Estimating Formation Effective Porosity and Mineral Composition

Using Common Geophysical Logs

By

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Abstract

This study is motivated by the need to estimate the effective porosity and mineral composition of sedimentary formations for the purpose of geologic carbon sequestration, based on common geophysical logs. Because there are generally more mineral types than the number of logs at a given site, current methods yield non-unique solutions and give ambiguous results.

In this study, I develop a new method to estimate effective porosity and as many as needed mineral fractions based on three common geophysical logs: Gamma Ray Log (GRL), Density Log (DL) and Neutron Porosity Log (NPL). The method utilizes a probability approach, based on our knowledge on global mineral abundance in sedimentary rocks, mineral co-existence in different depositional environments, diagenetic (as a function of age/depth, hence temperature, pressure, preservation) constraints, in the form of several “filters” to rule out unlikely scenarios, and to give more weights to more likely scenarios.

Comparisons of the new model results with core-lab measurements demonstrate significant improvements over existing petrophysics methods in porosity estimation, and the new model offers a new possibility that existing petrophysics methods cannot offer, i.e., estimating the fractions of as many as necessary number of minerals.

This new method can be extended to other situations where a different set of geophysical logs are available. The innovation of this new method lies in the systematic approach of implementing physical constraints to eliminate or downplay unlikely mathematical solutions, these physical constraints being the basic knowledge of sedimentary and diagenetic processes.

Acknowledgement

To my whole wonderful family.... Because of you and for you.

I acknowledge my Thesis Committee, Professors Ying Fan Reinfelder, Ken Miller and Don Monteverde, for the infinite help they have given to me, even when I do not deserve it. I have now the duty to behave as a person of honor to show that I deserve such help.

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1. Introduction

Geological carbon sequestration is one of the several proposed strategies to permanently reduce atmospheric CO$_2$ levels (Socolow and Pacala, 2006; Schrag, 2007). The process involves capturing the CO$_2$ from large point sources (such as power-generation plants), compressing the gas to supercritical fluids, and injecting the fluids into deep, porous and saline geologic formations. To estimate the formation storage capacity, hence carbon sequestration potential, we must rely on knowledge of the effective porosity (the portion of total porosity that can be displaced by another fluid), and the mineralogical makeup of the formation. Porosity and mineral composition also determine the formation permeability which controls the movement of the injected CO$_2$ away from injection points. Direct analysis of drill cores to determine effective porosity and mineral composition is costly and hence rarely done, reserved for providing calibration data only. Instead, common downhole geophysical logs, such as Gamma Ray Log (GRL), Density Log (DL), and Neutron Porosity Log (NPL), are routinely acquired. These common logs provide indirect information on the properties of the formation, and petrophysics models have been developed to translate these measurements into formation properties (e.g., Tiabb and Donaldson, 2004).

However, current petrophysical approaches have several shortcomings (Crain, 2017). The state-of-science petrophysics methods rely on a system of linear equations, with each geophysical log readings expressed as linear combinations of the signals of the minerals present, plus an equation stating that all fractions add up to one (Pirson, 1970; Crain, 2017). Because there are generally more unknowns (e.g., number of minerals present) than the number of logs (e.g., the above three common logs), the problem is mathematically ill-posed, i.e., with many possible solutions that satisfy the mathematical equations. This leaves the petrophysical solutions often ambiguous, and the results are not always physically meaningful.

Meanwhile, there exists a large body of knowledge on mineral occurrence and co-occurrence in sedimentary formations, and as functions of depth and age (diagenetic conditions/history). Such knowledge can help constrain the multiple solutions by “weeding out” those that are inconsistent with such knowledge. However, in order to incorporate empirical knowledge into quantitative methods, a probability-based approach is necessary. This is the primary objective of this study: to develop a probability-based method for estimating formation effective porosity and mineral fractions, using the three most common geophysical logs, and to be constrained by knowledge of sedimentary conditions. In addition, the new method will account for the presence of drilling fluid, which invades the formation and contaminate the geophysical log readings. The traditional petrophysics methods neglect drilling fluids.

In the follow, I will discuss the current petrophysical methods and their limitations (section 2), the new methods developed here (section 3), the results from each step of the new model development and comparison with the traditional petrophysics methods (section 4), ending with the summery and conclusions (section 5).
2. Current Approaches and Limitations

2.1. Classic Petrophysical Models

The state-of-science classic petrophysical approach, widely used in the petroleum and the groundwater industry (Schlumberger, 1989), is well described by Seker (2012) and Crain (2017). The most critical parameter for calculating fluid flow in porous media is the permeability $K$, a function of effective porosity and mineralogy. Permeability exhibits strong anisotropy (direction-dependence) in sedimentary formations, and thus is expressed as a tensor (i.e., a 3D vector). Following Ulgerez (1990), Wangen (1991) and Bjorlykke (1993) and assuming that the x-y-z coordinates align with the bedding plane, then:

$$K = k(\phi_e) \cdot \begin{bmatrix} k_{1,1} & 0 & 0 \\ 0 & k_{2,2} & 0 \\ 0 & 0 & k_{3,3} \end{bmatrix}$$

(1)

Where $k(\phi_e)$ is a function of effective porosity $\phi_e$. The values of $k_{1,1}$, $k_{2,2}$, and $k_{3,3}$ are coefficients of the permeability tensor, representing x, y, and z components of the tensor, and they are functions of the lithology-minerology of the formation (Ulgerez, 1990). Therefore, quantifying the effective porosity and mineral composition is required to estimate formation permeability.

However, direct laboratory measurements of effective porosity and mineral composition are time consuming, hence expensive, and impractical to be performed routinely. Downhole geophysics tools have been developed to provide indirect estimates aided by inversion methods. In essence, petrophysics tools invert the formation properties based on their signal loading onto the well log readings. For example, the most common method for calculating permeability is the Archie’s equation based on inverting either Induction Log (IL) or Resistivity Log (RL) readings (Schlumberger, 1989; Crain, 2017). For another example, according to Schlumberger (1989), Seker (2014), and Crain (2017), the combination of Gamma Ray Log (GRL) and Spontaneous Potential Log (SPL) can be interpreted as: high GRL + low SPL indicates that the rock is a shale, low GRL and high SPL indicates a limestone, evaporites, or others; and low GRL and high SPL indicates a sandstone.

The most-commonly used petrophysics methods for calculating effective porosity (hence forth just “porosity” for simplicity) are:

- Method I:

$$\phi_e = \begin{cases} \frac{2.71 - \rho + \phi_n}{1.69 + \frac{100}{100}}, & \text{if } \frac{2.71 - \rho}{1.69} \leq \frac{\phi_n}{100} \\ \frac{\sqrt{(2.71 - \rho)^2 + \left(\frac{\phi_n}{100}\right)^2} - 2}{1.69}, & \text{if } \frac{2.71 - \rho}{1.69} > \frac{\phi_n}{100} \end{cases}$$

(2)

$\rho = \text{density log (DL)}, \ \phi_n = \text{neutron porosity log (NPL)}$
Method II:

\[
\phi_e = \frac{2}{3} \phi_{de} + \frac{1}{3} \phi_{ne}
\]

\[
\phi_{de} = \frac{2.71 - \rho}{1.69} - V_{sh} \frac{2.71 - \rho}{1.69}
\]

\[
\phi_{ne} = \phi_n - \phi_{n,sh} V_{sh}
\]

\[
V_{sh} = \frac{GRL}{GRL_{max}}
\]

Where \(\phi_e\) = effective porosity, \(\phi_n\) = neutron porosity log (NPL), \(\phi_{n,sh}\) = NPL of shale rock with the highest gamma ray log (GRL), \(\rho\) = density log (DL), \(\rho_{sh}\) = DL of shale with the highest GRL, \(\phi_{de}\) = porosity calculated using only DL values, \(\phi_{ne}\) = NPL without contribution from the shale fraction, \(V_{sh}\) = shale fraction, \(GRL_{max}\) is the highest value of GRL in all shale rocks drilled.

The presence of fluids (water, oil, gas), including drilling fluids, interferes with the geophysical signals of the native rock properties. The presence of drilling fluids in the rock can be detected by using the Induction Log (IL) when the drilling mud is based on non-conductive freshwater, the Resistivity Log (RL) when the drilling mud is based on high-conductivity saltwater, plus the density log (DL) and the neutron porosity log (NPL) (Schlumberger, 1989; Seker, 2014; Crain, 2017). To characterize drilling fluid influence, the borehole is divided into three sections whose resistivity can be used to diagnose fluid presence (Schlumberger, 1989):

- The flushed zone, which is completely invaded by the drilling fluid, and whose resistivity is denoted as \(RL_{xo}\)
- The transition zone, which is partially invaded by the drilling fluid, and whose resistivity is called \(RL_i\)
- The virgin zone, which is uninvaded, and whose resistivity is \(RL_t\)

The classic criteria for determining the type of fluid is then the following:

- The formation is water-bearing and impermeable if the resistivity values of the three zones are equal.
- The formation is water-bearing and permeable if the resistivity values differ, with \(RL_{xo}\) being the maximum, and \(RL_t\) the minimum. If the drilling mud is saline water, then it is not possible to detect if the rock is permeable or not, since both formation water and drilling mud will have similar properties. However, if the drilling mud is fresh water based, then the behavior will be very similar to hydrocarbon-bearing and permeable formations, and the only way to distinguish from them is through spontaneous potential.
- The formation is hydrocarbon-bearing and permeable if the three resistivity values are different, with \(RL_t\) being the maximum, and \(RL_{xo}\) the minimum. DL and NPL then can be used in addition to determine if the fluid is gas or oil as below:
The above are examples of some of the standard petrophysics tools in charactering formation properties based on combinations of a variety of geophysical logs. Several deficiencies in these approaches are summarized below, which provide the motivation for the present study:

- The resulting lithological interpretation is ambiguous and often qualitative. In order to estimate permeability via Equ-1, quantitative information of effective porosity and mineral fractions are needed. Current methods cannot provide these quantitative estimates.
- These standard methods do not make use of the large body of knowledge on mineral occurrence and co-occurrence, thus can produce unrealistic solutions.
- These methods do not consider the post-deposition compaction and diagenesis constraints on mineral existence under different temperature and pressure conditions, both functions of depth/age.
- They do not correct for the effect of the drilling fluids which contaminate the log readings.
- The formula for calculating shale fraction \(V_{sh}\), an important parameter in Method II above for computing effective porosity, does not consider the possibility of the presence of Potash Feldspar in the rock, among other similar issues.
- Water, oil, and gas can coexist in the same rock but cannot be differentiated with existing methods. Also, without resistivity logs (RL), the presence of gas vs. halite cannot be differentiated because their effect on DL and NPL are the same.
- It is difficult to calibrate these methods using direct lab measurements of the cores where they do exist which can improve results to be consistent with local reality.

### 2.2. Recent Attempts for Improvement

To develop a more systematic and quantitative approach, Pirson (1970) and Crain (2017) used GRL, DL, NPL, and Sonic Log (SL) to build a system of linear equations for calculating porosity and mineral fractions. The equations are defined by each mineral signature as coefficients contributing to the 4 well log measurements, plus the conservation law (all fractions add up to 1). These yields 5 equations (4 logs, plus the conservation law). To obtain a unique set of solutions, there must be exactly 5 unknowns (e.g., porosity plus 4 mineral fractions), as formulated below:

\[
\begin{align*}
\text{Oil} & \quad \text{if} \quad \frac{(2.71-\rho)}{1.69} < \frac{\Phi_n}{100} \\
\text{Gas} & \quad \text{if} \quad \frac{(2.71-\rho)}{1.69} > \frac{\Phi_n}{100}
\end{align*}
\]

(4)
\[
\begin{bmatrix}
g_{r1} & g_{r2} & g_{r3} & g_{r4} & g_{r5} \\
d_1 & d_2 & d_3 & d_4 & d_5 \\
h_{i1} & h_{i2} & h_{i3} & h_{i4} & h_{i5} \\
v_1 & v_2 & v_3 & v_4 & v_5
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2 \\
x_3 \\
x_4 \\
x_5
\end{bmatrix} =
\begin{bmatrix}
GR \\
DL \\
NL \\
SL
\end{bmatrix}
\] (5)

Where \(x_1, x_2, x_3, x_4, \) and \(x_5\) are the 5 volume fractions the users choose to calculate; \(g_{r1}, g_{r2}, g_{r3}, g_{r4}, \) and \(g_{r5}\) are the signature of the 5 minerals in GRL; \(d_1, d_2, d_3, d_4, \) and \(d_5\) are the signatures in DL; \(h_{i1}, h_{i2}, h_{i3}, h_{i4}, \) and \(h_{i5}\) are the signatures in NPL; \(v_1, v_2, v_3, v_4, v_5\) are the signature in the SL readings.

This represents a significant step forward from the traditional and often semi-quantitative tools, in that it is conceptually sound, mathematically rigorous, and it allows for site-specific inversions. However, five constituents (including porosity as one) are too few in most settings to define a realistic mineral composition. This limits the applicability of the new, albeit quantitative method. Additionally, if porosity was one of the 5 variables in Equ-5, then one must identify the fluid type, because the signature of porosity is the signature of the fluids. Then it becomes necessary to obtain either Resistivity Log (RL) or Induction Log (IL) as discussed earlier.

More recently, new attempts are made to calculate porosity using neural networks (Konate et al., 2015, and Jamshidian et al., 2015). Both studies used RL (resistivity), SL (sonic), DL (density), and NPL (neutron porosity) data, obtaining excellent correlations between the calculated porosity and the core laboratory measurements. However, most wells do not have RL and SL. The SL was necessary for achieving the good correlations reported in Konate et al. (2015) and Jamshidian et al. (2015), since SL has the best correlation with lab-measured porosity values by far. Therefore, the neural network models are limited to situations where SL is available.

The above review of current approaches points to a need for a new method that (1) only requires readily available, common geophysical logs, (2) builds on and improve the rigorous mathematical approach of Crain (2017) (Equ-5), (3) corrects for drilling fluid signature, and (4) utilizes the available knowledge on mineral occurrence, co-occurrence, and other diagenetic constraints, based on a probability approach. The next chapter describes the new methods in detail.
3. A New Probability-Based Method

3.1. The Study Site and Data Constraints

This study is initiated by the need to estimate the carbon storage potential in the deep saline aquifers off the coast of New Jersey (Figure 1a), where the sedimentary structures have been well constrained by decades of seismic acquisitions and deep drilling. The Great Stone Dome is an attractive site for geologic carbon sequestration because of its depth and the dome structure that can trap the injected CO$_2$. To estimate the storage potential, to predict the injected CO$_2$ plume migration, and to assess the potential for long-term carbon sequestration through CO$_2$ dissolution and carbonate mineral precipitation, effective porosity, mineral composition, and permeability are required. The only well with complete core laboratory analysis is COST B-2 (Figure 1b), accompanied by three common downhole geophysical logs: Gamma Ray Log (GRL), the Density Log (DL), and the Neutron Porosity Log (NPL).

![Figure 1](a) Study area with seismic lines and deep drill cores, showing the Great Stone Dome, (b) the 3 logs and laboratory measurements of porosity and permeability at well COST B-2. The oval shapes represent depth to basement rock. Red lines indicate tracks of multichannel seismic lines. Green and blue circles represent shallow wells. Red circles denote deep wells. White circles represent both COST B-2 and COST B-3 wells (Monteverde et al., 2010).
Thus, this study is motivated, and constrained, by the available data at well COST B-2: laboratory measurements as the “ground truth”, and the 3 common geophysical logs as the “inputs” to the new model to be developed. These 3 logs are also common at other drill sites in the area, and thus the new method will allow for extrapolation of key formation properties across the region.

3.2. The Mathematical Problem

Given the 3 logs only, plus 1 conservation law, only 4 variables, such as the effective porosity plus 3 mineral fractions, can be uniquely determined. However, the COST-B2 report gives X-Ray Diffraction (XRD) results for quartz, feldspar (undifferentiated), calcite, dolomite, siderite or ankerite, illite, kaolinite, montmorillonite, pyrite, oxides, phosphates, evaporites, micas, and zircon, etc., the list far exceeding 3.

Consider the more general case with 24 most common minerals, including the effective porosity as one of the constituents (Table-1). Each of the 24 variables registers a signature on the 3 geophysical logs employed in this study; note that organic matter is not split into kerogen and coal since their signatures on the well logs are very similar. Following Equ-5, one can write the system of 4 equations based on the 3 available logs:

\[
\begin{bmatrix}
g_{r1} & g_{r2} & g_{r3} & g_{r4} \\
\rho_1 & \rho_2 & \rho_3 & \rho_4 \\
h_{i1} & h_{i2} & h_{i3} & h_{i4} \\
1 & 1 & 1 & 1
\end{bmatrix}
\begin{bmatrix}
x_1 \\
x_2 \\
x_3 \\
x_4
\end{bmatrix}
=
\begin{bmatrix}
GRL \\
DL \\
NL \\
1
\end{bmatrix}
\]

(6)

Where \(g_{r1}, g_{r2}, g_{r3},\) and \(g_{r4}\) are the signatures of each variable in the gamma log; \(\rho_1, \rho_2, \rho_3,\) and \(\rho_4\) are their signatures in the density log; \(h_{i1}, h_{i2}, h_{i3},\) and \(h_{i4}\) are their signatures in the neutron log; and \(x_1, x_2, x_3,\) and \(x_4\) are the fractions of the constituents. These signatures are given in Table 1. Thus, the state-of-art formulation can only yield the fraction of 4 variables.

**Table 1.** The 24 mineral constituents (including effective porosity), and the signature of each in the 3 logs: gamma log (GRL), density log (DL), and neutron porosity log (NPL) (Crain, 2017).

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Gamma (API units)</th>
<th>Density (g/cm(^3))</th>
<th>Neutron Porosity (HI-index)</th>
<th>Mineral</th>
<th>Gamma (API units)</th>
<th>Density (g/cm(^3))</th>
<th>Neutron Porosity (HI-index)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity</td>
<td>0</td>
<td>1.02</td>
<td>1</td>
<td>Moscovite</td>
<td>270</td>
<td>2.82</td>
<td>0.12</td>
</tr>
<tr>
<td>Quartz</td>
<td>0</td>
<td>2.65</td>
<td>-0.02</td>
<td>Biotite</td>
<td>275</td>
<td>2.99</td>
<td>0.21</td>
</tr>
<tr>
<td>Calcite</td>
<td>0</td>
<td>2.71</td>
<td>0</td>
<td>Chlorite</td>
<td>2.15</td>
<td>2.76</td>
<td>0.52</td>
</tr>
<tr>
<td>Dolomite</td>
<td>0</td>
<td>2.84</td>
<td>0.02</td>
<td>Apatite</td>
<td>0</td>
<td>3.16</td>
<td>0.0044</td>
</tr>
<tr>
<td>Potash Feldspar</td>
<td>220</td>
<td>2.52</td>
<td>-0.03</td>
<td>Hematite</td>
<td>0</td>
<td>5.18</td>
<td>0.11</td>
</tr>
</tbody>
</table>
One approach is to set up and solve Equ-6 for only 4 of the 24 variables at a time, and then obtain the average of solutions from all possible combinations of 4 variables. With a total of 24 variables to choose from, the number of combinations of 4 variables reaches \( \binom{24}{4} = \frac{24!}{4!(24-4)!} = 10626 \), which can be computed with a simple program. However, such blind averaging of mathematically possible solutions is not meaningful, because some of the solutions are more realistic than others, given known mathematical and mineralogical constraints. That is, some of the solutions should be given more “weight” than others, and these weights should be based on our knowledge of sedimentary formations.

In the absence of site-specific knowledge, the weights should reflect the overall probability of the mineral occurrence in sedimentary formations. For example, globally speaking, the probability of encountering quartz is higher than encountering pyrite, since quartz volume fraction is higher than pyrite fraction in sedimentary rocks globally. Therefore, an inventory of global abundance of minerals in sedimentary rocks can provide a first-order constraint, in the probabilistic sense, on the realism of the 10626 mathematical outcomes.

### 3.3. The Probability of Mineral Occurrence

In this section, I estimate the Average Volumetric Mineral Composition of Sedimentary Rocks (AVMCOSR), based on a synthesis combining-revising-harmonizing published results in the literature. There have been some attempts to estimate AVMCOSR. Folk (1980) obtained a preliminary estimate by volume, and Huckenholz in Angenheister (1982) presented an estimate by weight. Both are considered here for achieving more complete and accurate estimates. Regarding the weight fraction by Huckenholz in Angenheister (1982), the fractions of some mineral groups, such as oxides and others, are not defined. If they are included, they will represent almost entirely the sum of “accessory and miscellaneous” minerals in the estimates by Folk (1980). Mineral classification among the groups in Folk (1980) needs to be revised; for example, glauconite should be in the group of micas and clay minerals proposed in Huckenholz in Angenheister (1982), instead of “miscellaneous minerals” in Folk (1990); for another example, gibbsite should be in the group of oxides and hydroxides of Huckenholz in...
Angenheister (1982) instead of belonging to clay minerals in Folk (1980). Some authors (Pettijohn et al., 1987; Boggs, 2003; McKenzie, 2005) consider such regrouping reasonable while not substantially affecting the resulting estimates of mineral fractions. Here the group of oxides will consist hematite, limonite, and gibbsite, and the group “others” will consist of evaporates (halite, gypsum, anhydrite, sylvite), pyrite, and siderite. The “miscellaneous and accessory” minerals in Folk (1980) will include “oxides” and “others” from Huckenholz in Angenheister (1982), plus phosphates, which is apatite because the latter is the most abundant phosphate by far. These two sets of estimates, aided by information from several additional studies as discussed below, are combined to produce the values reported in Table 2.

Table 2. The Average Volumetric Mineral Composition of Sedimentary Rocks (AVMCOSR, in fractions, sum = 0.9984). They represent the global probability for the occurrence of a mineral.

<table>
<thead>
<tr>
<th>Mineral</th>
<th>Volume Fraction</th>
<th>Mineral</th>
<th>Volume Fraction</th>
</tr>
</thead>
<tbody>
<tr>
<td>Porosity</td>
<td>0.08</td>
<td>Muscovite</td>
<td>0.0656</td>
</tr>
<tr>
<td>Quartz</td>
<td>0.2704</td>
<td>Biotite</td>
<td>0.03</td>
</tr>
<tr>
<td>Calcite</td>
<td>0.0629</td>
<td>Chlorite</td>
<td>0.0171</td>
</tr>
<tr>
<td>Dolomite</td>
<td>0.0209</td>
<td>Apatite</td>
<td>0.0021</td>
</tr>
<tr>
<td>Potash Feldspar</td>
<td>0.0663</td>
<td>Hematite</td>
<td>0.0116</td>
</tr>
<tr>
<td>Salt/Sulfur</td>
<td>0.006</td>
<td>Limonite</td>
<td>0.0133</td>
</tr>
<tr>
<td>Gypsum</td>
<td>0.0052</td>
<td>Gibbsite</td>
<td>0.0192</td>
</tr>
<tr>
<td>Pyrite</td>
<td>0.0053</td>
<td>Sylvite</td>
<td>0.0001</td>
</tr>
<tr>
<td>Organic Matter</td>
<td>0.0092</td>
<td>Kaolinite</td>
<td>0.095</td>
</tr>
<tr>
<td>Anhydrite</td>
<td>0.0022</td>
<td>Montmorillonite</td>
<td>0.04</td>
</tr>
<tr>
<td>Siderite</td>
<td>0.006</td>
<td>Glaucnite</td>
<td>0.041</td>
</tr>
<tr>
<td>Plagioclase</td>
<td>0.009</td>
<td>Illite</td>
<td>0.12</td>
</tr>
</tbody>
</table>

The following logical and numerical calculations are performed to produce Table 2 (subscript v is by volume, w is by weight). Although the symbol % is used, the quantity refers to fraction (all <1.0).

\[
\% \text{miscellaneous}_v + \% \text{accessory}_v = \% \text{others}_v + \% \text{oxides}_v + \% \text{apatite} \quad (f)
\]

With the information from Folk (1980), it is deduced that:

\[
0.0154 \leq \% \text{miscellaneous}_v + \% \text{accessory}_v \leq 0.0674 \quad (g)
\]
Additionally, according to Huckenholz in Angenheister (1982), and give the density of apatite is 2.99 g/cm$^3$:

$$\frac{2.99 \times \% \text{apatite}}{\% \text{oxides}_w} = 0.5 = \frac{1}{13} \quad \text{and} \quad \frac{2.99 \times \% \text{apatite}}{\% \text{others}_w} = 0.5 = \frac{1}{5} \quad (h)$$

The heaviest mineral in the group “oxides” is hematite with density = 5.18 g/cm$^3$, and the lightest is gibbsite with density = 2.47 g/cm$^3$, which leads to the following inequality:

$$2.47 \times \text{oxides}_v \leq \text{oxides}_w \leq 5.18 \times \text{oxides}_v \quad (i)$$

Or:

$$\frac{1}{5.18 \times \% \text{oxides}_v} \leq \frac{1}{\% \text{oxides}_w} \leq \frac{1}{2.47 \times \% \text{oxides}_v} \quad (j)$$

Multiplying the above by 2.99 * %apatite (density x volume fraction):

$$\frac{2.99 \times \% \text{apatite}}{5.18 \times \% \text{oxides}_v} \leq \frac{2.99 \times \% \text{apatite}}{\% \text{oxides}_w} \leq \frac{2.99 \times \% \text{apatite}}{2.47 \times \% \text{oxides}_v} \quad (k)$$

Combining (h), we obtain:

$$\frac{2.99 \times \% \text{apatite}}{5.18 \times \% \text{oxides}_v} \leq \frac{1}{13} \leq \frac{2.99 \times \% \text{apatite}}{2.47 \times \% \text{oxides}_v} \quad (l)$$

$$\frac{13 \times 2.99 \times \% \text{apatite}}{5.18} \leq \% \text{oxides}_v \leq \frac{13 \times 2.99 \times \% \text{apatite}}{2.47} \quad (m)$$

$$7.51 \times \% \text{apatite} \leq \% \text{oxides}_v \leq 15.74 \times \% \text{apatite} \quad (n)$$

Similarly, we obtain:

$$3 \times \% \text{apatite} \leq \% \text{others}_v \leq 8 \times \% \text{apatite} \quad (o)$$

Subtracting (n) and (o) from (g):

$$0.0154 - 10.5 \times \% \text{apatite} \leq \% \text{apatite} \leq 0.0674 - 23.7 \times \% \text{apatite} \quad (p)$$

$$0.0013 \leq \% \text{apatite} \leq 0.0027 \quad (q)$$

The maximum value of 0.0027 agrees well with the weight fraction of apatite of 0.005 reported in Huckenholz in Angenheister (1982).

Next, we examine %oxides$_v$ and %others$_v$ as below:

$$0.008186 \leq \% \text{others}_v \leq 0.02183 \quad \text{and} \quad 0.02047 \leq \% \text{oxides}_v \leq 0.0428 \quad (r)$$

Combining the maximum of %apatite in (q) with (h), we obtain that %others$_w$ = 0.0408 and %oxides$_w$ = 0.1061.

Many authors consider hematite the most abundant iron ore mineral in sedimentary rocks (Pettijohn et al., 1987; Boggs, 2003; McKenzie, 2005). Therefore, based on analytical
optimization techniques the final values are: \%oxides_{v} = 0.0279, \%hematite = 0.0112, \%gibbsite = 0.0106, and \%limonite=0.00612

Now, we can follow a similar procedure for evaporite minerals based on halite representing 50%, gypsum 25%, anhydrite 20%, and sylvite less than 5% of the total volume of evaporite minerals (Boggs, 2003). The volume fraction and pyrite are practically the same (Boggs, 1992).

Since ankerite is much less common than siderite, its fraction in AVMCOSR is near zero (Bathurst, 1975; Moore, 2004). In the end, \%others_{v} = 0.013, \%pyrite = 0.002563, \%siderite = 0.002563, \%halite = 0.003938, \%gypsum = 0.001969, \%anhydrite = 0.001575, and \%sylvite = 0.000394.

According to Folk (1980),

\[ 0.0004 \leq \%muscovite + \%biotite \leq 0.0032 \quad (s) \]

and \% muscovite is much higher than \%biotite, so we can assume that

\[ \rho_{illite} \times \%illite + \rho_{muscovite} \times \%muscovite \cong \rho_{illite} \times \%illite \]
\[ \rho_{glauconite} \times \%glauconite + \rho_{biotite} \times \%biotite \cong \rho_{glauconite} \times \%glauconite \quad (t) \]

Additionally, halloysite is a very uncommon clay mineral so that,

\[ \rho_{montmorillonite} \times \%montmorillonite + \rho_{kaolinite} \times \%kaolinite + \rho_{halloysite} \times \%halloysite \geq \rho_{montmorillonite} \times \%montmorillonite + \rho_{kaolinite} \times \%kaolinite \quad (u) \]

Based on Weaver (1989), the Montmorillonite to Kaolinite ratio is 63/29.

To determine the organic matter volume fraction is straightforward since all the types of kerogen and coal have similar physical properties, and the volume fraction for each one is not known, so it is assumed a density value of 1.19 g/cc for the whole organic matter group.

Manger (1963) states that the value of 8.2% for the average porosity of sedimentary rocks is underestimated since the average porosity of shales has been underestimated too. However, when only the effective porosity is considered, the value of 8.2% is reasonable.

In summary, based on the above calculations, we derived a new AVMCOSR (Table 2), giving the global volumetric fraction of all the minerals we will use in this study. Some minerals, such as zircon, ilmenite, leucoxene, etc. are not included in Table 2 because their signatures in the 3 geophysical logs employed in this study are unknown (see Table 1). The volume fractions in Table 2 will be interpreted as the global probability of their occurrence in sedimentary rocks. Then it follows that the probability of finding any four minerals together, corresponding to each one of the 10626 solutions to Equ-6, is the product of the probabilities of the 4 variables:

\[ w_i = p_j \times p_k \times p_l \times p_m \quad (7) \]
Where \( w_i \) is the probability of the \( i^{th} \) solution (1 of the 10626) to be encountered in nature, and \( p_j, p_k, p_l, \) and \( p_m \) are the probabilities for the \( j^{th}, k^{th}, l^{th}, \) and \( m^{th} \) variables listed in AVMCOSR (Table 2). The value \( w_i \) will then be given as the weight to each solution when obtaining the average of all possible mathematical solutions.

But before the weighted averages are calculated, several “checks” must be performed to “weed out” meaningless or unrealistic solutions. These checks are described as “filters” below.

### 3.4. The Mathematical Filter

After solving Equ-6 for each combination of 4 variables, the resulting volume fractions should satisfy the following condition, that each fraction should be positive (≥ 0) and less than 100% (≤1):

\[
0 \leq x_{i,j} \leq 1 \quad 1 \leq i \leq 24 \quad 1 \leq j \leq 10626
\]  

(8)

Where \( x_{i,j} \) refers to the fraction of a mineral \( i \) (including effective porosity) obtained in combination \( j \) of 4 variables (of a total of 10626). The effect of this filter is to discard the solutions that are negative or greater than one before the final averaging.

### 3.5. The Minerology Filter

This section describes a set of filters based on knowledge of mineral diagenesis to “weed out” improbable mineral occurrence or co-occurrence in given sedimentary/diagenetic environments.

#### 3.5.1. Mineral Co-occurrence

Sedimentary environments and diagenesis define the mineralogy of the sedimentary rocks. The most common types of sedimentary environments are clastic, carbonates, and evaporites (Boggs, 2003; Reading, 1986). Clastic environments are controlled by hydromechanical energy which is responsible for the distribution of particles of various sizes; for example, sand and clay are difficult to find together when they are deposited, but carbonates and evaporites are consequences of chemical precipitation whose main factors are pH (acidity) and Eh (redox potential), and they can occur together.

Common mineral associations are considered here. Some associations can occur, but others are rare. We assume that some associations cannot occur, as summarized in Table 3.
**Table 3.** Unlikely associations of mineral groups based on deposition/diagenetic environments.

<table>
<thead>
<tr>
<th>Mineral Groups</th>
<th>Unlikely Associations</th>
<th>Reasons</th>
</tr>
</thead>
<tbody>
<tr>
<td>1   evaporates and carbonates</td>
<td>1 &amp; 3</td>
<td>difference in hydromechanical energy</td>
</tr>
<tr>
<td>2   pyrite and organic matter</td>
<td>2 &amp; 3</td>
<td>difference in hydromechanical energy</td>
</tr>
<tr>
<td>3   quartz and feldspar</td>
<td>2 &amp; 6</td>
<td>difference in redox conditions</td>
</tr>
<tr>
<td>4   micas</td>
<td>3 &amp; 4</td>
<td>difference in hydrodynamic energy, and in diagenetic stages</td>
</tr>
<tr>
<td>5   clays</td>
<td>3 &amp; 5</td>
<td>difference in hydrodynamic energy, and in diagenetic stages</td>
</tr>
<tr>
<td>6   oxides and hydroxides, cations</td>
<td>4 &amp; 5</td>
<td>micas become clays and clays become micas during diagenesis; one is destroyed to make the other</td>
</tr>
<tr>
<td>7   effective porosity</td>
<td>7 &amp; 1, 2, 4, 5</td>
<td>diagenesis of these groups destroys effective porosity</td>
</tr>
</tbody>
</table>

**3.5.2. Diagenetic Constraints**

Here the post-deposition diagenesis is considered. Figure 2 summarizes the main mineral fields according to depth and temperature following Burley (1993). Burley (1993) states that the main factors for conditioning diagenesis are pH, Eh, and temperature. However, it is difficult to predict the effect of pH and Eh in the diagenetic processes. So here we only consider depth since temperature can be predicted by depth and the geothermal gradient.

Figure 2 defines the depth and temperature range over which each minerals can exist in a stable state. It is organized by three rock fields (top row): mudstones, sandstones and evaporites-carbonates, with temperature on the left and depth on the right. For example, for mudstones, the clay mineral presence, mineral destruction, organic matter behavior, pore water changes and pore water expulsion all vary systematically with temperature and depth. This allows us to judge whether a mineral is stable and likely found at a given depth. A simple check is performed here to “weed out” the mineral combinations that include minerals which are not stable at the reported depth. This is different from the next step, where the depth information is used to estimate quantitatively the probability of mineral occurrence, as the weight of a particular solution in the final averaging.
3.5.3. Probability of Occurrence with Depth/Age – An Improved Mineral Filter

Here a more comprehensive and innovative approach is discussed, which takes into account of the probability of mineral occurrence as depended on depth and age. This new approach is expected to improve upon the previous diagenetic constraint filter above which simply discards the solutions that contain minerals unstable at the known depth, but do not assign a probability of occurrence to the mathematical solution. The new approach incorporates two bodies of knowledge: first, the volume/mass evolution of each mineral in geological times (Boggs, 2003; Glenn et al., 1994; Hay, 1990; Hazen et al., 2013; Horita et al., 2002; Kholodov et al., 2008; Mackenzie, 2005), and second, systematic changes in porosity in geological times and in the burying processes (Ehrenberg, 2006; Ehrenberg et al., 2009; Manger, 1963).

Boggs (2003) gives estimates of changes in volume fraction for many types of rocks and changes in deposition rate along geologic times (Figure 3). We assume constant average mineral composition and uniform deposition rate within each of the time intervals such as within the Quaternary, Tertiary, and Mesozoic; in the special case of evaporites, the ratio among them reported in Table-2 is kept here. The porosity data in Edwards (1963) was used to compute correlations between depth and porosity for rocks of Cretaceous to Quaternary age (Figure 3). This differentiates the mineral fractions reported in Table-2 into different depth ranges or age groups undergone varying degrees of compaction and diagenesis. Using these data, we obtain a new set of weights or probabilities for the presence of each mineral and porosity during each of those periods of time, replacing the simple approach described in section 3.3 and Table-2.
3.6. Correcting for Drilling Fluid Contamination

Salazar et al. (2005) and Gandhi (2013) demonstrated the importance of having detailed drilling fluid information to evaluate drilling fluid influence. However, the COST B-2 report by Smith et al. (1976) did not include quantitative information on circulation loss during drilling, but only mentioned the shortage of drilling fluids. That is, the drilling information is insufficient.

Figure 4 is an operational sketch of COST B-2 well, which fortunately shows the changes in parameters of the drilling fluid, such as chlorine and calcium concentration, pH, and density with increasing depth. Those parameters are useful for calculating their signatures in the Neutron Porosity log (hydrogen index). It is also known that the drilling mud used for COST B-2 was not radioactive, which means that their signature in gamma ray is zero (0). Therefore, we can take the drilling fluid parameters as the signature of a new variable, in addition to the 24 variables in
Table 1, so we now have 25 variables. The combination of 4 variables from a list of 25 is now 12650, instead 10626 initially. Finally, this new variable fraction is added to the porosity fraction since the drilling fluids occupy pore space but return different signals from native fluids.

![Operational diagram of COST B-2 well and the changing drilling fluid parameters with depth (from Smith et al. 1976).](image)

Figure 4. Operational diagram of COST B-2 well and the changing drilling fluid parameters with depth (from Smith et al. 1976).

3.7. The Final Weighted Average with Example Calculations

Here we describe, and illustrate with a simple example, how the up to 12650 mathematical solutions, after applying the filters to weed out unrealistic ones, are averaged based on their probabilities in sedimentary rocks in different depth/age ranges. We use the following notations:

\[ x_{ij} = \text{volume fraction of mineral i in solution j (i=1 to 24; j = 1 to 12650)} \]

N = the number of solutions whose solutions pass all the filters discussed above (N = 1 to 12650)

\[ n_i = \text{the total number of solutions in N where mineral i appears (n_i = 1 to 12650, n_i < N)} \]

\[ w_k = \text{the weight for solution k based on Table-2 (AVMCOSR) first and later Figure 3 (which differentiates the weight by depth). We use Table-2 first to evaluate the improvement due to this information alone, and later we apply Figure 3 to evaluate how adding depth/age information further improves the results. This is the probability of the 4 minerals occurring together, or the} \]
The weight for solution $k$ itself ($k = 1$ to $N$), as shown in Equ-7, obtained as the product of the values in Table 2 or Figure 3.

The total probability of the $N$ valid solutions is simply the sum of the probability of the $N$ solutions:

$$\sum_{k=1}^{N} W_k$$

The weight given to each mineral $i$ in solution $j$ is then:

$$\sum_{j=1}^{n_i} W_j \times x_{i,j}$$

Note that we use $j$ not $k$, because $n_i < N$ and this summation. Then the total volume fraction in the final solution for mineral $i$, $X_i$ will be

$$X_i = \frac{\sum_{j=1}^{n_i} W_j \times x_{i,j}}{\sum_{k=1}^{N} W_k} \quad (9)$$

Below is an example to demonstrate how Equ-9 is applied. Assume that only two solutions (two 4-mineral combinations) passed all the filters above and will be considered in the final solution ($N=2$). Refer to Table-4 below. The first solution contains porosity ($x_{1,1}$), quartz ($x_{2,1}$), potash feldspar ($x_{3,1}$), and plagioclase ($x_{4,1}$), but no hematite ($x_{5,1}=0$); and the second solution contains porosity ($x_{1,2}$), quartz ($x_{2,2}$), potash feldspar ($x_{3,2}$), with no plagioclase ($x_{4,2}=0$), but with hematite ($x_{5,2}$). Therefore, there are only five variables ($i=1$ to 5) in this 2-solution scenario ($j=1$ to $N$, $N=2$). These variables are listed in row-1 of Table 4.

Table 4 below illustrates the steps of applying Equ-8 in an excel worksheet. It contains five rows of values: row-2, volume fraction in AVMCOSR (Table 2) for each mineral present in the two solutions; row-3, mineral fraction from the first solution; row-4, mineral fraction from the second solution; row-5, weights for each mineral (column B-F); row-6, final weighted mean volume fractions across the two solutions. Column-G is the probability of each solution, obtained as illustrated below in Table 4, step by step.

**Table 4.** Example to illustrate the application of Equ-9.

(a) Computing the joint probability of the 4 minerals present in the first solution, as product of the values in row-2 for these minerals (from Table 2, AVMCOSR) (note: skipping column-F). See Equ-7.
(b) Computing the joint probability of the 4 minerals present in the second solution, as product of the values in row-2 for these minerals (from Table 2, AVMCOSR) (note: skipping column-E): See Equ-7.

Steps (a) and (b) give the $w_k$ in Equ-8, for solution-1 ($k=1$) and solution-2 ($k=2$).

(c) Computing the sum probability of the two solutions:

Step (c) gives the denominator of Equ-8 ($\sum_{k=1}^{N} w_k$). Here $N=2$.

(d) Assigning weight (probability) to each mineral fraction from each solution, by multiplying the mineral fraction from each solution by this solutions’ probability (Column G), and summing up across the 2 solutions:

This step gives the joint weight (probability) of “Porosity” in this 2-solution scenario. This is the numerator in Equ-8 ( $\sum_{j=1}^{n_i} w_j * x_{i,j}$ ), where $j = 1$ to 2 (the 2 solutions, $n_i = 2$), and $i = 1$ (Porosity).

This step gives the joint weight (probability) of “Quartz” in this 2-solution scenario. This is the numerator in Equ-8 ( $\sum_{j=1}^{n_i} w_j * x_{i,j}$ ), where $j = 1$ to 2 (the 2 solutions, $n_i = 2$), and $i = 2$ (Quartz).
This step gives the joint weight (probability) of “Potash Feldspar” in this 2-solution scenario. This is the numerator in Equ-8 \( \left( \sum_{j=1}^{n_i} w_j \times x_{i,j} \right) \), where \( j = 1 \) to 2 (the 2 solutions, \( n_i = 2 \)), and \( i = 3 \) (Potash Feldspar).

This step gives the joint weight (probability) of “Plagioclase” in this 2-solution scenario. This is the numerator in Equ-8 \( \left( \sum_{j=1}^{n_i} w_j \times x_{i,j} \right) \), where \( j = 1 \) to 2 (the 2 solutions, \( n_i = 2 \)), and \( i = 4 \) (Plagioclase).

This step gives the joint weight (probability) of “Hematite” in this 2-solution scenario. This is the numerator in Equ-8 \( \left( \sum_{j=1}^{n_i} w_j \times x_{i,j} \right) \), where \( j = 1 \) to 2 (the 2 solutions, \( n_i = 2 \)), and \( i = 5 \) (Hematite).

(e) Computing the weighted average mineral fraction from the two solutions, by dividing the weight of each mineral in row-5 (blue box) by the sum probability of the two solutions (red box). This is Equ-8 applied:
(f) Checking that the final mineral fractions add up to 1 (100%):
4. Results and Discussions

In this section, results from each step of the model development are presented. They are compared against core laboratory measurements of porosity and the mineral fractions at COST B-2, showing incremental improvements by implementing one step at a time.

First, Equ-6 is solved for each of the 12650 possible combinations of 4 variables (24 in Table 1, plus the drilling fluid). Then the Average Volumetric Mineral Composition of Sedimentary Rocks (AVMCOSR, Table-2) is used as the probability of occurrence of a particular variable, and the joint probability of a particular set of 4 variables occurring together is the product of the 4 probabilities independently. This joint probability is assigned as the “weight” of averaging among the 12650 solutions to obtain the estimates of porosity and mineral fraction. Then the various filters are applied to “weed out” the unlikely solutions based on common knowledge of sedimentary and diagenesis processes.

4.1. Improvement from AVMCOSR-Weighted Averaging and the Mathematical Filter

In this step, solutions with mineral fractions that are negative or greater than 1 are eliminated. Figure 5a plots the calculated effective porosity ($\phi_e$) against core laboratory measurements at well COST B-2. This is compared with the results from the classic-petrophysics methods I (Figure 5b) and II (Figure 5c), the latter methods were given in Equ-2 and 3.

Figure 5. Comparison of mathematical filtered results (a), petrophysics method I (b) and petrophysics method II (c) against core lab measurements of effective porosity.

Figure 5 shows that based on AVMCOSR-weighted averaging and removing mathematically spurious solutions alone, the new method performed slightly better than the petrophysics methods. The regression statistics (Table 5, red font) show that the new method gives higher $R^2$, slope closer to 1, and intercept closer to 0.
Table 5. Regression statistics of calculated vs. measured porosity using traditional petrophysics methods and the new method, with successive improvements.

<table>
<thead>
<tr>
<th>Methods</th>
<th>$R^2$</th>
<th>Slope</th>
<th>Intercept</th>
</tr>
</thead>
<tbody>
<tr>
<td>Petrophysics Method I</td>
<td>0.29</td>
<td>0.55</td>
<td>0.15</td>
</tr>
<tr>
<td>Petrophysics Method II</td>
<td>0.31</td>
<td>0.72</td>
<td>0.02</td>
</tr>
<tr>
<td>New Method AVMCOSR</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>with Math Filter Alone</td>
<td>0.35</td>
<td>0.70</td>
<td>0.05</td>
</tr>
<tr>
<td>Adding Cooccurrence Filter</td>
<td>0.36</td>
<td>0.78</td>
<td>0.01</td>
</tr>
<tr>
<td>Adding Drilling Fluid</td>
<td>0.53</td>
<td>0.95</td>
<td>0.03</td>
</tr>
<tr>
<td>Adding Diagenetic Constraints</td>
<td>0.87</td>
<td>0.97</td>
<td>0.01</td>
</tr>
</tbody>
</table>

4.2. Improvement from the Minerology Cooccurrence Filter

In this step, the probability of mineral co-occurrence is used to exclude unlikely combinations of 4 variable solutions, based on Table 3.

Figure 6a shows the comparison of the calculated (adding mineral filter) vs. lab-measured porosity. The regression statistics are improved (Table 5 above, green font) with higher $R^2$, a slope even closer to 1, and intercept closer to 0.

Figure 6. Results of (a) adding mineral co-occurrence constraints (Table 3), (b) drilling fluid as a new variable, and (c) diagenetic constraints of Burly (Figure 2), plotted against core lab measurements of effective porosity.
4.3. Improvement from Including Drilling Fluid

Figure 6b shows the results of including the drilling fluid as one of the variables. It resulted in further improvements of the regression statistics (Table 5, light blue font), but also gives some negative porosity values, calling for further improvements.

4.4. Improvement from Simple Diagenetic Constraints

In this step, simply diagenetic constraints by depth/temperature from Burly (1993) (see Fig 2) are used to eliminate solutions with minerals that are unstable at the reported depth/temperature. The results are shown in Figure 6c. This step produced the most significant improvement so far (Table 5, dark blue font), raising the R2 value to 0.87 and the slope to 0.97, and reducing the intercept to 0.01.

In the above, only porosity estimates are evaluated against core measurements, demonstrating the effect of each step of imposing mathematical and mineralogical constraints. Next, the results of mineral fractions, in addition to porosity, are presented. These estimates of mineral fractions have not been possible using traditional petrophysics tools. Since there are no traditional petrophysics tools to quantify mineral fractions, we can only compare with lab measurements. Table 6 below gives the regression statistics between the mineral fractions estimated using the new method vs. lab measurements at COST B-2.

**Table 6.** Regression statistics between the mineral fractions estimated using the new method vs. core lab measurements at COST B-2. It shows the incremental improvement by adding one constraint at a time: with drilling fluid correction, with simple diagenetic constraints (based on Figure 2), and with the final probabilistic constraints given age/depth (based on Figure 3).

<table>
<thead>
<tr>
<th>Variable /Method</th>
<th>With Drilling Fluid Correction</th>
<th>With Simple Diagenetic Constraints (Figure 2)</th>
<th>With Age/Depth Probabilities (Figure 3)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>R²</td>
<td>Slope</td>
<td>Intercept</td>
</tr>
<tr>
<td>Porosity</td>
<td>0.53</td>
<td>0.95</td>
<td>0.03</td>
</tr>
<tr>
<td>Quartz</td>
<td>0.73</td>
<td>0.67</td>
<td>0.22</td>
</tr>
<tr>
<td>Feldspar</td>
<td>0.52</td>
<td>0.77</td>
<td>0.02</td>
</tr>
<tr>
<td>Illite</td>
<td>0.70</td>
<td>0.96</td>
<td>0.00</td>
</tr>
<tr>
<td>Kaolinite</td>
<td>0.76</td>
<td>0.72</td>
<td>0.01</td>
</tr>
<tr>
<td>Montmorillonite</td>
<td>0.56</td>
<td>1.10</td>
<td>0.00</td>
</tr>
<tr>
<td>Calcite</td>
<td>0.73</td>
<td>0.73</td>
<td>0.02</td>
</tr>
<tr>
<td>Dolomite</td>
<td>0.86</td>
<td>0.78</td>
<td>0.00</td>
</tr>
<tr>
<td>Pyrite</td>
<td>0.67</td>
<td>1.87</td>
<td>0.00</td>
</tr>
<tr>
<td>Siderite</td>
<td>0.80</td>
<td>0.61</td>
<td>0.00</td>
</tr>
<tr>
<td>Anhydrite</td>
<td>0.98</td>
<td>0.71</td>
<td>0.00</td>
</tr>
<tr>
<td><strong>Average</strong></td>
<td>0.71</td>
<td>0.90</td>
<td>0.03</td>
</tr>
</tbody>
</table>
There is a significant improvement by adding the simple diagenetic constraint based on Figure 2 (the center block), compared to the first block. However, some of the low $R^2$ values (in red) prompted the next step, a new, quantitative, probability-based sedimentary and diagenetic constraint, derived from quantitative knowledge of mineral occurrence as a function of geologic time (age) and burial depth (see Figure 3), discussed next.

4.5. Improvement from Probabilistic Depth/Age Constraints

In this final step, quantitative data was compiled to generate the volume of mineral groups as a function of depth (temperature/pressure gradient) and geologic age (diagenesis and preservation), shown in Figure 3 earlier. The regression statistics are given in the right block of Table 6, showing significant improvement over the earlier mineral filters (co-occurrence and Burly 1993 constraints). On the average (last row of Table 6, blue font), the new method, in its final form (last block), offers highly accurate estimates of the effective porosity and 11 most abundant minerals at COST B-2. Figure 7 below shows the final porosity and mineral fraction estimates against lab measurements (thin line = regression, thick black line = 1:1 relation).
Figure 7. Final results using the new minerology filter of depth/age probability, compared to lab measurements. Thin line = regression, thick black line = 1:1 relation.
5. Summary and Conclusions

This study is motivated by the need to estimate the effective porosity and mineral composition of sedimentary formations for the purpose of geologic carbon sequestration, based on common geophysical logs. Because there are generally more mineral types than the number of logs at a given site, current methods yield non-unique solutions and give ambiguous results.

In this study, I develop a new method to estimate effective porosity and as many as needed mineral fractions based on three common geophysical logs: Gamma Ray Log (GRL), Density Log (DL) and Neutron Porosity Log (NPL). The method utilizes a probability approach, based on our knowledge on global mineral abundance in sedimentary rocks, mineral co-existence in different depositional environments, diagenetic (as a function of age/depth, hence temperature, pressure, preservation) constraints, in the form of several filters to rule out unlikely scenarios, and to give more weights to more likely scenarios.

Comparisons of the new model results with core-lab measurements demonstrate significant improvements over existing petrophysics methods in porosity, and offers an entirely new possibility that the existing petrophysics methods cannot offer, i.e., estimating the fractions of as many as necessary number of minerals.

This new method can be extended to other situations where a different set of geophysical logs are available. The innovation of this new method lies in the systematic approach of implementing physical constraints to eliminate or downplay unlikely mathematical solutions, these physical constraints being the basic knowledge of sedimentary and diagenetic processes.
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