Object-oriented approach for the pore-scale simulation of DC electrical conductivity of two-phase saturated porous media

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ABSTRACT

Archie’s empirical power laws are strictly valid only for homogeneous, water-wet (WW) rocks deprived of microporosity or substantial clay-exchange cations. When these conditions are not met, non-Archie electrical behavior arises whereby relationships among rock resistivity, porosity, and water saturation no longer exhibit power-law dependence. Currently, such an unreliable behavior of empirical laws can be quantified only through pore-scale modeling of electrical conductivity under specific sets of geometric assumptions and with substantial computation memory requirements. We introduce a new geometric concept to simulate direct-current electrical-conductivity phenomena in arbitrary rock models on the basis of 3D grain and pore objects that include explicit distributions of intragranular porosity, clay-exchange cations, nonwetting fluid blobs, thin films, and pendular rings. These objects are distributed in the pore space following simple heuristic principles of drainage/imbibition that honor capillary-pressure curves. They provide a simple way to parameterize the 3D pore space and to calculate the electrical conductivity of porous media saturated with two immiscible fluid phases by way of diffusive random walks within the brine-filled pore space. Not only is the random-walk method memory efficient but it also allows the inclusion of clay/brine cation exchange surfaces otherwise not possible with conventional pore-network models. By comparing results stemming from random-walk, pore-network, and percolation simulations, we show the importance of grain surface roughness and thin film thickness, even in water-wet rocks where those factors usually are neglected. For the case of strongly oil-wet rocks, we show that thin films, snap-offs, and pore microgeometry have a primary impact on hysteresis-dominated rock resistivity during imbibition (increasing water saturation). Our simulation method agrees well overall with percolation simulation results and is advantageously unaffected by assumptions concerning site-percolation imbibition.

INTRODUCTION

In situ quantification and monitoring of water saturation in hydrocarbon formations usually are performed using open-hole and time-lapse cased-hole well-log measurements of electrical conductivity in the kHz range. The traditional basis for quantification of water saturation from low-frequency resistivity measurements, water salinity, and rock porosity is established by the well-known Archie’s relations (1942) and by their calibration to core measurements. These empirical formulas relate a fully water-saturated electrical-forming factor $F_R$ and a partially water-saturated electrical-resistivity index $I_R$ to power laws of porosity $\phi$ and water saturation $S_w$. Letting $\rho$ be the value of electrical resistivity, such relations are written as

$$F_R = \frac{\rho_{S_w=100\%}}{\rho_{\text{brine}}} = \frac{a}{\phi^m}$$

and

$$I_R = \frac{\rho_{S_w<100\%}}{\rho_{S_w=100\%}} = \frac{1}{S_w^n}$$

(1)

where $a$ defines the so-called tortuosity factor, $m$ the lithology (or cementation) exponent, and $n$ the saturation exponent. Similar power laws have been derived for shaley sands with exponents corrected for the presence of clay double-layer electrical conduction, as reviewed by Argaud et al. (1989).
With the resistivity measurements published by Sweeney and Jennings (1960) on oil-wet (OW) carbonate samples or by Wei and Lile (1991) on siliciclastic cores successively imbibed and drained with water and kerosene, it has been recognized that Archie’s relations are accurate only in the case of rocks that are strongly water wet (WW) and exhibit homogeneous granular morphology. For instance, complex rock morphology such as vugular and intragranular porosity, clay cation-exchange surfaces, and oil-wetting films at the grain surface affect the values of $m$ and $n$ in conflicting manner over the entire water saturation range (Stalheim et al., 1999; Fleury, 2002). Fluid distribution, recovery, and multiphase flow displacement also are affected directly by the degree of water wettability in reservoir rocks (Hirasaki, 1991).

The factors that influence the electrical response of saturated rocks are so varied that pore-scale models are required to describe — and, in some simple cases, quantitatively predict — these measurements. Models based on site- and bond-percolation theories (Zhou et al., 1997) seem very efficient to reproduce the electrical behavior of generic rocks, including behavior under OW conditions. However, it is out of their scope to incorporate grain-morphology information. At the other end of the spectrum of pore-scale models, pore networks (PN) extracted from high-resolution rock tomography (Oren and Bakke, 2003) or reconstructed stochastically (Liang et al., 2000) aim to honor accurate grain topology but reach practical limitations because of limited voxel resolution, simplified pore-throat and pore-body shapes, and inability to include cation-exchange clay surfaces.

An alternative way to compute electrical conductivity from such digital rocks is to mesh the pore volume of a nominal bulk rock volume with finite elements (Adler et al., 1992) and solve Laplace’s equation for the electrical potential at steady state. However, the computational requirements of such applications remain prohibitive for several million voxels. Complex multiscale technical issues also arise when dealing with nanometer-thin wetting films in pores as large as tens or hundreds of microns.

Therefore, one can consider a different numerical approach that incorporates explicit grain-morphology description, including microporosity and clays, that overcomes spatial resolution limitations, and that can be run without a complex parallel computation algorithm? This paper introduces the use of diffusive random walks (RW) and a simple grain- and pore-based geometric model as a viable solution to circumvent such problems for the simulation of direct-current (DC) electrical conductivity in porous media with two-phase fluid saturation. The next sections illustrate the flexibility of the method and compare corresponding simulation results to other simulation methods as well as typical measurements reported in the open technical literature for, respectively, single-phase, two-phase water-wet, and two-phase oil-wet granular rocks. We discuss the practical implications of these results in a final section.

**OBJECT-ORIENTED GEOMETRY**

Over the years, diffusive random walks have been used successfully to simulate single-phase measurements of nuclear magnetic resonance (NMR), electrical conductivity, and hydraulic permeability in fully saturated soils and rocks for a variety of pore geometries (Schwartz and Banavar, 1989; Kim and Torquato, 1990; McCarthy, 1990a, 1990b; Kostek et al., 1992; Ioannidis et al., 1997; Ramakrishnan et al., 1999). However, there has been no reported attempt to use the same principles to simulate electrical conduction effects caused by multiphase fluid saturations, saturation history, and variable wettability.

**Integrating grain morphology and pore-scale fluid distribution as geometric objects**

Following Schwartz’s geometric simulation models (Johnson et al., 1986; Schwartz and Banavar, 1989; Ramakrishnan et al., 1999), we define porous rocks as disordered packings of solid or microporous spherical grains which limit the free diffusion of random walkers in the pore space. Once a pack of given grain-size distribution is constructed, the grains are homogeneously overgrown to replicate the effects of rock diagenesis, overburden pressure, and cementation. As illustrated in Figure 1, pore units are defined by the void space left between each tetrahedral group of the four closest grains. A Quickhull algorithm (Barber et al., 1996) is used to partition the bulk volume into a Delaunay tessellation of such conforming tetrahedra (Bryant and Pallat, 1996).

In Figure 1, we consider a consolidated version of Finney’s pack of monodisperse grains (Finney, 1970). For simplicity, each pore size is assimilated to the size of the largest sphere that can be positioned among the four surrounding grains. Each pore shape, however, remains defined accurately by the 3D asymmetric star-shaped volume complementary of the four surrounding grains. Likewise, pore throats between two neighboring tetrahedra are assigned the size and center of the largest disk that can be positioned among the three grains of the corresponding triangular section while retaining their exact 2D star shape. This strategy ensures that the entire pore space is encoded by only the position and size of each grain, with no compromise on the actual pore and throat shapes probed by the random walkers. Finally, pendular rings (PR) of wetting fluid are defined where grains meet in the pore space.

We increase the complexity of the tortuous diffusion pathways within the granular model with intragranular porosity features controlled by the type of grains used in the packing. Figure 2 illustrates the different grain objects considered in our approach. Solid grains (type 1) are made of spheres at the contact of which the random walkers rebound. Microfractured grains (type 2) feature unidirectional slit-type microfracture along the direction of maximal overburden stress across the packing and passage of random walkers within the slit. Microporous grains (types 3-4) capture purely geometric intragranular rock microporosity (as encountered in carbonate micrites or microporous cherts) and are approximated with consolidated cubic-centered packings of micrograins. If that microporosity is connected openly to the intragranular pore space, it is deemed “coupled,” following the work of Ramakrishnan et al. (1999). On the contrary, if microporosity is isolated from intragranular porosity by cement or crystal overgrowth, it is considered “uncoupled.”

Clay-bound microporosity is considered in a different manner. Because pore size between clays is extremely small and because of the presence of exchange surface charges and cation double layers, we assign effective wet-clay volumes with an equivalent electrical conductivity. The value of this equivalent “clay conductivity” might differ from that of pore brine, depending on brine ionic content and clay type. Several publications have described this dual-conductivity approach. Argaud et al. (1989) considered the macroscopic effect of the ratio of “excess conductivity associated with the clay conductor” and the bulk brine conductivity in pores. They measured the ratio between these conductivities to be in the range 0.02–2 for a vari-
Pore-scale simulation of DC resistivity

Fluid-distribution model and capillary-pressure hysteresis

To illustrate our method, we distribute the pore objects described above across the entire pore space according to simple drainage and imbibition heuristics. Elaborate fluid-flow algorithms could be used interchangeably, such as the one developed by Gladkikh and Bryant (2005). For the sake of generality, we use simple displacement heuristics to model the electrical response of the saturated medium.

Specifically, we consider two mechanisms of pore-to-pore piston-like propagation and film growth in agreement with the scenarios suggested by Knight (1991) and implemented by Kovscek et al. (1993). The two mechanisms are known to alternate depending on capillary number and therefore on flow rate, fluid viscosity, and porous-medium properties (Lenormand and Zarcone, 1988; Lenormand et al., 1988; Vizika and Payakates, 1989). Kovscek et al. (1993) assume that only film growth occurs during imbibition in the presence of asphaltenic oil and subsequent alteration of grain surface wettability into oil wet. We model this main assumption for compar-

Figure 1. Example of a 1000-grain cubic subset from the Finney pack constructed with 200-μm-diameter grains and uniformly consolidated to reach 20% porosity: (a) 3D view of the grain pack and (b) corresponding Delaunay tessellation where each tetrahedron describes a pore unit bounded by four grains. (c) Graphical description of one cell which defines one pore, four throats, and six pendular rings (PR).
ison purposes. Unlike the mixed-wettability model of Kovscek et al. (1993), whereby a size cutoff discriminates populations of smaller OW pores from larger WW pores, we enforce the additional physical constraint that pores must be connected hydraulically to allow fluid displacement from pore to pore. We implement six saturation cycles of drainage and imbibition, whether alternate or successive. In the following, drainage refers to displacement of the dominant wetting phase by the NW phase, and imbibition refers to the opposite. Such an idea becomes ambiguous in the presence of mixed-wet pores after wettability alteration. We illustrate these saturation mechanisms in Figure 6, whereas the resulting hysteretic loops of pseudocapillary pressure (PCP) are shown in Figure 7 for the pistonlike displacement cycles and compared to the analytic results of Kovscek et al. (1993).

- Cycle 1: Drainage of the WW medium model through pore-to-pore pistonlike oil propagation (Figure 6c and d). Starting from the inlet face of the simulation domain (x = 0 in Figure 1a), we assume oil blobs (pore type 2, Figure 4) that invade the pores on a neighbor-to-neighbor basis, using nested conditional loops which test the two following criteria: (1) The oil blob reaches the throat that separated the two pores, and (2) the size of that throat is larger than a given throat-size threshold (TST). Once the outlet faces other than those at x = 0 are reached, the distribution of pore types 1 and 2 within the pore space defines the fluid geometry for the random walkers at a given value of water saturation. Drainage continues by decreasing the TST. Figure 8 illustrates the propagation of the NW phase, tetrahedron by tetrahedron, for a value of NW-phase saturation equal to 22%. At each saturation stage, the pseudocapillary pressure (PCP) is calculated from the

![Figure 2](image-url)  
**Figure 2.** Illustration of the six grain types considered in the geometric framework of this paper. Color is used to code the diffusivity values enforced during random walk by zones (blue: \(D_w\); yellow: \(D_{\text{clay}}\) — disconnected from the blue-connected brine; green: \(D_{\text{clay}}\)). Dotted lines: passage allowed via probability of passage, equation 8. Plain lines: surface rebound of the random walker.

![Figure 3](image-url)  
**Figure 3.** Illustration of the geometry of two-phase fluid saturation in a Delaunay tetrahedron. A nonwetting blob occupies the intersection between the pore space and a sphere of radius \(R_o\) concentric with the pore shown in Figure 4. Thin wetting films of thickness \(T_w\) are included between the blob and the grains.

![Figure 4](image-url)  
**Figure 4.** Illustration of the four pore types: (1) WW, water saturated; (2) WW (water films of thickness \(T_w\)), invaded with hydrocarbons; (3) OW, oil saturated; (4) OW (oil films of thickness \(T_o\)), invaded with water.

![Figure 5](image-url)  
**Figure 5.** Illustration of the effect of surface roughness on effective thickness of brine-wetting film for an equivalent smooth surface. (a) Relatively smooth grain surface. (b) Rough grain surface. Single-headed arrows identify electrical conduction currents through the brine film.
inverse of the TST, whereas water saturation $S_w$ is obtained by counting the proportion of randomly generated points in the water phase. As shown in Figure 9, depending on the value of $\alpha_w$, $S_w$ reaches a critical value (irreducible saturation) below which the PCP increases sharply. The value of $\alpha_w$, therefore, is calibrated to meet objective irreducible water saturation located in the pendular rings and the least accessible pores that cannot be reached by oil blobs. In this example, the value of $\alpha_w$ is considered homogeneous for all pores and is set at 2.25 to reach 13% irreducible water saturation. Before each subsequent cycle, the TST is reset to a large value.

- **Cycle 2**: Imbibition of the WW medium through pore-to-pore water propagation (Figure 6d and e). Water is injected from the inlet face $x = 0$ (pores of type 2 revert to type 1) and propagates from pore to pore when a new TST is met between two pores. The inverse of the imbibition TST then is subtracted from the PCP at the imbibition onset (point B) to yield new values of PCP for this cycle. Such a value of TST is decreased until $S_w$ remains constant (point C). Irreducible oil saturation is located within type-2 snapped-off pores trapped between type-1 pores. Figure 10a shows the evolution of the number of snap-offs with TST. The hysteresis ABC of Figure 7a agrees very well with the capillary-pressure hysteresis expected for a homogeneous rock.

- **Cycle 3**: Imbibition of the WW medium through film thickening (Figure 6f-h). This cycle is an alternate of cycle 2 and models the fluid distribution resulting from incremental growth of the wetting films by thickness $T_w$ (Kovscek et al., 1993). As the films grow, the NW phase includes increasingly elongated shapes. A parameter $\beta_w$ is defined to account for a possible truncation of these elongated shapes as $T_w$ increases, such that the radius of the blob is reduced by $\beta_w T_w$. Starting from point B (Figure 7a) at 30 nm, $T_w$ and $S_w$ increase in similar relative proportions (Figure 10b) while the blob radius decreases in the connected pores. When $T_w$ becomes as large as the pore throats, the NW phase is snapped off and becomes isolated from the inlet. The NW phase then is trapped, and films stop thickening in those pores. The value of $T_w$ continues to increase in the pores where oil remains connected to the inlet. Coefficient $\beta_w$ controls the maximal water saturation of the cycle (i.e., the saturation of snapped-off oil or gas). For the 20%-porosity Finney pack, values of $\beta_w$ were distributed homogeneously amid the pores. Values equal to 0.5 and 1 yielded irreducible oil saturation values of 27% and 13%, respectively. The simulation results presented in this paper use $\beta_w = 0.5$. Film thickness and PCP are not immediately related, whereupon capillary pressure during cycle 3 is not considered in Figure 7a.

- **Cycle 4**: Drainage of the OW medium through pore-to-pore pistonlike water displacement after assumed wettability alteration, following the completion of cycle 1 (Figure 6i-k). All the type-2 pores are converted arbitrarily into type-3 pores, and then water is put into contact with the inlet face $x = 0$. This process is similar to that of cycle 1 except that pores change from type 3 to type 4 as water advances across the pore space. The only criterion for water propagation across a pore throat is that its size meets a new TST. The PCP derived for this cycle is taken equal to the onset PCP (point B) minus the inverse of TST. In Figure 7a, cycle 4 de-

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**Figure 6.** Two-dimensional description of the saturation mechanisms considered in this paper. (a) Real rock topology from a thin section (white is quartz and blue is pore space). (b) Model idealization including the grains (yellow circles) and the Delaunay cells (dashed triangles). (c) and (d) Successive stages of drainage (cycle 1). Spheres (blue circles) of radius $R_s = \alpha_s R$ delimit the oil-saturated volume within each pore of size $R_s$. (e) Result of imbibition through pistonlike displacement of oil blobs (cycle 2) starting from stage (d) and leading to irreducible oil saturation in the top left corner of the pore space. (f-h) Successive stages of imbibition through incremental growth of the water films (cycle 3) starting from stage (e); in (g), snap-off occurred between the NW phase inlet and blobs to the left of the pore space, yielding irreducible oil saturation in (h). (i-k) Alternatively from cycles 2 and 3, cycle 4 assumes wettability alteration of stage (d) and successive drainage by pistonlike displacement of water blobs. (l) Imbibition of the OW medium through oil film growth (cycle 5) starting from stage (k). Note the evolution in the connectivity of pendular rings to the inlet water during cycles 4 and 5.
scribes the segment BDE and reaches PCP = 0 at point D. The end point E almost reaches $S_{wir} = 100\%$ because the only oil volume left in the rock is formed by the 30-nm-thin films. Oil-wet, oil-filled pendular rings would be required in the model to reach both curvature and irreducible oil saturation obtained by Kovscek et al. (1993) in Figure 7b.

- **Cycle 5:** Imbibition of the OW medium through oil film thickening (Figure 6k and l). This displacement process is identical to cycle 3 by defining a new blob-truncation coefficient $\beta_0 = 0.5$ equivalent to $\beta_w$ in the WW case. Likewise, no PCP is derived for this cycle. The segment EF considered in Figure 7a only illustrates the transition between cycles 4 and 6.

- **Cycle 6:** Secondary drainage of the OW medium through pore-to-pore pistonlike water displacement. This cycle starts from a spatial configuration wherein most pores are filled with thick oil films and with water left at their center, disconnected from the inlet (point F in Figure 7a). Water again is put into contact with the inlet face and propagates pore by pore as long as a new TST is met, thereby reconnecting the snapped-off water to the bulk water. The PCP for this cycle is taken equal to the inverse of that TST (segment FG). Overall, The OW segments BDE and FG agree well with the results of Kovscek et al. (1993) (Figure 7b) despite the absence of significant irreducible oil saturation in our model.

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**Figure 7.** Comparison of the mixed oil-wet capillary-pressure curves (a) simulated with our model and (b) derived by Kovscek et al. (1993) for identical values of $S_{wir}$ reached after cycles 1 ($S_{wir} = 13\%$) and 5 ($S_{wir} = 23\%$).

**Figure 8.** Visualization of the Delaunay tetrahedra invaded by oil during cycle 1 to reach 22% oil saturation for the pack of 100-μm grains shown in Figure 1 (17-μm throat-size threshold). The oil inlets are located at face $x = 0$ (circled 1). Breakthrough is reached at faces $x = 1600$ μm (circled 2), $y = 0$ (circled 3), $z = 0$ (circled 4), and $z = 1600$ μm (circled 5). The color scale describes the $x$-coordinate of the pore centers.

**Figure 9.** PCP curves calculated for primary drainage in the pack of Figure 1. The curves describe pseudocapillary pressure values as a function of water saturation for different NW blob-size factors $\alpha_o$ involving different values of $S_{wir}$.
Random-walk simulation of DC electrical conductivity

Having described the brine-filled pore space in a manner consistent with fluid-displacement mechanisms and capillary pressure, we now review how diffusive random walkers are used to compute formation factor and resistivity index for arbitrary porous media. If one defines as $\sigma$ the locally homogeneous DC electrical conductivity in a subregion and $\nabla \Phi$ the gradient of electrical potential across that region, then macroscopically, Laplace’s equation for the electric potential $\Phi$ is satisfied across the entire volume considered, i.e.,

$$\nabla \cdot (\sigma \nabla \Phi) = 0. \quad (2)$$

The macroscopic conductivity value that satisfies equation 2 for the apparent electrical gradient taken across the entire volume is $\sigma_{\text{eff}}$. In a similar manner, the material balance for a diffusing species of locally homogeneous self-diffusivity $D$ across a subregion of local concentration gradient $\nabla C$ macroscopically satisfies the equation

$$\nabla \cdot (D \nabla C) = \frac{\partial C}{\partial t}. \quad (3)$$

The macroscopic diffusivity value that satisfies equation 3 for the apparent concentration gradient taken across the entire volume is $D_{\text{eff}}$. In the steady-state limit ($t \to \infty$) where $C$ converges asymptotically, the diffusion problem of equation 3 is equivalent to the DC electrical-conduction problem of equation 2 by setting $D$, $C$, and $D_{\text{eff}}$ as equivalents of $\sigma$, $\Phi$, and $\sigma_{\text{eff}}$, respectively.

Simultaneously, the diffusion problem can be solved in three dimensions with random walkers reproducing thermal agitation. Particles within a fluid phase of self-diffusivity coefficient $D$ describe trajectories through iterative microscopic displacements of length $\delta r$ and duration $\delta t$ related by Einstein’s equation (Einstein, 1956)

$$(\delta r)^2 = 6D\delta t. \quad (4)$$

If $r$ is the position vector of a walker in the pore space and $t$ is the walk time, the effective diffusivity of the fluid is related to the mean-square displacement over all walkers, i.e.,

$$D_{\text{eff}}(t) = \frac{\langle |r(t) - r(0)|^2 \rangle}{6t}. \quad (5)$$

The effective conductivity across the porous medium is therefore proportional to the late-time asymptote of effective diffusivity of the conductive phase calculated with random walkers across the porous medium.

From this equivalence, it can be shown (Rasmus, 1986; Clennell, 1997) that the formation factor $F_R$ and resistivity index $I_R$ defined in equation 1 are proportional to the following diffusivity ratios:

$$F_R(S_w) = \frac{\sigma_{\text{water}}}{\sigma_{S_w=100\%}} = \frac{1}{\rho D_{\text{water}}} \frac{D_{\text{water}}}{t \to \infty}$$

and

$$I_R(S_w) = \frac{\sigma_{S_w=100\%}}{\sigma_{S_w<100\%}} = \frac{1}{S_w D_{\text{water}}} \frac{D_{\text{water}}}{t \to \infty},$$

where $\sigma_{\text{water}}$ and $D_{\text{water}}$ designate the electrical conductivity and diffusivity of the bulk electrolyte, respectively, and $\sigma_{S_w}$ and $D_{S_w}$ designate the corresponding effective values across the porous medium saturated with water saturation equal to $S_w$.

Given the scale contrasts between the relevant length scales of rock and fluid (nm-thick films, sub-µm micro pores, m-scale pores, sub-µm grains, µ-scale vugs), we dynamically adjust the step size to be smaller than the smallest surrounding length scale (e.g., the throat size of an occupied pore or the film thickness within a wetting-water film). Once a walker is determined to belong to the pore volume formed by one of the grain or pore objects defined previously, distances are calculated between random-walker location and pore center and grain centers. The length of an RW step is equal to the smallest quantity between one-twentieth of the pore radius and one-fifth of the smallest open throat size of that pore, whereas that within a wetting film is equal to $T/3$. To optimize the number of random walkers necessary to determine the asymptote $D_{S_w}(t \to \infty)$, we perform the simulations sequentially with series of 10 to 50 walkers.

The resulting late-time effective diffusivities are averaged across as many series of walkers as needed to obtain a smooth time-decay curve and for simulation times long enough ($10^6$ to $10^7$ ms equivalent diffusion time, for $D_{\text{water}} = 2 \mu$m$^2$/ms) to reach asymptotic convergence within reasonable repetition error. Figure 11 shows the time decay of effective water diffusivity computed in the consolidated Finney pack described in Figure 1a, for different values of $S_w$. Our simulation error is usually on the order of $\pm 5\%$ in WW cases or for large $S_w$ values, and it falls within the size of the markers used to indi-

Figure 10. Evolution with water saturation of the fraction of oil-saturated snapped-off pores with (a) throat-size threshold during cycle 2 and (b) incremental water-film thickness during cycle 3.

Figure 11. Examples of diffusivity time decays simulated for water molecules at different values of water saturation $S_w$ in the grain pack shown in Figure 1.
cate RW simulation results. For most OW simulations, $S_{w}$ values lower than 30%, or in the presence of intragranular microporosity (grain type 3), much longer simulation times are necessary to reach convergence of $D_{s}(t \rightarrow \infty)$. When appropriate, correspondingly higher error bars for calculated values of $F_{k}$ and $F_{e}$ are indicated on the plots which follow.

Inclusion of conductive clays in the model (grain types 5 and 6) implies conductivity contrasts (i.e., diffusivity contrasts for RW purposes) between pore water and clay volumes, as shown in Figure 2. Each time a random walker reaches such an interface between pore water and conductive clay volume, it is subject to a probability of passage adapted from McCarthy’s work (1990a, 1990b):

$$p = \frac{D_{\text{clay}}}{D_{\text{water}} + D_{\text{clay}}}.$$  (8)

If that probability is honored, then the random walker crosses the interface and its self-diffusivity value is changed, thereby affecting the clock increment $\delta \tau$ for a given step size $\delta r$, after equation 4. If not, then the random walker bounces back in the original region. However, no rigorous demonstration exists for that probability of passage (McCarthy, 1990a), whereby any probability that honors the limits

$$p \to 0 \quad \text{when } D_{\text{clay}} \to 0$$  (9a)

and

$$p \to 1/2 \quad \text{when } D_{\text{clay}} \to D_{\text{water}}$$  (9b)

should be acceptable. Equation 8 precisely differs from that of McCarthy’s (1990a) by a factor of two, because his expression of $p$ tends to one in condition 9b. On the contrary, we believe that $p$ should be unbiased (tend to 1/2) when clay volumes are as conductive as pore water. Further investigation is in process to correctly calibrate clay-coating thickness $D_{\text{clay}}$ and $p$ in pore-scale models with respect to electrical-conductivity measurements in shaley sands (Jin et al., 2007).

**SIMULATION RESULTS**

Single-phase saturation with clustered grains and clay inclusions

We uniformly overgrow the Finney pack shown in Figure 1a to reduce its porosity from 39% to 7%. As indicated in Figure 12a, the values of the formation factor derived from the RW simulation via equation 6 compare very well to those obtained using a pore network with the same Finney pack (Bryant and Pallatt, 1996) and to published measurements of clay-free sandstones (Doyen, 1988). The lithology exponent $m$ is defined as the slope of the bilogarithmic plots of Figure 12. Bryant and Pallatt’s (1996) original PN model considered the balance of electrical flux (Kirchhoff’s law) at the surface of the same tetrahedral cells indicated in Figure 1b and weighted by the pore-throat section shown in Figure 1c. Samples measured by Doyen (1988) are considered representative of generic sandstone rocks with negligible clay or microporosity conductivity. The assumption of uniform grain growth of the Finney pack entails good agreement between simulated and measured formation factors at porosity values below 15%. Above 15% porosity, however, the simulated values of formation factors are lower than expected in real rocks. Additional simulation work in Figure 12b indicates that variable grain clustering (or, similarly, nonuniform grain overgrowth) affects the electrical formation factor and yields better agreement between grain-pack simulations and rock measurements than uni-

Figure 12. Comparison of formation-factor curve measurements and simulations (a) for an unclustered clay-free grain pack: measurement on similar sandstone samples (Doyen, 1988) and simulation on the Finney pack (Figure 1a) with pore network (PN) (Bryant and Pallatt, 1996) and random-walk (RW) techniques; (b) for clustered clay-free grain packs: measurement on similar sandstone samples (Doyen, 1988) and RW simulation with packs of normally distributed grain sizes and different degrees of grain clustering (pack 1 is the least clustered and pack 3 is the most); (c) for clay-coated grain pack: RW-simulation results with different contrasts of clay-to-brine electrical conductivity.
form grain overgrowth for porosities above 15%. The grain packs numbered 1 through 3 considered in Figure 12b were constructed with a realistic normal grain-diameter distribution in the range of 50 to 320 μm (Figure 13). Clustering then was enforced by defining attracting grains toward which all other grains displace by a distance \( d/r^2 \), where \( d \) is a constant and \( r \) is the distance between the grains and the attractors. Grain packs 1 through 3 are characterized by increasing values of \( d \).

The RW approach allows one to include conducting clay coats embedded in the grain-pack skeleton. We illustrate such application by varying the cation-exchange capacity of the clay coatings in Figure 12c. Thirty percent of the grains are randomly assigned a 3-μm clay coat (as described in the type-4 grains of Figure 2) so that the corresponding clay volume amounts to 2% of total solids in the synthetic sample. The porosity is reduced by homogeneously growing all the grains, whereas the 3-μm clay coat thickness is maintained as constant. As brine salinity decreases, the contrast ratio \( D_{\text{clay}}/D_{\text{water}} \) increases to values of 1:1000, 1:10, and 1:1, and \( m \) decreases to values as low as 1.5 when clays become as conductive as the pore brine (a situation common in low-salinity shaly sands). Two-phase-fluid applications of this model and their implications in quantifying the impact of geometric clay distribution on shaley-sand resistivity models are described elsewhere (Devarajan et al., 2006; Jin et al., 2007).

Two-phase saturation with water-wet grains (saturation cycles 1 through 3)

Figure 14 shows the resistivity-index curve simulated as a function of \( S_w \) from equation 7 for drainage cycle 1. Archie’s \( n \) saturation exponent appears as the negative slope of the bilogarithmic plot assuming a constant tortuosity factor \( a = 1 \). Figure 14a indicates good agreement among (1) RW simulations performed on the Finney pack with a film thickness of 30 nm, (2) measurements performed on a 20%-porosity clay-free sandstone sample (core T1 from Argaud et al., 1989), and (3) PN simulations performed on the same smooth Finney pack (Bryant and Pallatt, 1996). The latter model assumes pistonlike displacement of the oil phase and homogeneous electrical conduction through pendular rings but not through wetting films. Except for the jump in resistivity index observed at \( SW = 50\% \), this agreement suggests that the contribution of thin-film electrical conduction is negligible in smooth, water-wet porous media. In the presence of substantial surface roughness, however, the effective thickness of wetting films becomes as large as hundreds of nm (Figure 5) and, as shown in Figure 14b, their presence becomes essential for accurate simulations.

In that figure, RW simulations emphasize that \( n \) decreases from 2 to 1.3 as \( S_w \) becomes lower than a critical value \( S_{\text{crit}} = 55\% \). This behavior agrees with observations by Diederix (1982), whereby surface roughness offered by the clay texture in salt-saturated shaley sandstones was interpreted as the origin of differences between the resistivity behaviors observed in two wells within the same field (Figure 14b). This interpretation was supported by experiments on smooth and rough water-wet glass-bead samples. The same argument justifies the choice of a 30-nm brine film thickness at the surface of our smooth, spherical grains to represent moderate grain roughness, instead of the 5- to 10-nm thickness expected for a flat rock/water/oil interface (Hirasaki, 1991).

Figure 14b also shows a similar non-Archie behavior previously modeled by Zhou et al. (1997) using percolation arguments in a generic 3D cubic pore network. That model assumes that the conductivity enhancement caused by corners or crevices in WW rocks is a bond-percolation mechanism. However, the non-Archie effect seems too exacerbated in the absence of explicit surface roughness or other microporosity, and the authors acknowledge that solely considering bond percolation is an oversimplification. Put in the context of the RW simulations, we now understand that solely bond percolation at low values of \( S_w \) captures the additional effect of rock-surface roughness but is not appropriate for smooth-grain rocks that exhibit no microporosity.

Figure 13. 3D view of one of the clustered grain packs used for the calculations of formation factors shown in Figure 12b.

Figure 14. Comparison of primary-drainage resistivity-index measurements and simulations. (a) In the absence of surface roughness or thick wetting films, measurements in clay-free sandstone (Argaud et al., 1989) and simulations with PN (Bryant and Pallatt, 1996) and RW techniques for the Finney pack shown in Figure 1. (b) In the presence of surface roughness or thick film thickness: RW-simulation results with thick 300-nm films, percolation simulations (Zhou et al., 1997), and well-log measurements of salt-saturated shaley sandstones containing smooth grains (as in Figure 5a: well 4 data from Diederix, 1982) and rough grains (as in Figure 5b: well 1 data from Diederix, 1982).
Next we consider the imbibition processes proposed in cycles 2 and 3 of our model. Figure 15 shows that adopting either imbibition process after drainage (cycle 1 end point) yields a distinct resistivity-index hysteresis. The hysteresis formed by cycles 1 and 2 is hardly noticeable and remains within the range of numerical-simulation error with a constant $n$ equal to 2.1. The other hysteresis formed by cycles 1 and 3 exhibits values of $n$ higher than 2 for $S_w < 25\%$ and down to 1 for $S_w > 30\%$. Even though measured values of $n$ are rarely that low, it is not unusual to encounter values of $n$ lower than 2, depending on experimental conditions (Knight, 1991; Longeron et al., 1989; Grattoni and Dawe, 1998). Imbibition resulting from a combination of the phenomena described by cycles 2 and 3 could explain why these measurements exhibit values of $n$ lower than 2.

Two-phase saturation with oil-wet solid and microporous grains (saturation cycles 1, 4, and 5)

Depending on the pH, thermodynamic conditions, and chemical oil composition, the grain surface can become oil wet. Figure 16a shows the resistivity-index curves calculated along saturation cycles 4, 5, and 6 for the 20%-porosity Finney pack, side by side with the percolation-simulation results of Zhou et al. (1997) (Figure 16b) computed for the same 3D cubic pore network as in the WW case. Similar to the WW case, Zhou et al. (1997) assume electrical conductivity as a bond-percolation phenomenon during drainage. As $S_w$ decreases during imbibition in OW rocks, electrical conductivity subtly depends on the presence of brine in adjoining pore bodies (site percolation) and adjoining pore throats (bond percolation) and by site-to-bond correlation. Zhou et al. (1997) then approximate electrical conductivity as a site-percolation process below an arbitrary SW = $50\%$. Numerical results for both RW and percolation models exhibit striking similarities, including a constant slope $n = 3$ during drainage cycle 4 and a sudden increase of $n$ as $S_w$ decreases below a critical value $S_{wcrit}$ about $40\%$ during imbibition cycle 5. These models are in good agreement with the electrical behavior measured by Wei and Lile (1991) in a 19%-porosity clay-free sandstone sample and shown in Figure 16c, whereby a succession of resistivity-index hysteresis appears among cycles 4, 5, and 6. The value of $S_{wcrit}$ constitutes the main difference between simulation results ($S_{wcrit} = 40\%$) and measurements ($S_{wcrit} = 55\%$).

In the absence of more information on the microstructure of Wei and Lile’s (1991) sample, we do not expect that simulations with the Finney grain pack will accurately match measurements and, specifically, $S_{wcrit}$ values. We do observe, however, that rock porosity and morphology substantially influence $S_{wcrit}$, as indicated by the next panels of Figure 16. Simulations performed on an overgrown 7%-porosity Finney pack constructed with solid grains exhibit a higher value of $S_{wcrit}$ (60%) (Figure 16d). On the other hand, a 22%-porosity microporous pack constructed from a 14%-porosity overgrown Finney pack with 30% solid grains and 70% microporous grains yields a high value of irreducible water saturation (45%), a negative curvature of $n$ for decreasing values of $S_w$, and a high value of $S_{wcrit}$ (72%) (Figure 16e). This partially microporous simulation example yields values of resistivity index that are similar to measurements performed by Sweeney and Jennings (1960) on strongly oil-wet carbonates and characterized by very high values of $S_{wcrit}$ (Figure 16f).

As in previous cases, no details are reported on the microstructure of the measured samples, whereupon the coincidence of the results might or might not be related to the presence of microporosity. Notwithstanding, the object-oriented approach developed in this paper enables the new combination of enough microstructural elements to reproduce resistivity hysteresis in strongly OW rocks with a wide range of critical saturation values which can be explained by variations of rock morphology.

**DISCUSSION**

Despite the simplicity of the geometric model introduced in this paper, quantitative comparison of our results against those obtained using alternative approaches reveals interesting properties. In particular, the coincidence of our results in the 20%-porosity Finney pack with the percolation results of Zhou et al. (1997) suggests that our pore-object approach properly captures the effect of fluid distribution on electrical conductivity for a generic dense, porous medium. By introducing microporous grain objects and varying the model porosity, we added morphological information that was missing in the percolation approach to describe the net effect of rock structure and fluid distribution (including wettability) on electrical measurements. Particularly, in their method, Zhou et al. (1997) had to assume that site percolation becomes predominant in OW rocks below $S_w = 50\%$, whereas the variation of $S_{wcrit}$ observed with the RW simulations suggests that such a cutoff value should vary as well. It is encouraging that our mechanistic conductivity assumptions for OW rocks agree well with percolation theory.

Comparison of our simulation results to those of earlier PN models based on the same WW Finney packs emphasizes the importance of thin films and pendular rings for electrical-conductivity modeling. Bryant and Pallatt (1996) ignored the presence of thin conductive films but did allow full electrical conduction between hydraulically disconnected pores because of common pendular rings. Those assumptions for a WW medium are similar to our assumptions for an OW medium except that we enforce constriction of the electrical pathways at the pendular rings. The drastic change of the resistivity index observed around $S_w = 13\%$ between (1) Bryant and Pallatt’s (1996) PN results at the cycle end point (Figure 14) and (2) our simulation results at the onset of cycle 4 (Figure 16a) therefore can be attributed to the constriction of pendular rings. Regarding the results shown in Figure 14, it is remarkable that almost the same values of resistivity index are obtained in the WW case using the two simulation approaches (absence of wetting films but connection through pendular rings versus presence of wetting films and constriction of pendular rings).

Snap-offs also comprise important components of pore-scale immiscible displacement. In agreement with the general percolation
work by Zhou et al. (1997), our model explains the high values of resistivity index obtained for OW media at low values of water saturation (cycles 5 and 6) based on the existence of snap-offs. It therefore might seem contradictory that Gladkikh and Bryant (2005) concluded that snap-off phenomena had no impact on immiscible displacements in the Finney pack. To reach that conclusion, Gladkikh and Bryant (2005) performed calculations of the interface curvatures and determined the onset of fluid displacement and snap-offs from the geometric coalescence of fluid menisci and nearby pendular rings. Their calculations, however, assume (1) perfect grain curvature, which for a given contact angle constrains the meniscus curvature at the interface between the two fluid phases, and (2) knowledge of pendular ring sizes and locations in the pore space. Based on these restrictive assumptions, it is unclear to what extent their approach should be generalized to real subsurface rock conditions. Such a technical point also questions the universality of grain packs to simulate transport processes through dense, compacted soils and rocks.

Our modeling philosophy is different. Rather than accurately simulating the displacement processes occurring in smooth bead packs, we consider the grain packs as geometric proxies for grain arrangements in real subsurface conditions. The object-oriented approach is intended to reproduce trends known to occur in rocks to simulate DC electrical conductivity resulting from superposition of complex grain morphologies, saturation history, and wettability effects. Segmentation of high-resolution rock-tomography images into grain packs (Saadatfar et al., 2005) offers new possibilities to quantitatively compare and calibrate our object-based approach to more detailed but computationally impractical voxel-based simulation techniques. In particular, such models could be used to accurately simulate fluid flow and distribute fluids in capillary equilibrium. Subsequently, the parameters $\alpha$, $\beta$, and $\gamma$ of an equivalent RW model could be adjusted on a pore-to-pore basis so that the same amounts of fluid saturate the same pores with the same accessibility to surrounding pores. As a result, the grain-based RW model could conform quantitively to measurements performed on real rocks.

Numerical models such as the one introduced in this paper are useful tools for analyzing the sensitivity of resistivity measurements of rocks to different conditions of surface roughness, wettability, and other microstructural factors. However, the predictive ability of numerical models is hindered by our own ability to characterize these elements reliably and accurately — for instance, when scanner resolution does not resolve pore microstructure or when connectivity between pores is unclear. Simulation time is also quite variable from one numerical method to another, depending on both the complexity of the rock model and the accuracy of the fluid-distribution algorithm. The RW method, for instance, proposes a memory-light alternative to heavier high-resolution voxel-based approaches that are not amenable to calculations on contemporary desktop computers. However, the diffusion time and number of walkers necessary to reach asymptotic behavior involves minutes, hours, or even days of computation time as conductive pathways become more and more tortuous when both $S_c$ and porosity decrease. Notwithstanding, these numerical simulation times still remain practical vis-à-vis schedules required for laboratory measurement of electrical properties of rock samples, which often can take months.

Beyond simulating the asymptotic DC electrical conductivity of saturated rocks, the RW simulation technique combined with object-oriented geometry offers unique opportunities to study time-domain transient behavior. Specifically, following the approach of Cortis...
and Knudby (2006) adopted for hydraulic permeability, we expect that the RW approach could be used to simulate both time-domain induced polarization and electrical conductivity frequency dispersion of rocks at pore scale. The numerical framework introduced in this paper also provides a direct way to simulate the nuclear magnetic resonance response of saturated rocks by solving Bloch’s equations along 1D segments of RW diffusion pathways (Toumelin et al., 2007).

CONCLUSION

This paper confirms the value of simple geometric models to explain the complex electrical behavior of saturated rocks. Specifically, complex grain morphologies, clay inclusions, and fluid configurations were considered as pore-scale objects, which we defined with a few geometric parameters in consistency with capillary-pressure curves and established thermodynamic models of immiscible fluid displacement. By enforcing simple drainage and imbibition mechanisms, the RW approach introduced in this paper quantitatively reproduces the resistivity hysteresis of generic two-phase saturated rocks and describes non-Archie behavior in oil-wet rocks as the combined effects of saturation history, wettability, and rock morphology. Thus far, pore-scale modeling is the only method available to quantify such a breakdown of Archie’s power laws. The RW results described in this paper are consistent with existing results stemming from pore-network and percolation simulations. However, only the RW approach remains amenable to combine variable wettability and explicit rock morphology, including intragranular microporosity and clay surface conductivity.

We showed that the accuracy of the algorithm used to distribute immiscible fluids at pore scale is contingent on the objective of the simulation model. For electrical conductivity calculations, grain surface roughness, thin films, pendular rings, and snap-offs need to be incorporated consistently in the model geometry. The combination of diffusive RW simulation and object-oriented pore geometry permits accurate simulation of the electrical behavior of saturated rocks, not only under steady-state conditions but also in transient regimes, as well as their NMR response.

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