

PORE-SCALE ANALYSIS OF THE WAXMAN-SMITS SHALY SAND CONDUCTIVITY MODEL

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ABSTRACT

Waxman-Smits and dual-water models of electrical conductivity in shaly sands account for the dual conductive pathways formed by pore brine and clay mineral exchange cations, while Archie's equations describe the electrical conductivity behavior of shale-free rocks. These empirical models have enjoyed great success in the interpretation of electric-log responses of homogeneous reservoir rocks. However, the models are not explicit in their predictions of electrical conductivity with respect to rock structure, spatial fluid distribution in the pore space, wettability, or clay mineral distribution. This paper quantifies the influence of petrophysical, textural, and fluid factors on the electrical conductivity of shaly siliciclastic rocks by calculating excess conductivities associated with clay minerals for explicit pore geometries of brine- and hydrocarbon-saturated shaly granular rocks.

We construct synthetic pore-scale models to represent homogeneous shaly sands that include the structural effects of compaction, cementation, and distribution of dispersed clay minerals. Exchange cations associated with these clay mineral distributions in the pore space are assigned effective conductivities which vary with brine salinity. Two-phase immiscible fluids are also geometrically distributed in the pore space consistent with capillary pressure and drainage cycles. Waxman-Smits Formation Factors and Resistivity Indices are calculated from the late-time diffusion asymptotes of random walks enforced within the conductive space formed by the pore water and clay mineral exchange cations.

The fully explicit pore-scale geometrical approach developed in this paper allows one to calculate accurate rock conductivity as function of amount and spatial distribution of clay minerals and their exchange cations, fluid saturation, and brine salinity for the homogeneous shaly sand case. We show that significant changes in excess electrical conductivity can be observed with

realistic perturbations of water saturation, salinity, and clay mineral distribution.

INTRODUCTION

The most fundamental empirical relationship for interpreting conductivity measurements in rocks was advanced by Archie (1942) as

$$F = \frac{\sigma_w}{\sigma_o} = \frac{a}{\phi^m}, \quad (1)$$

where F is referred to as the formation factor, ϕ is the porosity, $a \approx 1$ is a lithological factor and m is the cementation (lithology) exponent, usually ranging between 1.3 and 3.5. The symbols σ_w and σ_o designate the conductivities of the pore fluid and the rock, respectively (mho cm^{-1}). However, this expression is applicable only to clean or clay mineral-free sands, i.e., non-conductive rock matrices. When clay minerals are present, imperfections in their lattices result in an excess of negative charges near the clay mineral surface. Electrical neutrality requires hydrated cations from the pore electrolyte. These hydrated cations on the surface of the clay minerals are in rapid exchange with those in the pore electrolyte. The behavior of such exchange cations under the influence of an electric field has been described by an empirical model developed by Waxman and Smits (W-S), 1968. Another interpretation of these exchange phenomena is that the hydrated cations form a thin "double layer" close to the grain surface. Because of the exclusion of anions, such a layer is often referred to as "salt-free." This double-layer concept led to the development of another empirical model for electrical behavior of shaly sands, the Dual-Water model of Clavier *et al.* (D-W), 1984.

The W-S model is characterized by the equation

$$\sigma_o = \frac{1}{F^*} (\sigma_w + BQ_v), \quad (2)$$

where F^* is the shaly sand formation factor, Q_v is the cation concentration per unit pore volume (equivalent liter⁻¹ or meq ml⁻¹) and B is the average mobility of the counterions close to the grain surface (mho $\text{cm}^2 \text{meq}^{-1}$). One important assumption in the W-S model is that the

electrical tortuosity associated with the hydrated-clay-mineral (HCM) counterions is the same as that of the bulk ionic current due to the rapid exchange of the hydrated cations between the clay mineral surface and the pore electrolyte. However, the D-W model assumes a spatial separation between the HCM counterions that are concentrated near the surface and the electrolytic ions that are uniformly distributed over the remaining pore space. When the formation does not behave as a clean sand, the ratio σ_w/σ_0 represents an apparent formation factor that is not related in a simplistic manner to the porosity, ϕ . Eq. (1) predicts a linear variation of σ_0 with σ_w for a given rock sample. For shaly sands, plots of σ_0 vs. σ_w are nonlinear at low values of salinity while becoming linear at high values of salinity. An essential requirement of all empirical models is to capture such a nonlinear (convex-upward) behavior of the σ_0 curve at low values of salinity. The W-S model captures this behavior by allowing the counterion mobility, B , to increase exponentially at low values of σ_w until it attains a constant and maximum value at high values of salinity. Using a diffusion current model, Sen (1987) demonstrated that the nonlinearity of σ_0 vs. σ_w follows naturally as a consequence of distribution of electric field between the two regions. Revil *et al.* (1998) suggested an effective medium theory that accounts for the different behavior of anions and cations in the two conductive regions. Bussian (1983) proposed a general model describing conductivity of heterogeneous mixtures and then applied a similar theory to describe the electrical conductivity of shaly sands.

RANDOM-WALK ALGORITHM

In this paper, we estimate rock conductivity based on random walks enforced in a synthetic porous medium comprised of insulating spherical grains as described by Toumelin *et al.* (2005) and Schwartz *et al.* (1989).

Rock model: The simulation domain consists of 1000 uniformly sized grains of radius 110 microns whose spatial coordinates were obtained from Finney's dimensionless dataset (Finney, 1970). This pack yields a porosity of 18%. All grains are then uniformly grown by 5 or 10 microns to obtain lower porosities such as 12% or 7%, respectively. In subsequent sections of this paper, a clay mineral "coat" and its corresponding hydrated exchange cations are added to the insulating spheres. Figure 1 shows the simulation domain containing the grain pack. An important parameter included in the random walk simulation is D , the self diffusivity of the finite conducting medium. Walkers are randomly generated in the pore space and move in any direction within the pore formation fluids. The time step, Δt , of each walk is related to the displaced

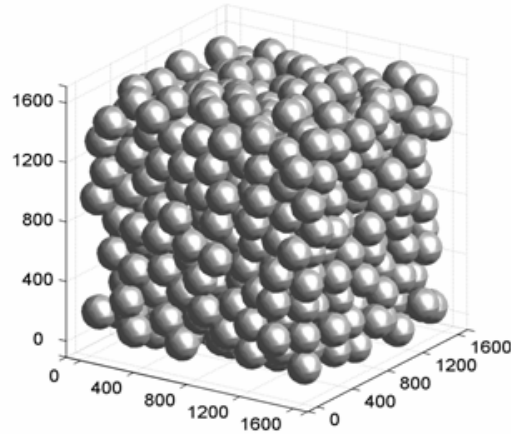


Figure 1: Schematic description of a "Finney" pack with mono-sized grains. All dimensions are given in μm .

distance, Δr , via Einstein's relation (Schwartz and Banavar 1989; Tobochnik *et al.*, 1990):

$$\Delta r^2 = 6D_{w,bulk}\Delta t, \quad (3)$$

where $D_{w,bulk}$ is the self-diffusivity of the brine. Length steps of a random walker are dictated by geometrical considerations such as the smallest surrounding pore opening or HCM exchange cation-coating thickness. If the walker lands in an insulating region – grain, oil, etc., then the step is cancelled and the walker is returned to the starting position, but the clock time is incremented (Schwartz and Banavar, 1989). The mean-squared displacement averaged over a sufficiently long time yields the estimate of D , i.e. the effective diffusivity of the rock. For the clay mineral-free case, the conductivity of the grain pack is calculated as

$$\frac{\sigma_0}{\sigma_w} = \phi \left(\frac{D_\infty}{D_{w,bulk}} \right), \quad (4)$$

where D_∞ is the long-time slope of average mean-squared distance plotted against time. Averages are estimated for an ensemble of random walkers, typically 500. Figure 2 shows the diffusivities obtained at various simulation times and the corresponding asymptotic value, D_∞ . The intrinsic formation factors for single-phase saturation in clay mineral-free rocks is then calculated as

$$F = \frac{1}{\phi} \left(\frac{D_{w,bulk}}{D_\infty} \right). \quad (5)$$

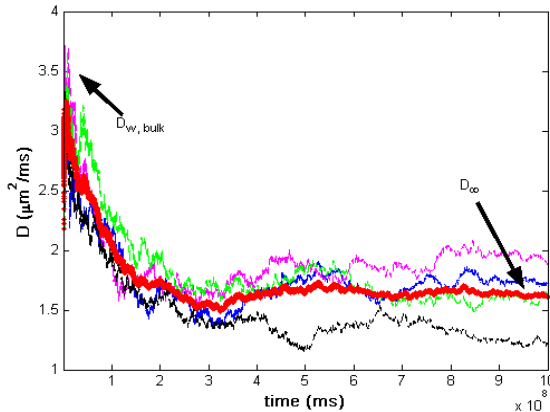


Figure 2: Change in effective diffusivity with increasing simulation time. The thick line describes an ensemble average while multiple thin lines describe simulation results for sets of 50 walkers each.

RANDOM-WALK MODEL FOR SANDS CONTAINING CLAY MINERALS

Dispersed clay minerals in sandstones are of three morphological types: (1) pore lining, (2) pore bridging, and (3) discrete particles. A discussion of the above clay mineral morphologies can be found in Neasham (1977). Pore-lining clay minerals usually occupy 8-20% of the bulk volume with Q_v values ranging from 0.1 to 0.7 meq ml⁻¹. Some pore-lining clay minerals can be idealized using a grain-coating geometry. Lima and Sharma (1990) used the coating clay mineral model to generate a composite grain conductivity that was subsequently used to calculate rock conductivity. Johnson *et al.* (1986) implemented the same strategy with random walks to quantify the effect of surface conduction on rock conductivity. The rock geometry for the above models consists of insulating spherical grains coated with a shell of thickness δ , conductivity σ_{clay} , and the bulk pore electrolyte of conductivity σ_w . The W-S model assumes a uniform pore electrolyte with a bulk conductivity that has been enhanced due to cation exchange phenomena. However, an alternate interpretation of these electrochemical concepts leads to the concept of different values of conductivity to exist close to the grain surface than in the bulk pore fluid. Almon (1979) suggests that this shell conductivity be an order of magnitude larger than the bulk pore water conductivity even for moderately saline waters. A decrease in salinity is expected to escalate the relative contribution from the HCM counterions, regardless of the model interpretation.

Revil *et al.* (1998) and Leroy *et al.* (2004) assign a specific surface conductivity in lieu of a clay mineral continuum by integrating the “anomalous” surface

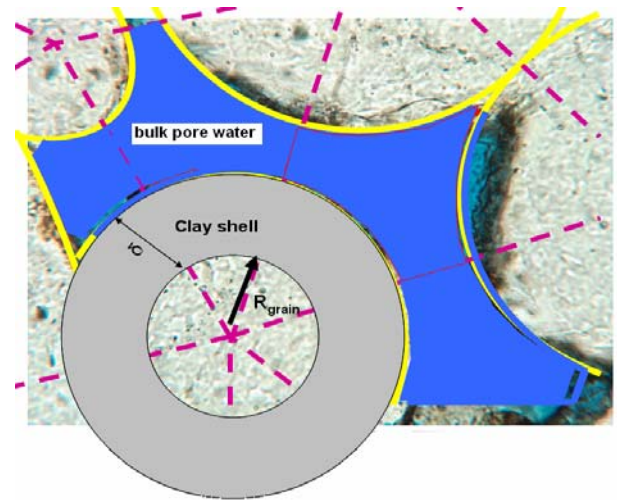


Figure 3: Idealized grain-coating clay mineral morphology showing the spatial separation between the HCM exchange cations and bulk electrolyte regions. The size of the HCM exchange cation shell relative to the grain radius has been exaggerated for better illustration.

conductivity over the double-layer thickness. Essentially, the shaly sand problem with underlying assumptions of homogeneous coating clay mineral morphology reduces to a multi-component conductivity problem similar to those discussed by Kim and Torquato (1990) and McCarthy (1990). An analogous approach has been used by Garboczi *et al.* (1995) for modeling the interfacial zone in mortar conductivity. However, there are characteristics specific to the double layer that warrant a careful appraisal of parameters chosen and results obtained. One such aspect is that δ is not the true thickness of an individual HCM cation double layer. This is unlike the mortar conductivity problem (Garboczi *et al.* 1995) where the width of the interfacial zone is comparable to the grain radius. Clay minerals do stack up on top of one other to form layers as thick as 12- μm . However, individual double-layer thicknesses are still in the sub-micron range. Thus, δ is the thickness of a representative volume continuum that would describe the cumulative effect from surface phenomena at each double layer. Likewise, there is no simplistic relation that associates surface conductance with volumetric excess HCM exchange cation conductivity. Parameter calibration is crucial owing to the freely varying nature of δ . Most measurements made to quantify electrical properties of HCM exchange cations involve the determination of Q_v . Waxman and Smits (1968) provided a comprehensive data set of shaly sands containing HCMs and their resulting conductivities tabulated with measured values of Q_v . Another parameter of interest is the “excess conductivity” associated with the HCM exchange

cations. For better understanding, eq. (2) is rewritten in its general form as

$$\sigma_0 = \frac{\sigma_w}{F^*} (1 + X), \quad (6)$$

where X is the dimensionless excess conductivity associated with the HCM counterions and is a characteristic variable used directly or otherwise included in most shaly sand conductivity models (Worthington, 1985). In the W-S model, $X = BQ_v/\sigma_w$, and becomes a simple additive excess. Grain conductivity models (Bussian 1993; Lima and Sharma, 1990) use this ratio in power laws involving the cementation exponent. Realistic values of X at low values of salinity vary from 2-10 depending on Q_v . At very high values of salinity this ratio approaches zero. **Figure 4** shows the values of X calculated as a function of BQ_v/σ_w , where B at 25 degC is evaluated from an empirical fit given by Waxman and Smits (1968) to be

$$B = [1 - 0.6 \exp(-\sigma_w / 0.013)] 0.046 \text{ mho cm}^2 \text{ meq}^{-1}. \quad (7)$$

While B represents the well understood electrochemical phenomena of ionic mobility, it is the one free parameter that is used in the empirical Waxman-Smits regression. Regardless of the phenomenological accuracy of eq. (7), it is worthwhile recognizing that the product BQ_v represents the experimental excess conductivity due to the HCM exchange cations at various values of salinity and can be used in calibrating a proposed conductivity model.

SINGLE-PHASE SIMULATION

We use the same random-walk scheme described in the previous section with the only change being the inclusion of a homogeneous HCM exchange cation shell of thickness δ and diffusivity D_{clay} surrounding each grain. As done earlier, bulk water is assigned a diffusivity equal to D_w and the composite rock conductivity is calculated from Eq. (4). **Figure 3** shows a schematic of the idealized grain coating model. In the rock model described earlier (mono-sized spheres of radii 110- μm), homogeneous intrusions of thickness 10- μm are included in each grain. The resulting grain pack contains spherical grains of radii 100- μm , an interfacial HCM exchange cation zone of thickness 10- μm , and the bulk pore water.

This “clayey” pack has a porosity of 21.5%, representing an increase from the earlier value of 18% due to smaller grain size, i.e., uniform compaction.

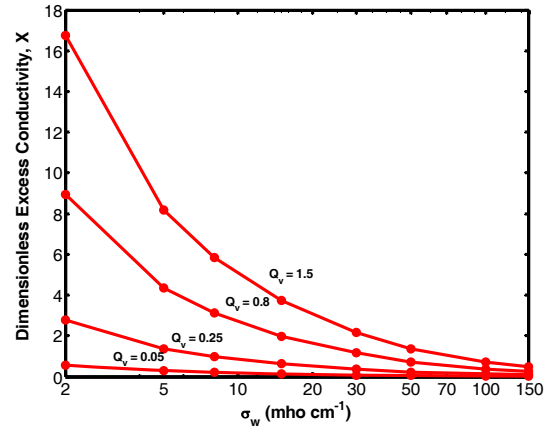


Figure 4: Plots of dimensionless excess conductivity generated from the Waxman-Smits' data set for a range of Q_v values, and $F^* = 12$.

Table 1 describes the porosity increment along with the shaly sand formation factor (F^*) for each configuration. The value of F^* is calculated by assigning $D_{clay} = D_w$ during the simulation. It will be observed later that values of the diffusivity contrast, D_{clay}/D_w , are close to 1 when the pore electrolyte is highly conductive. The value of F^* from the W-S equation corresponds to the slope of the linear portion in the σ_0 vs. σ_w plot, that occurs at high values of σ_w .

Table 1: Values of additional porosity generated when clay minerals and their hydrated exchange cations are added to the grain. All results are normalized using corrected formation factors for the new porosities.

	ϕ	F^*	% “clay bound” water	% connected bulk water
$R_{\text{grain}} = 110 \mu\text{m}$	18.4%	11.5-12.3	0	100
$\delta = 5 \mu\text{m}$	21.5%	9.8-10	22	78
$\delta = 10 \mu\text{m}$	25%	7.9-8.2	38	62

If the bulk fluid conductivity and diffusivity are assigned the value of unity, then the rock conductivity can be calculated directly as $\sigma_0 = \phi D_\infty$. Eq. (6) is used to compare our results to the W-S model. **Figure 5** shows the simulated values of excess conductivity for two values of δ and a range of D_{clay}/D_w values. The HCM exchange cation layer cannot be strictly treated as a continuum of finite conductivity. The conductivity of HCM exchange cation decreases from a “surface value”

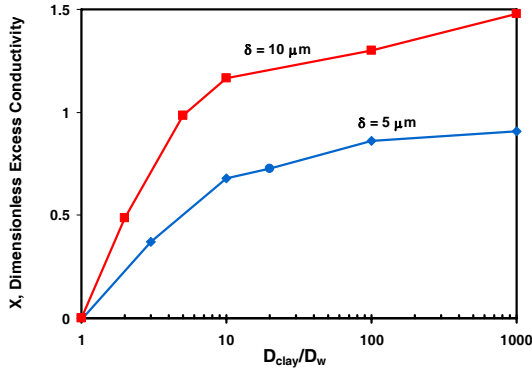


Figure 5: Simulated values of X as a function of model parameters - D_{clay}/D_w and δ .

to the bulk value and, as illustrated by Schwartz *et al.* (1989a), is a function of normal distance from the grain surface. This gradation provides insight into the probability scheme that needs to be used for the inter-zonal walks. We suggest that there be no biased probability for the walker to move from the bulk water to the HCM exchange cation region and vice versa. Non-biased walks are consistent with the rapid exchange of the HCM counterions near the grain surface with those in the pore electrolyte, especially at high values of salinity. Comparison of **Figs. 4 and 5** indicates that at low values of salinity, D_{clay} must be several orders of magnitude greater than D_w . If a biased probability is enforced based on the relative conductivity of the two phases i.e. D_{clay}/D_w (Kim and Torquato, 1990) or the harmonic mean of D_{clay} and D_w (McCarthy, 1990), there is considerable “locking” of the walker within the HCM exchange cation shell. Locking not only induces non-uniqueness to the solution, since there is significant uncertainty when assessing the long-time asymptote, but is also physically unrealistic when the clay mineral does not form a continuous electrical pathway. Using no bias for stepping across the phase boundaries, (probability = 0.5), we obtain a smoothed-out effective conductivity function and a stable long-time asymptote. **Figure 6** shows results of the simulation applied to a rock with $Q_v = 0.45$. The value of σ_0 is calculated by choosing appropriate values of D_{clay}/D_w at different σ_w 's thereby resolving the dimensional excess conductivity from **Fig. 5**. It is interesting to note that the chosen diffusivity contrasts are proportional to $1/\sqrt{\sigma_w}$ at high values of salinity but proportional to $1/\sigma_w$ at low values of salinity.

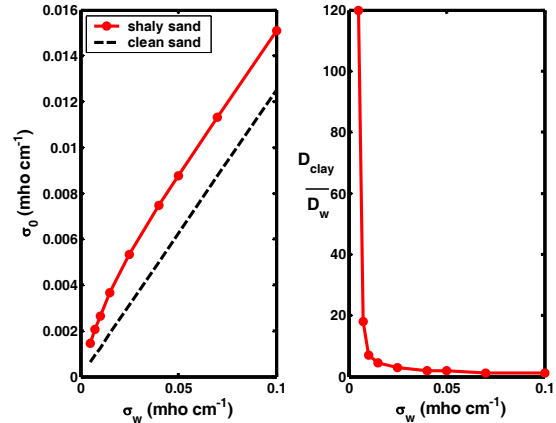


Figure 6: Plot of σ_0 vs. σ_w for the case of a sample shaly sand with $Q_v = 0.45$ meq/ml. Values of D_{clay}/D_w are chosen to yield excess conductivity consistent with W - S model predictions. Chosen values for the diffusivity contrast are shown alongside the σ_0 plot.

Reasonable parametric values can be surmised from a better understanding of the relationship between diffusivity contrasts and pore fluid conductivity, σ_w . For $Q_v = 0.45$ meq/ml, we have used the $\delta = 10$ - μm plot from **Fig. 5** to obtain D_{clay}/D_w . For low values of Q_v , e.g. 0.25, $\delta = 5$ - μm is an appropriate choice. **Figure 7** shows diffusivity contrasts that were used for $Q_v = 0.25$ for $\delta = 5$ - μm and 10 - μm .

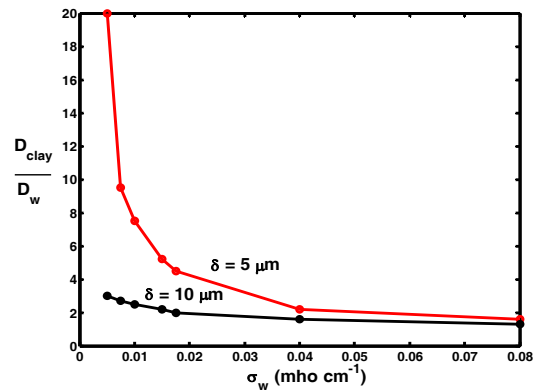


Figure 7: Diffusivity contrasts chosen to yield W - S model results for the case of a shaly sand with $Q_v = 0.25$ meq/ml.

From Fig. 7 it is clear that the desired value of D_{clay}/D_w at different values of salinity is influenced by the choice of δ . For the case of $\sigma_w < 0.04$ mho/cm, the value of δ exerts a strong influence on the diffusivity contrast that needs to be chosen. The ratio D_{clay}/D_w can be maintained relatively constant if δ is allowed to increase with decreasing values of salinity. This is in keeping with increases in double-layer thickness that have been found to occur below a critical value of salinity (Clavier *et al.* 1984; Sen, 1987; Bassiouni, 1994; Hill *et al.* 1979). Silva and Bassiouni (1988) calculate fractional volume occupied by the double layer as a function of far-water conductivity. A decrease of far-water conductivity below a value of 0.03-mho/cm is accompanied by a drastic increase in volume occupied by the double layer. This further justifies the selection of higher values of δ at low values of salinity while maintaining invariant diffusivity contrasts. For the case of very shaly sands ($Q_v > 1$ meq/ml) and under low equilibrating brine conductivity ($\sigma_w < 0.03$ mho/cm), the desired excess conductivity is realizable only when δ is comparable to the bulk/pore dimensions. The ratio D_{clay}/D_w can then be as low as 1, which eventually reduces to Waxman and Smits' (1968) assumptions of a uniformly enhanced pore electrolyte. The variation of the apparent formation-positivity exponent, m_a , defined as

$$F_a = \frac{1}{\phi^{m_a}} = \frac{\sigma_w}{\sigma_0} \quad (8)$$

is also of interest. Excess conductivity generated by the HCM counterions results in decreased values of m_a at low values of salinity. As salinity increases, m_a reaches a constant value as the relative contribution of HCM conductivity diminishes. Fig. 8 describes the variation of m_a with pore fluid conductivity. The variation of m_a closely resembles the trends in log-log plots of F_a/F vs. σ_w described by Worthington (1985).

TWO-PHASE SIMULATION

Primary drainage – The water-saturated formation described in the previous section is invaded with non-wetting hydrocarbons. A thin water film of thickness 30nm is maintained in contact with each grain while non-wetting oil blobs percolate starting from one end of the grain pack. The extent of hydrocarbon percolation is controlled by adjusting the pore aperture threshold beyond which non-wetting (NW) phase percolation is allowed. When this criterion is satisfied, the pore is occupied by a NW blob leaving formation-water in the thin-films and pendular rings (Toumelin *et al.* 2005). The percolation of NW phase blobs is consistent with

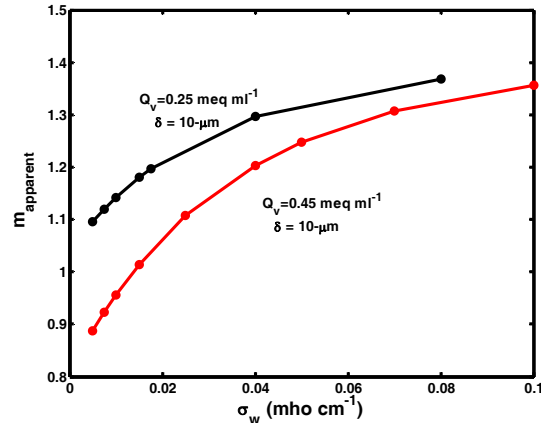


Figure 8: Values of m_a calculated from simulation results as a function of pore fluid conductivity.

capillary pressure vs. saturation curves. In addition, the clay mineral bound water is retained in its interfacial layer and is not affected by the percolating oil blobs. When the formation is partially saturated, the exchange cations are densely packed within the clay mineral zone and hence, the relative contribution to overall rock conductivity from the HCM layer is expected to increase. Waxman and Smits (1968) predict this excess contribution to be inversely proportional to the value of water saturation. The resistivity index, I_R , is used to quantify the effect of partial saturation on rock conductivity and is defined as

$$I_R = \frac{\sigma_{0(S_w=100\%)}}{\sigma_{0(S_w < 100\%)}} \approx S_w^{-n}, \quad (9)$$

where n is defined as the saturation exponent and is typically ≈ 2 for clean sands. However, n varies with amount of clay minerals present and represents an apparent saturation exponent when calculated using eq. (9) for shaly sands. We have calculated this apparent saturation exponent for three values of water saturation using a D_{clay}/D_w ratio of 10. As seen before, this value of diffusivity contrast represents conduction at low values of σ_w . Calculated values of $n_{apparent}$ are between 1.0 – 1.6. The abnormal decrease in the value of n at low values of water saturation close to 60% has been discussed by Diederix (1982). Waxman and Smits (1968) formulated an empirical relationship that interrelates I_R and S_w with a constant exponent, n^* , with the inclusion of the effect of the HCM exchange cations through the function, BQ_v/S_w as

$$I_R = S_w^{-n^*} \left[\frac{\sigma_w + BQ_v}{\sigma_w + \frac{BQ_v}{S_w}} \right]. \quad (10)$$

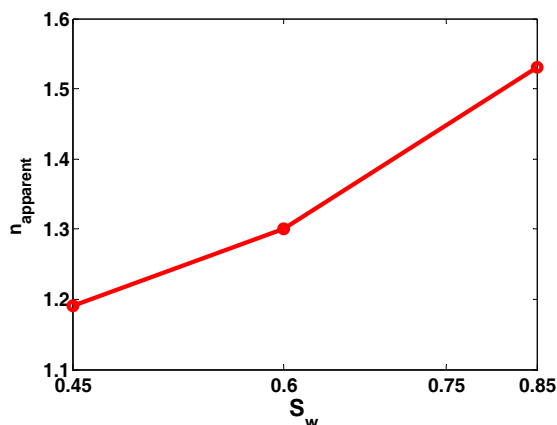


Figure 9: Variation of n with decreasing values of water saturation using $D_{\text{clay}}/D_w = 10$.

Figure 9 shows the variation of n ($= n_{\text{apparent}}$) with decreasing values of saturation. The value of n decreases with decreasing values of S_w , implying that the resistivity associated with lower values of formation water saturation is offset by the conductivity enhancement arising from densely-packed HCM exchange cations.

CONCLUSIONS

We have used a random-walk model to demonstrate the pore-level phenomena governing electrical conduction in shaly sands. We have been able to reproduce realistic values of excess conductivities associated with the HCM exchange cations at various electrolyte conductivities. Our model can be extended to various clay mineral morphologies since we have made no assumptions regarding continuous electrical pathways for the HCM cations. Many earlier works on this subject did not consider the effective volumetric contribution to excess conductivity resulting from surface conductivities associated with the HCM cations. We have shown that the relationship between interfacial clay mineral conductivity and effective excess conductivity of the HCM exchange cations needs to be calibrated using the width of the volume continuum, δ . The requirement of increasing values of δ with a decrease in electrolyte salinity is consistent with observed swelling of the anion-free layer at low values of salinity. By maintaining constant diffusivity contrasts while allowing only δ to increase, we have simulated the entire range of measured excess conductivities associated with moderately shaly sands. The fact that the thickness of the clay mineral zone, δ , needs to be comparable in size to the pore dimensions

at low values of salinity, verifies W-S assumptions of a uniform pore electrolyte. For fresh water shaly sands, i.e. for low values of σ_w and high values of Q_v , it can be concluded that the W-S model is the one that best predicts experimentally observed values of rock conductivity. When the formation is partially saturated with non-wetting hydrocarbon phase, the simulated values of the apparent saturation exponent, n , are lower than the typical value of 2, and consistent with computed values of n^* . This behavior is also consistent with observed decreases in values of n for shaly fresh water sands and the computed values of n^* . The ability of our pore-scale method to correctly predict the σ_o vs. σ_w curves and the subsequent sensitivity to model parameters lends credence to the physical consistency of the approach. Future work will involve studying the effects of wettability, saturation cycles, and varying rock geometry on the model parameters.

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