Pore-Level Analysis of the Relationship Between Porosity, Irreducible Water Saturation, and Permeability of Clastic Rocks

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Abstract

Permeability is one of the most important, most spatially variable, most uncertain, and hence least predictable transport properties of porous media. Various empirical models, such as Tixier’s, Timur’s and Coates’ equations, are widely used to quantify permeability from well-log calculations of porosity and irreducible water saturation. However, these models do not explicitly include the role played by rock structure, spatial fluid distribution in the pore space, wettability, or clay mineral distribution on permeability. We present a pore-scale approach to investigate the influence of these factors on the permeability of clastic rocks for explicit pore geometries of brine-saturated granular rocks.

Synthetic pore-scale models are constructed to represent granular sands with variable grain-size distributions. These models include the structural effects of compaction, cementation, and distribution of dispersed hydrated clay minerals. Irreducible water is geometrically distributed on grain surfaces of the synthetic rocks. Permeability is calculated from lattice-Boltzmann flow simulations. A nonlinear relationship between permeability, porosity, and irreducible water saturation is established for these computer-generated rocks. We compare calculated permeability values of computer-generated rocks and laboratory measurements of core samples to those estimated from different empirical approaches, such as Tixier, Coates, and Timur models. It is found that the latter models cannot be applied to general cases of clastic rocks even if their free parameters are adjusted to fit core measurements. Our simulations also show that spatial distributions of clay minerals and irreducible water play a fundamental role in establishing an accurate correlation between permeability, porosity, and irreducible water saturation. Specific deterministic equations must be established for rock formations that exhibit distinct grain-size distributions, clay types, structural clay distributions, and grain cementation.

Introduction

Permeability governs the displacement of fluids through the pore space of porous media. It is one of the most important and least predictable transport properties of porous media in reservoir characterization. Permeability is usually evaluated from core samples and/or well tests. However, core samples and well-test data are often only available from few wells in a reservoir while well logs are available from the majority of wells. Therefore, accurate and reliable evaluation of permeability from well-log data embodies a significant technical and economic advantage.

Various empirical models have been proposed to infer permeability from well-log data, based on calculations of porosity, water saturation, capillary pressure, and formation resistivity factor. Permeability is estimated via correlations among other rock petrophysical properties. In many cases, there may exist deterministic relationships among these properties, but such correlations usually are empirically derived for a given formation in a given area, are often statistical in nature and, therefore, cannot be applied to general cases.
Permeability has also been observed to be a strict function of porosity and/or residual water saturation in certain reservoirs. A general empirical relationship proposed by Wyllie and Rose relates the permeability, \( k \), of a porous medium to its porosity, \( \phi \), and irreducible water saturation, \( S_{wi} \), as

\[
k = a \phi^b \frac{S_{wi}}{c}.
\]

where \( a, b, \) and \( c \) are statistically determined model parameters. Based on this general expression, various empirical relationships have been proposed to calculate permeability from values of porosity and irreducible water saturation derived from well logs, including:

**Tixier:**

\[
k = 62.5 \phi^6 \frac{S_{wi}}{S_{wi}},
\]

**Timur:**

\[
k = 8.58 S_{wi}^4 \frac{S_{wi}}{S_{wi}},
\]

and

**Coates:**

\[
k = 4.90 \phi^4 (1 - S_{wi})^2 \frac{S_{wi}}{S_{wi}},
\]

where the unit of permeability is Darcy (D). The units of porosity and irreducible water saturation are expressed in terms of fraction of bulk volume and pore space volume, respectively. Despite their widespread use, existing models used to calculate permeability from porosity and irreducible water saturation do not explicitly include the role played by rock structure, grain geometry, grain-size distribution, wettability, and spatial distribution of irreducible water in the pore space.

Laboratory studies have shown that permeability depends on a long list of parameters: porosity, pore size and shape, pore size distribution, clay content, fluid type, and saturation – a nearly overwhelming complexity. The objective of this paper is to investigate the influence of rock microstructure and spatial distribution of clay minerals on the permeability of clastic rocks for explicit pore geometries of brine-saturated granular rocks. Hydrated clay minerals are responsible for the presence of excess irreducible water whose spatial distribution in the pore space further conditions the geometry of pore throats.

Therefore, presence of clays in sands can substantially affect the relationship between porosity, irreducible water saturation, and permeability in ways that depart from standard parametric models such as those of Tixier, Timur, and Coates (see Eqs. (2)-(4)).

The macroscopic properties and detailed microstructural information of a porous medium can be obtained from experiments. However, the associated experiments are often time-consuming and expensive. In addition, routine laboratory testing is not easily applied to damaged core material or drill cuttings and often reservoir conditions cannot be reproduced in the laboratory. As an alternative to both experimental determination of rock properties and petrophysical correlations, we make use of a numerical approach in this paper.

We construct synthetic pore-scale models to represent granular sands with variable grain-size distributions. These models include the structural effects of compaction, cementation, and distribution of dispersed hydrated clay minerals. A D3Q19 lattice-Boltzmann algorithm is used to simulate viscous flow of the single-phase fluid in the pore space of computer-generated rock samples. Permeability is calculated directly from the simulated velocity field using Darcy’s equation. We compare the permeability calculated from computer-generated rocks and laboratory measurements of core samples to those estimated from different empirical models, such as those introduced by Tixier, Coates, and Timur.

**Numerical Methods**

In general, sedimentary rocks originate by deposition of grains followed by compaction and cementation. The latter two processes determine the final pore-space geometry and connectivity. A physics-based depositional model serves to reconstruct natural sedimentary rocks, and generates 3D images of the pore space at an arbitrary degree of spatial resolution. This model provides detailed microstructure of the rock, and makes it possible to calculate the steady-state velocity field for single-phase fluid flow. Figure 1 illustrates the simulation procedures used to construct numerical rock samples with this method.

Dispersed clay minerals in sandstones are of three mor-
phological types: (1) pore lining, (2) pore bridging, and (3) discrete particles. Pore-lining clays are attached to pore walls to form a relatively continuous and thin clay mineral coating. In this paper, we assume that clay minerals, independent of its composition, are homogeneously deposited on grain surfaces within the sample according to a proposed cement overgrowth algorithm. Figure 2 shows the idealized patterns of clay mineral distribution on grain surfaces in two dimensions. Two different patterns are used: (1) PU growth: clay minerals grow uniformly in all directions on grain surfaces; and (2) PT growth: clay minerals preferentially grow in narrow grain-contact regions.

Clay shell (region of blue color in Figure 2), which is composed of exceedingly fine-grained particles, often exhibits very high porosity. Water held in this shell is responsible for presence of irreducible water saturation. Different volumes of the clay shell correspond to different values of irreducible water saturation. In addition, because pores and pore channels are equally small, for all practical purposes clay shells exhibit zero permeability. Therefore, we model clay shells as highly porous, but impermeable layers in numerical simulations. A no-flow boundary condition is enforced at fluid-solid interfaces.

We use the D3Q19 lattice-Boltzmann algorithm to simulate viscous flow of a single-phase fluid in the pore space of computer-generated rock samples. In this paper, we use the improved incompressible lattice-Boltzmann model together with a pressure boundary condition enforced on the inlet and outlet faces. Simulations are performed individually for each of the $x-$, $y-$, and $z-$directions. Absolute permeability is derived directly from the simulated velocity field using Darcy’s equation. Effective absolute permeability is defined as the arithmetic average of the calculated absolute permeabilities in the $x-$, $y-$, and $z-$directions. Only effective permeability is considered in this paper.

**Results and Analysis**

Five different grain-size distributions, shown in Figure 3, are used to generate numerical rock samples with different degrees of compaction and cementation. Total volume of all grains with the same size is expressed in terms of fraction of total solid volume in the rock. Only one rock sample is constructed from each of the types 1, 2, and 4, respectively. Type 3 is used to generate two rock samples with different porosities. There are 371 samples with different porosities and clay morphology constructed from the same grain-size distribution, type 5.
Table 1—Initial values of porosity $\phi$, average radius $R_a$, and absolute permeability $k$ of samples A-F. The average radius is calculated from the expression $V_t = N \frac{4}{3} \pi R_a^3$, where $V_t$ is the total volume of all grains, and $N$ is total number of grains in the pack. Permeability is calculated with lattice-Boltzmann flow simulations.

<table>
<thead>
<tr>
<th>Sample</th>
<th>$\phi_t$ (%)</th>
<th>$R_a$ (mm)</th>
<th>$k$ (Darcy)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>27</td>
<td>0.42</td>
<td>98.1</td>
</tr>
<tr>
<td>B</td>
<td>34</td>
<td>0.21</td>
<td>82.6</td>
</tr>
<tr>
<td>C</td>
<td>29</td>
<td>0.24</td>
<td>45.4</td>
</tr>
<tr>
<td>D</td>
<td>40</td>
<td>0.24</td>
<td>199.0</td>
</tr>
<tr>
<td>E</td>
<td>25</td>
<td>0.25</td>
<td>40.1</td>
</tr>
<tr>
<td>F</td>
<td>-</td>
<td>0.10</td>
<td>-</td>
</tr>
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</table>

For highly porous, we further assume that the volume of clay shells is equal to the volume of irreducible water in the rock pore space. Therefore, different volumes of clay shells correspond to different values of irreducible water saturation in the simulations.

Figure 4 describes variations of the calculated permeability for different values of irreducible water saturation, $S_{wi}$, for samples A-E. We note that rock permeability decreases with increasing values of irreducible water saturation for all samples A-E. For increasing values of irreducible water saturation, all samples exhibit a similar trend of decreasing permeability. Figure 5 displays the calculated permeability of samples F for different values of porosity and irreducible water saturation. There are 184 computer-generated samples in which clays exhibit the PU growth pattern, and 187 samples in which clays exhibit the PT growth pattern.

To establish a general relationship between permeability, $k$, porosity, $\phi$, and irreducible water saturation, $S_{wi}$, for these numerical rocks, we use the generalized form, described by Eq. (1). All simulation data in Figures 4 and 5 are used to calculate the parameters $a$, $b$, and $c$ in Eq. (1). We have obtained the following forms for samples A-F with the PU growth pattern and PT growth pattern, respectively:

**PU pattern:**

\[ k = 1.68 \times 10^2 \phi^{0.07} S_{wi}^{0.97}, \]  

(5)

and

**PT pattern:**

\[ k = 5.53 \times 10^2 \phi^{5.09} S_{wi}^{1.03}, \]  

(6)

where the unit of permeability is Darcy. Porosity and irreducible water saturation are expressed in terms of fraction of bulk volume and pore space volume, respectively. Different values of model parameters $a$, $b$, and $c$ indicate that similar correlations derived for a given formation in a given
Figure 6—Calculated permeabilities from lattice-Boltzmann simulations (LBS) compared to those calculated with different empirical models (COR), Eqs. (2)-(6), for all computer-generated rock samples with different clay-growth patterns (a) PU pattern, and (b) PT pattern.

Figure 7—Permeability from lattice-Boltzmann simulations on computer-generated rock samples (SIM) and laboratory measurements on core samples (EXP), together with the corresponding values calculated via correlation, Eq. (6).

Figure 8—Measured permeabilities from core samples (EXP) compared to those estimated with different empirical models (COR), Eqs. (2)-(6). Note that experimental data are from Salazar et al.’s paper20 (Figure 1).

To further verify and compare empirical models discussed previously, we have chosen core data from a tight-gas reservoir consisting of sand units of turbidite origin.20,21 Core samples were acquired from a shallow interval of A1-A5 m and a deep interval B1-B5 m. Laboratory measurements on these samples, including porosity, irreducible water saturation, and permeability, were well conducted and documented. Figure 7 displays the measured permeability of core samples, together with the calculated permeability of computer-generated rock samples F with PT clay morphology. These calculated/measured values are compared to the estimated values determined from the developed correlation in this paper, Eq. (6). Our model overestimates the permeability of core samples. This dis-
crepancy may be caused by different grain size distributions and different types of clays present in the core samples and computer-generated samples. It is well known that different clay morphologies significantly affect rock porosity/permeability, capillary pressure curve, and associated pore-size distributions in various ways. Different values of these parameters in Eqs. (5) and (6) further confirm the effect of the spatial distribution of irreducible water on specific parameters included in the calculations.

Figure 8 shows the overall comparison of permeability between laboratory measurements on core samples and those estimated with empirical models, Eqs. (2)-(6). We observe that Timur’s model gives the best estimate of permeability, while Tixier’s and Coates’ equations underestimate the permeability, and our correlation, Eq. (6), overestimates the measured permeabilities.

In Figures 9 and 10, we observe more clearly the difference between permeability estimates for different models, where permeability is plotted as a function of depth. The length of each tick mark in depth is 5 m. Timur’s predictions of permeability are in excellent agreement with laboratory measurements for both depth intervals, while our model overestimates the permeability approximately by one order of magnitude, and Tixier’s model underestimates it by one order of magnitude. Coates’ predictions nearly match experimental data in the deep depth interval B1-B5, but underestimate slightly their values in the shallow interval A1-A5.

The above discrepancy is due to different values of free parameters included in Eqs. (2)-(6). Table 2 lists all the free parameters together for comparison. Compared to values in Timur’s (or Coates’) model, we observe that the value of $b$ in Tixier’s model is larger (the difference is about 2), whereas the coefficient $a$ is also one order of magnitude larger. Average values of porosity and irreducible water saturation of core samples studied in this paper are about 10% and 50%, respectively. Therefore, Tixier’s model would underestimate the permeability by approximately one order of magnitude, as reflected by the plots of Figures 9 and 10. Similarly, our equation (PT pattern) yields larger values of $a$ (about 2 order of magnitude larger) and $b$ (the difference is about 1). It also yields a smaller value of $c$ (the difference is about 1). These differences of parameters in our equation contribute to overestimate the permeability of core samples by approximately one order of magnitude.

However, we note that the fact that Timur’s model yielded a better estimate of permeability for core samples does not indicate that it is superior to other empirical models and that this model gives the best estimates of permeability for all types of rock formations. Moreover, we emphasize that our equations (5) and (6) were derived from computer-generated samples, which exhibit the same uniform grain size distribution. Our approach to assign the
This study: $k, mD$

Tixier: $k, mD$

Timur: $k, mD$

Coates: $k, mD$

<table>
<thead>
<tr>
<th>Depth, m</th>
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<tbody>
<tr>
<td>B1</td>
</tr>
<tr>
<td>B2</td>
</tr>
<tr>
<td>B3</td>
</tr>
<tr>
<td>B4</td>
</tr>
<tr>
<td>B5</td>
</tr>
</tbody>
</table>

Figure 10— Measured permeability of core samples compared to their estimated values from different empirical models: Tixier: Eq. (2), Timur: Eq. (3), Coates: Eq. (4), and this study: Eq. (6). Core samples were acquired in the deep interval of B1-B5 m. The length of each tick mark in depth is 5 m.

Table 2— Values of parameters $a$, $b$, and $c$ in the general form $k = a \phi^b S^c w_i$, for different empirical models. The unit of permeability is Darcy. Porosity and irreducible water saturation are expressed in terms of fraction of bulk volume and pore space volume, respectively.

<table>
<thead>
<tr>
<th>Empirical model</th>
<th>$a$</th>
<th>$b$</th>
<th>$c$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tixier</td>
<td>62.5</td>
<td>6</td>
<td>2</td>
</tr>
<tr>
<td>Timur</td>
<td>8.58</td>
<td>4.4</td>
<td>2</td>
</tr>
<tr>
<td>Coates</td>
<td>4.90</td>
<td>4</td>
<td>~2</td>
</tr>
<tr>
<td>This study, PU</td>
<td>$1.68 \times 10^2$</td>
<td>4.07</td>
<td>0.97</td>
</tr>
<tr>
<td>This study, PT</td>
<td>$5.53 \times 10^2$</td>
<td>5.09</td>
<td>1.03</td>
</tr>
</tbody>
</table>

spatial distribution of irreducible water on grain surfaces ignores many complications and, of course, may not accurately represent the real distribution of irreducible water saturation in complex rock formations.

**Discussion and Conclusions**

We introduced a pore-level procedure to investigate the relationship between rock permeability, porosity, and irreducible water saturation. We first constructed synthetic rock samples using a physics-based depositional model. Starting with an unconsolidated random grain pack, we simulated rock compaction and cementation. The spatial distribution of clay-bound water was geometrically determined using a simple approach, similar to that of the cement overgrowth algorithm. Single-phase fluid flow within computer-generated rocks was simulated using the lattice-Boltzmann method. Absolute permeability of the sample was estimated directly from the velocity field using Darcy’s equation. Such an approach provided detailed rock microstructure and distribution of irreducible water in the pore space, thereby enabling the study of their influence on the permeability of clastic rocks.

We established a relationship between permeability, porosity, and irreducible water saturation for our computer-generated rock samples. To test and compare existing empirical models, such as Tixier’s, Timur’s and Coates’, we compared permeability values predicted with these models to permeability values of both computer-generated rocks and laboratory measurements performed on core samples. We found that all existing models underestimated the permeability of our numerical rocks. For core samples, Timur’s predictions were in excellent agreement with laboratory measurements, while our model overestimated the permeability by approximately one order of magnitude, whereas Tixier’s underestimated them by one order of magnitude. Coates’ estimates nearly matched experimental data for core samples acquired in a deep interval, and it underestimated them for core samples acquired in a shallow interval.
Our correlations were derived from computer-generated rocks, in which we used the same uniform grain-size distribution and spherical grains. A simple but flexible cement-growth algorithm was used to geometrically distribute irreducible water on grain surfaces. This approach ignores many complications, and of course, may not represent the real distribution of irreducible water in the pore space. We expect that all these factors will play a significant role in establishing a correlation between permeability, porosity, and irreducible water saturation. Therefore, we emphasize that the correlation developed in this paper is only valid for our numerical rocks and is not universal.

It is well known that permeability is dominated by the smallest portions (pore throats) of flow channels in the rock pore space, while porosity and water saturation are controlled by the volume of large pores, not by pore throats. Irreducible water saturation may be closely related to the solid surface area of a rock. Hence, correlations for permeability may be inherently limited in their accuracy and reliability when assuming specific correlations with porosity and water saturation, or with any other rock property, that is not strongly affected by the pore throats of porous media. These factors explain why empirical permeability models are not universal; different predictive equations must be established for different types of rocks. Therefore, it is necessary to address these factors suitably when establishing a correlation among rock properties to calculate permeability.

In addition, empirical permeability models, such as Tixier’s, Timur’s and Coates’, relates the permeability of a porous medium to its porosity with only one constant parameter for all values of porosity. Laboratory measurements performed on Fontainebleau sandstones� have shown that the correlation between permeability and porosity has two different families (low and high porosities) for which the correlation law has the same mathematical shape, but not the same characteristic parameters. Therefore, we also do not expect that a simple correlation between permeability, porosity, and irreducible water saturation would work well for all rock formations with different values of porosity.

Our fully-explicit pore-scale geometrical approach enables one to study the sensitivity of permeability to amount and spatial distribution of hydrated clay minerals and their exchange cations, brine salinity, and irreducible water saturation for clastic rocks with variable grain-size distributions. Compared to laboratory measurements, this numerical approach is particularly attractive, due to its low cost and high speed of calculation. Our study is but a first step toward applying pore-scale models to well-log interpretation.

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References


