the level of maturity of the organic matter, as is stated by *Equation* (9). However, it was not possible to get such information directly from lab measurements, therefore using *Equation* (9) proposed by Passey et al. (1990) is not feasible. Consequently, a modification to the technique has been made. Instead of using *Equation* (9), in the regression analysis the procedure between TOC measured values and delta log R was conducted adjusting a best-fit linear curve expressed as follows:

$$TOC = A \cdot \Delta \log R + B. \tag{11}$$

The results from applying the linear approximation methods to Well 1 are shown in *Table 1*. It can be stated that the input variable delta log R distance is strongly correlated to the TOC core by the linear estimation model. The pair resistivity/neutron and resistivity/density present the highest value of correlation among the pairs; however, the difference between the other linear models is not significant, excluding the density log as an input variable, where the correlation between the density log and the TOC from the core is especially poor or uncorrelated at 0.24.

After the correlation analysis was done, the TOC log curves were estimated and are shown in *Figure 4*. Despite of the correlation constraint imposed on the methodology (*Figure 2*), for illustrative purposes, the density method results were used to calculate a TOC log curve.

Table 1

Method	Α	В	r
U-Spectral Gamma Ray	0.4324	0.7131	0.84
Density	117.58	-44.049	0.24
Clay Indicator	10.4795	0.2638	0.86
Passey (Sonic)	2.4006	0.9303	0.90
Passey (Neutron)	2.4895	0.8973	0.91
Passey (Density)	3.2447	0.8816	0.91

Regression analysis results. A and B are the regression coefficients, and r is the Pearson's correlation coefficient.



Discriminant function and estimated TOC logs. TOC P-Sonic: Passey's resistivity/sonic method; TOC P-Neutron: Passey's resistivity/neutron method; TOC P-Density: Passey's resistivity/density method; TOC Clay In: Clay Indicator method; TOC Density: Density Method; and TOC U-SGR: Uranium Method.

From *Figure 4* it is visually clear that estimated TOC log curves follow a similar trend to the values of TOC from core data. A more precise analysis was done when calculating the coefficient of determination and root-mean-square error, which compared the estimated TOC log curve values to TOC from cores. Results are shown in *Table 2*.

Table 2

i	root mean-square error (RMSI		
Method	\mathbf{R}^2	RMSE	
U-Spectral Gamma Ray	0.71	0.8701	
Density	0.02	2.0268	
Clay Indicator	0.74	0.7110	
Passey (Sonic)	0.76	0.6400	
Passey (Neutron)	0.81	0.8655	
Passey (Density)	0.78	0.6134	

Statistical analysis: Coefficient of determination (R²) and root mean-square error (RMSE) From *Table 2* it is clear that the resistivity-neutron pair from Passey's method gives the highest coefficient of determination value, 0.81, and a 0.8655 RMSE. The resistivity/density pair gives the lowest RMSE value, 0.6134, with a 0.7805 coefficient of determination. Uranium and Clay methods show a good performance, with 0.71 coefficient of determination and 0.8701 root-mean-square error, and 0.74 coefficient of determination and 0.7110, respectively. The Schmoker method shows poor performance in predicting data for Well 1, with a coefficient of determination of 2.27% and an RMSE of 2.0268.

It can be seen that visually there is quite a good match between measured and estimated TOC values, but summarized uncertainties show higher values. An explanation to this can be that with TOC range uncertainties varies, that is to say, as we go down, especially below 2.0% wt. TOC, uncertainties become even higher and errors will grow apparently. Thus, to prove that lower TOC values can caused uncertainties, a TOC cut-off higher than 2.0% was considered for calculating the accuracy between measurements and estimations.

Table 3

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Method	\mathbb{R}^2	RMSE
U-Spectral Gamma Ray	0.83	1.1554
Density	0.94	1.4865
Clay Indicator	0.81	1.3359
Passey (Sonic)	0.91	1.1475
Passey (Neutron)	0.83	1.139
Passey (Density)	0.97	0.7018

Statistical analysis for a 2.0% wt. TOC cut-off: Coefficient of determination (R^2) and root- mean-square error (RMSE)

Comparing the results from *Tables 2* and *3* it can be confirmed that intervals with poor TOC content make uncertainties higher, and thus, errors will grow significantly. For example, estimation from Passey's method using the sonic log considering the TOC cut-off presents a higher R^2 (i.e., 0.91) than without the cut-off ($R^2 = 0.76$). Also, the Schmoker method proved a much precise estimation in intervals where TOC content is higher than 2.0%, giving $R^2 = 0.94$; this might be explained by this method being based on the assumption of a high organic-rich, low-porosity and low-permeability shale formation.

5. CONCLUSIONS

Different methods for estimating TOC content by means of wireline logs were analyzed showing relevance for particular cases. This is due to the fact that different petrophysical properties of the formation are taken into account in different well-log records. An important step for source rock potential evaluation is the delimitation of the formation into organic-rich source rocks and organic-lean rocks; the use of a discriminant function has proved to be a certain tool to visually trace the boundaries between non-source and source rock intervals. The Uranium Spectral Gamma Ray method has shown good performance for estimating TOC content when compared against TOC values from the core, where U-SGR reading were available. This method is one of the first methods to be developed and is based on the fact that an increase in spectral gamma-ray readings can be highly correlated to TOC content in a shale formation, mainly considering lithological factors. However, careful evaluation should be done in the case of complex radioactive mineralogical formations.

The Clay indicator method not only takes into account the radiative response of the organic matter measured by the gamma-ray log, but also includes the effect of the kerogen, by means of the neutron and density porosity used to calculate the clay index curve. This method has given good results for Well 1 ($R^2 = 0.74$), Well 2 ($R^2 = 0.70$), and Well 5 ($R^2 = 0.56$).

The Passey method has shown to be the most reliable method of the empirical approaches since it takes into account not only the effect of the kerogen reflected in the porosity logs but also considers the compaction and burial history of the formation, by means of increasing resistivity response with a higher level of organic maturity. This last fact also appears to be limiting for applying this method, as in this study no data for LOM were available. However, following a good calibration procedure, it was possible to establish models for estimated TOC content.

The Schmoker method shows, in general, low performance based on R^2 values. This might be implied by the fact that this method requires some assumptions to be fulfilled such as that mineral composition is constant and porosity of the shale is low and constant all over the formation, so that variations in the density log can be attributed to the presence or absence of low-density organic matter. In general, it was noticed that the Schmoker method underestimates the TOC content in the source rock interval.

Finally, it is highly recommended to employ a combination of different techniques for estimating TOC content due to the fact that each well-log tool responds to different petrophysical properties, so results are ensured to be more accurate when compared against others. Borehole conditions should be checked by means of a caliper and borehole bit size since the quality of the porosity logs can be highly affected by this.

The Clay, Uranium, and Schmoker methods have demonstrated that they are acceptable as an alternative when there is a lack of resistivity data or abnormal R_T readings and the Passey method cannot be performed. Also, those methods are LOM-independent estimations of TOC content.

In addition, it is suggested to implement a more complex model that relates not just two wireline logs or parameters but using all the data available – uranium gamma-ray spectroscopy, density, neutron, sonic, and resistivity logging – applying multivariate statistical regression and inversion methods, i.e., the interval inversion suggested by Dobróka et al. [17] and further developed by Szabó and Dobróka [7]. This is recommended since the petrophysical model used in the studied methods oversimplifies the reality, and it would allow more complex and accurate models to be used considering not only the non-clay minerals, silt and clay, and the water

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volume, but also mobile, capillary and clay-bound water, also in addition to free hydrocarbons and absorbed gas in the porosity.

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