Modeling and inversion of petrophysical properties using Monte Carlo method in coquinas of the Morro do Chaves Formation (Sergipe-Alagoas Basin)

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Abstract

Petrophysical characterization of reservoirs is crucial for the accurate assessment of their properties. The discovery of large hydrocarbon accumulations in the pre-salt coquinas of the Santos Basin has motivated research in accessible analogues, such as the coquinas of the Morro do Chaves Formation in the SE-AL Basin. This study employs geophysical inversion methods to model and predict petrophysical parameters, using well log data and laboratory data from well 2-SMC-02-AL, drilled in the Atol Quarry, in São Miguel dos Campos, Alagoas. The main objective was to estimate a continuous porosity profile well correlated with the porosity measured in the laboratory. To achieve this, the observed density data were adjusted to the total density of the samples. Using the Markov Chain Monte Carlo (MCMC) method, we determined the coefficients of the Gardner equation (1974) - *a*, *b*, *c* - which allowed us to generate a continuous density profile ($\rho_{GardnerFIT}$) and subsequently a porosity profile ($PhiE_{DENFIT}$). The equations of Raymer et al. (1980) and Wyllie et al. (1956) were employed as alternative methods to estimate porosity profiles from the sonic log. The resulting porosity profiles were correlated with laboratory data (Phi_{LAB}), demonstrating that $PhiE_{DENFIT}$ provided the best fit. The results demonstrate the effectiveness of the MCMC method combined with the Gardner equation for predicting petrophysical properties, validating it as an interesting approach when essential curves for the characterization of complex carbonate reservoirs are absent.

Keywords: coquinas, porosity, modeling, inversion, Monte Carlo method

1 Introduction

The discovery of hydrocarbon accumulations in pre-salt coquinas has made these rocks important exploration targets in the Santos Basin. Several studies have been conducted on analogs to understand the complex porous system of carbonate rocks [1-4]. The hybrid coquinas of the Morro do Chaves Formation (Fm.) in the SE-AL Basin are considered analogous to the coquina reservoirs of the Campos and Santos Basins due to lithological similarities and depositional context. Investigating these rocks provides valuable insights and contributes to developing new methodologies for carbonate rock characterization, especially considering the high costs and challenges associated with pre-salt exploration.

The absence of essential well logs in the study area makes the precise estimation of porosity at depth, and consequently, the characterization of hybrid carbonate rocks, challenging. Modeling and inversion techniques emerge as alternatives to estimating petrophysical properties, such as density and porosity, by integrating laboratory and well-log data. Over the past 30 years, various inversion approaches have been used to calculate petrophysical parameters, with the development of nonlinear inversion algorithms for more accurate interpretation

[5,6]. As presented by Tarantola and Valette [7], Bayesian inversion provides model parameter estimates from a statistical perspective leveraging prior information and dealing with multiple local minima, applicable to many geophysical problems [eg. 8,9]. The MCMC method is efficient for characterizing the posterior probability distribution in complex and high-dimensional model spaces.

Therefore, this work aims to estimate a continuous porosity profile at depth, correlating it with the porosity data measured in plugs during laboratory analysis. For this purpose, MCMC simulations were applied to estimate the coefficients of Gardner's Polynomial Equation [10], resulting in a satisfactory fit between the measured and predicted density data. With the estimated density profile at depth, it will be possible to calculate a porosity profile. Finally, the equations of Wyllie [11] and Raymer-Hunt [12] were modeled based on the sonic log to estimate two porosity profiles, to compare which approach provides a better fit with the measured porosity. Additionally, a statistical evaluation was performed to analyze the accuracy and effectiveness of the applied models.

2 Study area

The Sergipe-Alagoas Basin is located on the continental margin of the northeastern region of Brazil, encompassing parts of the states of Sergipe and Alagoas. On a map, it appears elongated in the NE direction, with a length of 350 km and a narrow width ranging from 20 to 50 km. This basin covers a total area of 44,370 km², with one-third being onshore and two-thirds submerged up to the 3,000 m isobath [13]. To the north, it is bounded by the Maragogi High in the Pernambuco-Paraíba Basin, and to the south, in the onshore portion, by the Estância Platform in the Jacuípe Basin and by the Vaza-Barris fault system in the offshore portion [13].

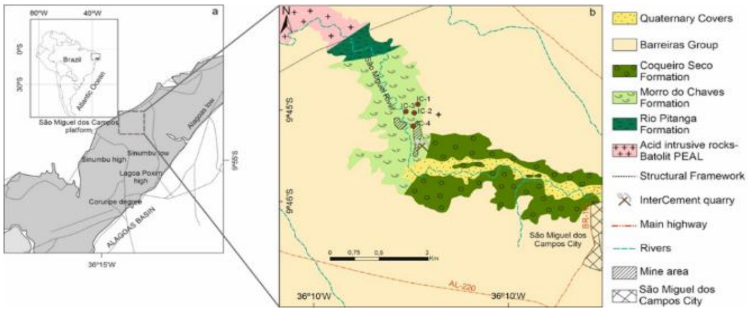

Figure 1. a) Location of the Alagoas Sub-Basin in northeastern Brazil showing the São Miguel dos Campos platform in detail. b) Geological map of Upper Cretaceous of Alagoas Sub-Basin (Modified from [14]).

In this study, we are interested in the coquinas of the Morro do Chaves Fm. (Barremian - Aptian) outcropping in the Atol Quarry region, located in São Miguel dos Campos, Alagoas (Fig. 1). The Morro do Chaves Formation is characterized by intercalated coquinas with laminates, sandstones, and conglomerates [15]. The intercalation of these carbonate and siliciclastic rocks reflects variations in environmental and climatic conditions over geological time. This occurrence of hybrid rocks significantly influences porosity and permeability, resulting in greater heterogeneity. Coquinas are carbonate rocks composed wholly or partly of transported shells and shell fragments [16], or any accumulation of skeletal remains [17], containing up to 50% terrigenous matrix [18]. The coquinas interval of the Morro do Chaves Fm. is considered a potential analog to the coquinas found in pre-salt reservoirs [19], due to their lithological similarity and depositional timeframe [20]. Therefore, various studies utilize these rocks to enhance understanding, by analogy, of the porous system in deep-water reservoirs.

3 Methodology

The data used for the development of this research consisted of geophysical well logs and laboratory data of rocks corresponding to the coquina interval of the Morro do Chaves Fm. These data belong to the Laboratory of Sedimentary Geology at UFRJ (LAGESED) and originate from well 2-SMC-02-AL drilled at the Atol Quarry. The primary objective was to estimate a continuous porosity profile at depth and correlate it with the porosity measured in the laboratory. This enabled the recognition of porosities between intervals where plugs were recovered for routine analyses (RCAL). Inversion using MCMC simulations was performed to estimate the coefficients of Gardner's Polynomial Equation, producing a satisfactory fit between the observed and measured density (Phi_{LAB}). Subsequently, modeling was carried out to estimate porosity using the Wyllie [11], Raymer-Hunt

[12], and Gardner [10] equations. The employed workflow consisted of six stages, as represented below.

3.1 Basic Petrophysics

Routine Core Analysis (RCAL) was performed by Solintec©, following API RP 40 standards, to obtain porosity, permeability, and grain density for 34 plugs from the Morro do Chaves Fm. Using the Law of Mixtures, the total density of the rock was calculated from the weighted average of the densities of its components, such as solid grains and pore fluid, considering their proportions. Therefore, based on the porosity (ϕ) values, grain density (ρ_{grains}) of each sample, and assuming the fluid density (ρ_{fluid} = 1.03 g/cm³), the total density (ρ_{total}) was estimated using eq. (1).

$$\rho_{total} = \rho_{grains}(1-\phi) + \rho_{fluid}\phi \quad (1)$$

3.2 Data selection, loading, and quality control

Well logs such as depth (DEPTH), caliper (CALI), gamma rays (GR), spontaneous potential (SP), compressional sonic transit time (BHC), total porosity (PhiT), and effective porosity (PhiE), as well as rock data such as grain density (ρ_{grains}), laboratory porosity (Phi_{LAB}), and estimated total density (ρ_{total}), were loaded into the Interactive Petrophysics (Geoactive) software.

Using the inverse of the transit time log, it was possible to obtain a P-wave velocity (Vp) profile through eq. (2). The transit time curves are in µs/ft. Therefore, the calculated Vp values were multiplied by the constant 304.8 to convert the units to km/s, according to Gardner's equation [16].

$$\mathrm{Vp} = \frac{1}{\mathrm{BHC}}\mathrm{x}304.8 \quad (2)$$

3.3 Clay volume estimation

The clay volume present in the rocks negatively influences porosity and is a crucial parameter for estimating the effectively connected porosity [21]. The most common method for estimating this parameter is based on using the gamma-ray log (GR) to determine the clay index (IGR), as shown in eq. (3).

$$\mathrm{IGR} = \frac{GR_{log}-GR_{min}}{GR_{max}-GR_{min}} \quad (3)$$

Where GR_{log} is the value read from the gamma-ray log; GR_{min} is the minimum value on the gamma-ray log; GR_{max} is the average of the maximum values on the gamma-ray log.

Next, the clay volume is estimated using Larionov's equation [22]. Considering that the rocks under analysis date back to the Cretaceous Period, eq. (4) was used.

$$\mathrm{Vcl}_{Larionov} = 0.33(2^{2\,IGR}-1) \quad (4)$$

3.4 Estimating the continuous density log

Gardner's Polynomial Equation [10] is an empirical relationship used to estimate rock density (ρ) from P-wave velocity (Vp). Table 1 illustrates the specific coefficients of the equation for different lithologies and the Vp intervals, in km/s, for which these coefficients are valid.

Table 1. Polynomial forms of the velocity-density relationships by Gardner et al. (1974) as presented by Castagna et al. (1993). The units are km/s and g/cm³ for velocity and density, respectively.

Lithology	*a*	*b*	*c*	Vp range (km/s)
Shale	-0.0261	0.373	1.458	1.5-5.0
Sandstone	-0.0115	0.261	1.515	1.5-6.0
Limestone	-0.0296	0.461	0.963	3.5-6.4
Dolomite	-0.0235	0.390	1.242	4.5-7.1
Anhydrite	-0.0203	0.321	1.732	4.6-7.4

Therefore, eq. (5) with coefficients from limestones was used to estimate a total density profile ($\rho_{Gardner}$), considering only the depths with Vp values between 3.5 – 6.4 km/s, as shown in Tab. 1.

$$\rho_{\mathrm{Gardner}} = a\mathrm{V_P^2} + b\mathrm{V_P} + c \quad (5)$$

3.5 Markov Chain Monte Carlo (MCMC) simulation

The estimation of the parametric terms in eq. (5) was conducted by solving the inverse parameter estimation problem. A Bayesian approach was adopted, utilizing all available information to reduce the uncertainty associated with the problem. New information was combined with previously available data for the statistical calculation of terms using Bayes' theorem, based on three principles: all parameters of the mathematical model were modeled as random variables; the degree of information regarding these variables was encoded by probability distributions; and the solution to the inverse problem was the posterior probability distribution [23-24]. Thus, parameter estimation involves obtaining a statistical distribution for each parametric term. In this research, the calculated total density profile was fitted to the theoretical curve provided by Gardner's model. The MCMC method, using the Metropolis-Hastings algorithm for likelihood calculation [24-25], was applied to estimate the posterior distributions of the parameters *a*, *b*, and *c* of Gardner's model. In this context, a study of metrics was carried out to evaluate the performance of the MCMC method results, including the R^2, which indicates the proportion of the variability of the dependent data that is explained by the model, and the RMSE, which provides a measure of the average difference between the predicted values and the observed values.

3.6 Porosity estimates

Porosity estimates were made using the Wyllie [11] and Raymer-Hunt [12] equations, utilizing the sonic log (BHC) and removing the effects of clay content. Wyllie's equation assumes that the measured transit time (Δt) is a weighted average of the transit times of the solid matrix (Δt_{matrix}) and the pore fluid (Δt_{fluid}), proportional to the rock's porosity. Thus, effective porosity is given by a linear relationship with the transit time of the rock components, as shown in eq. (6).

$$\mathrm{PhiE_{wyllie}} = \frac{\Delta t_{log} - \Delta t_{\mathrm{matrix}} - V_{clay}(\Delta t_{clay} - \Delta t_{matrix})}{(\Delta t_{\mathrm{fluid}} - \Delta t_{\mathrm{matrix}})Cp} \tag{6}$$

Where: Δt_{log} is the transit time read directly from the sonic log; Δt_{matrix} = 47.5 μs/ft is the transit time in the rock matrix considering a limestone matrix; Δt_{fluid} = 188 μs/ft is the transit time in the fluid considering pores saturated with slightly brackish water; Δt_{clay} = 70 μs/ft is the transit time in the clay present in the rock matrix; V_{clay} is the clay volume estimated from the gamma-ray log; C_p = 0.7 is the empirical compaction factor. This correction factor, typically ranging from 0.7 to 1.0, adjusts the simple linear relationship of Wyllie's equation to improve accuracy, especially in formations with intermediate porosity.

Raymer-Hunt [12] proposed a new empirical correlation that relates transit time and porosity, with the same parameters defined in Wyllie's equation [11]. For rocks with porosity below 37%, the Raymer-Hunt equation [12] is given by eqs. (7), (8), and (9) below:

$$\mathrm{Phi_{clay}} = \frac{(2\,V_{matrix} - V_{fluid}) - \sqrt{(2\,V_{matrix} - V_{fluid})^2 - 4V_{matrix}(V_{matrix} - V_{clay})}}{2\,V_{matrix}} \tag{7}$$

$$\mathrm{Phi_{son}} = \frac{(2\,V_{matrix} - V_{fluid}) - \sqrt{(2\,V_{matrix} - V_{fluid})^2 - 4V_{matrix}(V_{matrix} - V_{log})}}{2\,V_{matrix}} \tag{8}$$

$$\mathrm{PhiE_{Hunt}} = \mathrm{Phi_{son}} - \mathrm{Phi_{clay}}V_{clay} \tag{9}$$

Where: $V_{matrix} = 1/\Delta t_{matrix}$; $V_{fluid} = 1/\Delta t_{fluid}$; $V_{log} = 1/\Delta t_{log}$.

Subsequently, porosity was calculated from the density log ($\rho_{GardnerFIT}$) estimated using Gardner's Equation [10] with the coefficients adjusted by the MCMC technique in the previous step. Porosity from the density log ($PhiE_{DENFIT}$) is given by eq. (10):

$$\mathrm{PhiE_{DENFIT}} = \frac{(\rho_{\mathrm{matrix}} - \rho_{\mathrm{bulk}} - V_{clay}\,(\rho_{\mathrm{matrix}} - \rho_{\mathrm{clay}}))}{(\rho_{\mathrm{matrix}} - \rho_{\mathrm{fluid}})} \tag{10}$$

Where: ρ_{bulk} is the density obtained directly from the estimated density log ($\rho_{GardnerFIT}$); ρ_{matrix} is the density of the rock matrix. A value of 2.71 g/cm³ was used, representing the average density of the rock matrix in the formation; ρ_{clay} = 2.55 g/cm³ is the density of the clay present in the rock; ρ_{fluid} is the density of the fluid present in the pores. A value of 1.03 g/cm³ was used, considering slightly brackish water.

Finally, a comparison was made between the porosity measured in the laboratory and the estimated porosity logs $PhiE_{Wyllie}$, $PhiE_{Hunt}$ and $PhiE_{DENFIT}$. A series of statistical measures were calculated to quantitatively evaluate which of the estimated porosity logs best fits the measured porosity (Phi_{LAB}). The root mean square error (RMSE) and the correlation coefficient (R^2) were used to assess the model's accuracy and correlation. Additionally, central tendency measures such as mean, median, mode, and dispersion measures such as standard deviation (SD) were employed.

4 Results and Discussions

Overall, the caliper log shows a stable response throughout the formation. However, wellbore wall collapses are observed in intervals with the presence of laminates (green highlight – Fig. 2). These rocks are more susceptible to failures and collapse due to chemical alterations promoted by the interaction of the water-based drilling fluid with the clay minerals present in the rock, and the relationship between low interlayer cohesion and wellbore wall stress caused by differential pressure during drilling. The gamma-ray log allowed for the identification of laminite intercalations, which exhibit anomalous peaks higher than 140 gAPI associated with high radioactivity and clean limestones represented by coquinas with an average of 15 gAPI. This radioactive anomaly is characteristic of laminates as they have a finer and more argillaceous composition, resulting in a high clay volume. Consequently, this impacted the available porosity logs, as observed in the reduction of total porosity (PhiT) compared to effective porosity (PhiE) in these clay-rich intervals (Track 9).

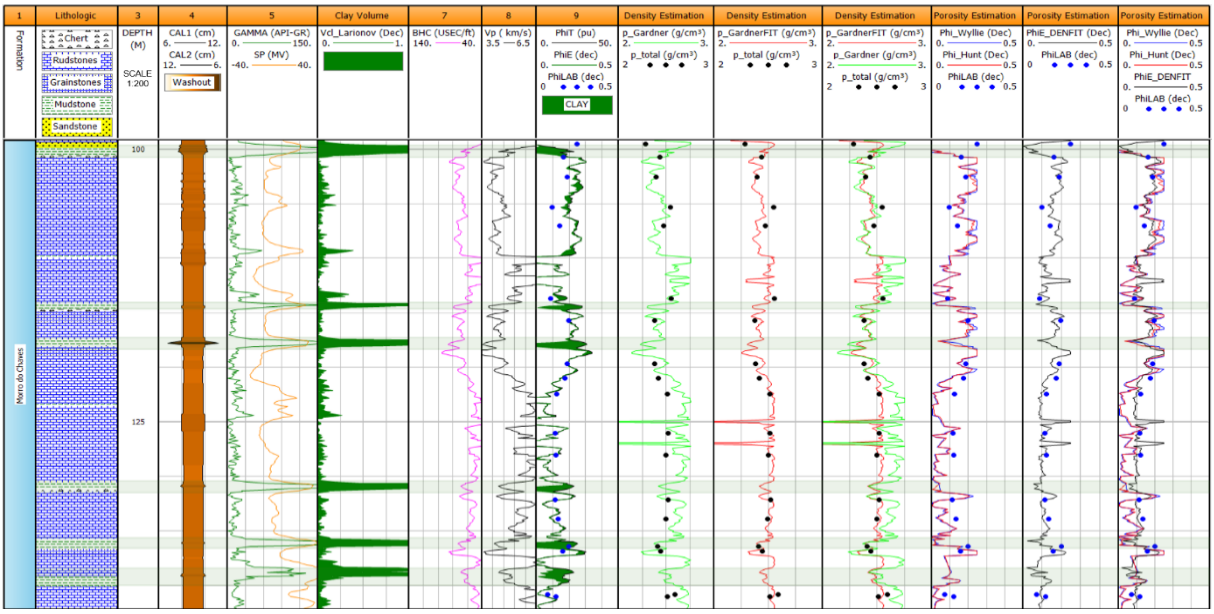

Figure 2. Geophysical logs of well 2-SMC-02-AL. Tracks: 1) Morro do Chaves Fm.; 2) lithological log (Lithologic); 3) DEPTH; 4) caliper (CALI); 5) gamma rays (GAMMA) e spontaneous potential (SP); 6) clay volume ($Vcl_{Larionov}$); 7) compressional sonic transit time (BHC); 8) P-wave velocity (Vp); 9) total (PhiT) and effective (PhiE) porosities logs; 10-12) total density estimates ($\rho_{Gardner}$ e $\rho_{GardnerFIT}$); 13-15) estimates and comparison of sonic effective porosity ($PhiE_{Wyllie}$ and $PhiE_{Hunt}$) and effective porosity by density ($PhiE_{DENFIT}$).

The application of the MCMC method to estimate the coefficients of Gardner's Polynomial Equation resulted in average values of a = -0.021, b = 0.294, and c = 1.535, derived from the generated statistical distributions. As illustrated in Fig. 3, these coefficients provided a satisfactory fit between the total density data (ρ_{total}) and the calculated density curve ($\rho_{GardnerFIT}$). Table 2 presents the statistical comparison of the density estimates using the coefficients for limestones as originally proposed by Gardner ($\rho_{Gardner}$) and the coefficients adjusted through the MCMC method ($\rho_{GardnerFIT}$). The $\rho_{GardnerFIT}$ estimate shows mean, median, and mode values that are close to each other and similar to the values found for ρ_{total}, indicating a symmetrical distribution with little influence from outliers. In contrast, the $\rho_{Gardner}$ profile shows higher values for these measures, with a mode of 2.75 g/cm³, which is higher than the average grain density of 2.71 g/cm³ of the samples. Additionally, the $\rho_{GardnerFIT}$ estimate has the lowest root mean square error (RMSE), reflecting greater model accuracy, and a positive and intermediate correlation coefficient (R^2), but relatively higher compared to $\rho_{Gardner}$. This small difference of 0.023 in favor of $\rho_{GardnerFIT}$ indicates a marginal improvement in the explanatory capacity of the adjusted model, even though $\rho_{GardnerFIT}$ explains a larger fraction of the data variability. These results highlight the superiority of the fit obtained with the MCMC method.

Table 2. Comparison of density estimates using coefficients proposed by Gardner (1974) and coefficients adjusted by the MCMC method.

Estimated	SD	Mean	Median	Mode	RMSE	R^2
ρ_{total}	0.08	2.42	2.50	2.54	-	-
$\rho_{Gardner}$	0.13	2.56	2.58	2.75	13.04	0.366
$\rho_{GardnerFIT}$	0.08	2.48	2.50	2.55	5.72	0.389

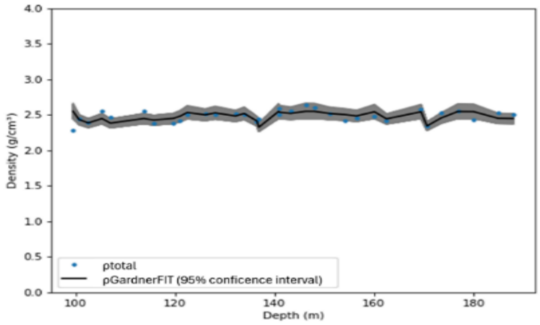

Figure 3. Fitting the measured total density (ρ_{total}) to the density curve calculated with the estimated parameter values ($\rho_{GardnerFIT}$).

Table 3 presents the basic statistics for the different estimated porosity logs. It is observed that the sonic porosities using equations (6) and (9) show similar values to each other but are much lower than the measured porosity. The $PhiE_{Wyllie}$ and $PhiE_{Hunt}$ curves resulted in RMSE values of 7.52 and 6.85, respectively, indicating how far these estimates are from Phi_{LAB}. This behavior occurs because the sonic log may encounter difficulties when reading porosity in carbonate rocks. The coquinas of the Morro do Chaves Fm. exhibit different types of pores—intergranular, interparticle, moldic, vugular, and fractures—that contribute to the increased complexity of the pore system. In these rocks, secondary porosity can predominate over primary porosity, and the sonic tool may not adequately capture this influence, underestimating the transit time and impacting the porosity estimates.

With an SD of 4.42, a mean of 12.62, a median of 11.75, and a mode of 9.50, the $PhiE_{DENFIT}$ profile demonstrates values statistically close to those obtained from laboratory measurements of Phi_{LAB}. Additionally, it has the lowest RMSE of 3.34 and the highest R^2 of 0.423 among all the estimates evaluated. Although the R^2 does not reach very high values, it still indicates a moderate positive correlation, which is significant considering the complexity of the pore system in these coquinas. Figure 2, track 15, illustrates the comparison between the different porosity estimates, highlighting the $PhiE_{DENFIT}$ profile for its better fit to the measured porosity data (Phi_{LAB}). Both statistically and graphically, greater efficacy in predicting porosity is observed using the density profile adjusted by the MCMC method compared to the sonic porosity profiles. These results reinforce the superior fit and greater accuracy in porosity estimation, validating the application of the MCMC method combined with Gardner's Equation as a robust approach for predicting porosity in coquinas.

Table 3. Basic statistics and metrics were adopted for the estimated porosity logs.

Estimated	SD	Mean	Median	Mode	RMSE	R^2
Phi_{LAB}	4.66	13.47	12.75	11.50	-	-
PhiT	7.87	15.56	15.60	18.50	6.70	0.379
PhiE	7.11	13.55	13.40	15.50	6.21	0.301
$PhiE_{Wyllie}$	7.96	9.51	7.62	1.50	7.52	0.366
$PhiE_{Hunt}$	7.35	9.48	8.12	1.50	6.85	0.366
$PhiE_{DENFIT}$	4.42	12.62	11.75	9.50	3.34	0.423

5 Conclusion

The application of the MCMC method proved effective for porosity estimation in the coquinas of the Morro do Chaves Fm. The coefficients of Gardner's Polynomial Equation, adjusted via MCMC, resulted in a density curve ($\rho_{GardnerFIT}$) that provided a superior fit to the total density data, with a lower root mean square error (RMSE) and a higher correlation coefficient (R^2) compared to Gardner's original coefficients. The sonic porosity estimates, such as $PhiE_{Wyllie}$ and $PhiE_{Hunt}$, were less accurate, resulting in higher RMSE and lower correlation with the measured porosity (Phi_{LAB}). In contrast, the $PhiE_{DENFIT}$ profile, derived from the MCMC technique, showed the lowest RMSE and the highest R^2 among all the estimates evaluated, indicating a moderate yet significant positive correlation considering the complexity of the pore system. These results validate the use of the MCMC method in combination with Gardner's Equation as a robust approach for predicting petrophysical properties in complex environments. The technique demonstrated greater accuracy in porosity and density estimation, highlighting its value as a tool for characterizing hybrid coquinas.

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Authorship statement. The authors hereby confirm that they are solely responsible for the authorship of this work, and that all material included herein as partes of the present paper is either the property (and authorship) of the authors or has the permission of the owners to be included here.

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