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Alain Tabbagh, Cédric Panissod, Roger Guérin, Philippe Cosenza. Numerical modeling of the role of water and clay content in soils' and rocks' bulk electrical conductivity. *Journal of Geophysical Research: Solid Earth*, 2002, 107, 10.1029/2000JB000025 . hal-04110483

HAL Id: hal-04110483

<https://hal.science/hal-04110483>

Submitted on 31 May 2023

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Numerical modeling of the role of water and clay content in soils' and rocks' bulk electrical conductivity

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Received 23 October 2000; revised 17 May 2002; accepted 24 June 2002; published 23 November 2002.

[1] The influence of clay and water content in the electrical conductivity of rocks and soils has been experimentally established and is expressed by simple empirical laws: the Archie's law and the addition law between volume water conductivity and surface shale conductivity. Two independent numerical modeling techniques, the moment method and the finite difference method, are presented here and are used, first, to verify the agreement between Maxwell's equation based theoretical approaches and the empirical laws and, second, to begin to investigate for a possible effect of the microscopic geometry over macroscopic conductivity. A good agreement between simulation results and Archie's law is obtained when both randomly distributed isotropic and elongated microvolumes of conducting water are considered and a slight difference appears between these two microstructures. For low clay contents in clay-dispersed media, the clay-associated conductivity is shown to be proportional to a specific clay area, which is in good agreement with the addition empirical law. *INDEX TERMS:* 3914 Mineral Physics: Electrical properties; 0619 Electromagnetics: Electromagnetic theory; 0644 Electromagnetics: Numerical methods; 0999 Exploration Geophysics: General or miscellaneous; *KEYWORDS:* numerical modeling, electrical conductivity, water content

Citation: Tabbagh, A., C. Panissod, R. Guérin, and P. Cosenza, Numerical modeling of the role of water and clay content in soils' and rocks' bulk electrical conductivity, *J. Geophys. Res.*, 107(B11), 2318, doi:10.1029/2000JB000025, 2002.

1. Introduction

[2] Electrical conductivity plays a determinant role in two complementary aspects of the exploration of the ground: surface measurements and well-logging measurements. This property exhibits the widest range of variation among all the properties used in exploration geophysics. It is directly related to the water content and thus constitutes an indirect but quantitative source of information about the presence of fluids and the transfer properties of the ground.

[3] Interpretation of electrical or electromagnetic (EM) surface measurements as well as resistivity logging corresponds to a two step processes: first, the spatial variations of the electrical resistivity value must be determined and second, a geological model deduced from the physical meaning of this property and its variations must be proposed. To perform this second step much experimental and theoretical work has been undertaken over the past seventy years [Serra, 1979; Keller, 1988]. Experimental studies established empirical laws that describe the role of water and clay content. They show that resistivity of porous, water-saturated clean rocks follow Archie's empirical law, namely [Archie, 1942],

$$F = \frac{\sigma_w}{\sigma} = a\varphi^{-m} \quad (1)$$

where F is called the formation factor, σ is the bulk conductivity, σ_w is the conductivity of the water filling the

pores, φ is the porosity, a depends on the lithology and lies between 0.6 and 2.0 [Keller and Frischknecht, 1970] and m is the cementation or tortuosity factor which depends on the shape of the pores and of their connections, it is not far from 2.0. In unsaturated rocks, the gas volumes play the same role as the solid volumes and the product (φS_w) replace φ in equation (1), S_w is the water saturation.

[4] In presence of fine grains, a surface conductivity corresponding to the displacement of the external counter ions of the grain-surface double layer has to be considered. In a series of experiments undertaken in petroleum industry on oil-bearing shaly sands [Waxman and Smits, 1968] concluded that the bulk conductivity of the rock is the sum of the water volume conductivity and of the shale surface conductivity. They fitted their observations with the empirical formula:

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

where σ is the bulk conductivity, σ_w the water conductivity, B a coefficient, Q_v the cation exchange capacity and F^* the formation factor in shaly sand. Other studies have confirmed the simple summation of the two types of conductivities [Johnson and Sen, 1988].

[5] In soil studies the role of both volume conductivity of water (soil solution), σ_w , and surface conductivity of fine grains, σ_s , was also recognized [Rhoades et al., 1976]. Again the bulk conductivity corresponds to their sum. The volume conductivity depends on the soil solution conductivity and on the volumetric free water content, θ , through a

dimensionless “transmission coefficient”, T , the empirical expression of which is $T = \alpha\theta + \beta$, α and β being empirical constants. The final expression is thus:

$$\sigma = \sigma_w(\alpha\theta^2 + \beta\theta) + \sigma_s \quad (3)$$

and it is not different from that used for rocks ($\alpha = 1$ and $\beta = 0$).

[6] Others experiments are in agreement with these formulas, and the general conclusion for large series of earth material are the followings: (i) the bulk conductivity is the sum of the water volume and clay surface conductivities, (ii) the exponent of the water content in the formation factor is not far from -2 .

[7] Various theoretical works have been performed to fit a physical model with the previous empirical laws. As for the dielectric permittivity, most theoretical models can be gathered in two groups: effective medium approximations and statistical models.

[8] In the first group, inclusions, representing either pores or solid grains, are embedded in a uniform matrix [Maxwell-Garnett, 1904; Bruggerman, 1935; Sen et al., 1981; Mendelson and Cohen, 1982; Bussian, 1983; Sen and Chew, 1983; Madden and Williams, 1993; Chelidze and Guéguen, 1999]. Models of partly molten upper mantle refer to this group [Waff, 1974; Glover et al., 2000] as well as hydrocarbon clean formations where the rock matrix conductivity can be assumed to be negligible. In this group, although the coupling between inclusions (i.e. EM interactions) is roughly approximated, resulting analytical expressions of the macroscopic effective conductivity depend on porosity and inclusion shape [De Kijper et al., 1996] and Archie’s law is derived for granular media [Sen et al., 1981; Mendelson and Cohen, 1982].

[9] In the statistical approach, the medium is considered as a three dimensional network of resistors and/or capacitors [Dullien, 1992]. Following this approach, the path of an electric charge in the network is a function of the volume fraction of the components [Madden, 1976; Suman and Knight, 1997]. Jonas et al. [2000] have attempted to introduce a more realistic description of porous medium by using its statistical properties. Rothman [1988] and Kuntz et al. [2000] applied an analogy with gas flow in porous media where the electrical conductivity is described by the motion of particles over a lattice with different sets of collision rules. All results lead to power law relationships between formation factor and porosity in fair agreement with Archie’s law. Other models were also proposed: in the work of Herrick and Kennedy [1994], the electrical conduction occurs through small tubes of nonuniform section and complex paths and Adler et al. [1992] used a numerical finite difference scheme to solve the Laplace equation in an artificial medium which shares same statistical properties as the real sandstone medium.

[10] Finally multiple different modeling methods have shown that they can simulate the Archie’s law response for rocks and it seems difficult to extract the details of the distribution of water in a rock from macroscopic measurements.

[11] The role of grain surface conductivity has been theoretically studied by Revil and Glover [1997, 1998]. Revil et al. [1998] developed an electrical conductivity

equation based on Bussian’s model and accounting for the different behavior of ions in the pore space. Electrical conductivity calculated with this equation is favorably compared with published data. This theoretical equation based on a differential effective medium theory does not allow distinguishing different modes of clay distribution at the microscopic scale, however.

[12] The approach we adopted hereafter is based on numerical solutions of Maxwell’s equations written at the microscopic scale. It allows: (i) the EM coupling between the different components to be treated without assumptions, and thus constitutes a physics-based method (ii) to investigate the role of water and clay content and distribution in the bulk electrical conductivity.

[13] Following such an approach to understand the physical meaning of the empirical relation between the relative dielectric permittivity value and the water content, we undertook numerical modeling [Tabbagh et al., 2000] and established that to fit the values and the curvature of the empirical curve the elementary volumes of water become more elongated as the water content increases. In a similar way, we present here an attempt to apply physics-based methods to the modeling of electrical conductivity (or resistivity) of heterogeneous media. Both moment and finite difference methods are used. They are presented in the two first parts of this paper. Our objective is to know if these numerical models of very simple microstructure are in accordance with the empirical laws and, in the case of clean rocks, to observe if the microscopic geometry of water cells may influence the bulk conductivity. In presence of clay, see the fourth part below, our aim is to check that a microscopic dispersed distribution of clay corresponds to a macroscopic addition law.

2. Modeling Using the Moment Method

[14] The moment method (MoM) was proposed by Harrington [1968] in EM. It establishes the equivalence between the presence inside a given volume of heterogeneity of differing properties and the presence of a “secondary” source of current. It has been used widely in EM geophysics to model 3D structure representing conductivity, magnetic susceptibility or permittivity contrasts, and was also extended to the static case [Dabas et al., 1994]. In the present modeling, we follow this extension.

[15] Consider a body of electrical conductivity σ_b located in a uniform medium of electrical conductivity σ_0 , one notes (\mathbf{E}, \mathbf{H}) as the total EM field and $(\mathbf{E}_p, \mathbf{H}_p)$ as the “primary” field, the field that would exist in the absence of the heterogeneity. Both fields satisfy the Maxwell’s equations, and their difference, the secondary field $(\mathbf{E} - \mathbf{E}_p, \mathbf{H} - \mathbf{H}_p) = (\mathbf{E}_s, \mathbf{H}_s)$ satisfies:

$$\nabla \times (\mathbf{E} - \mathbf{E}_p) = \mathbf{0} \quad (4)$$

$$\nabla \times (\mathbf{H} - \mathbf{H}_p) = \sigma_0(\mathbf{E} - \mathbf{E}_p) + (\sigma_b - \sigma_0)\mathbf{E} \quad (5)$$

[16] In equation (5), the term $(\sigma_b - \sigma_0)\mathbf{E}$ associated to the heterogeneity appears as a secondary current source. Thus, the heterogeneity can be considered as equivalent to the presence of a secondary current density $\mathbf{J} = (\sigma_b - \sigma_0)\mathbf{E}$, proportional to the total field. In the presence of a series of different bodies, a series of corresponding sources

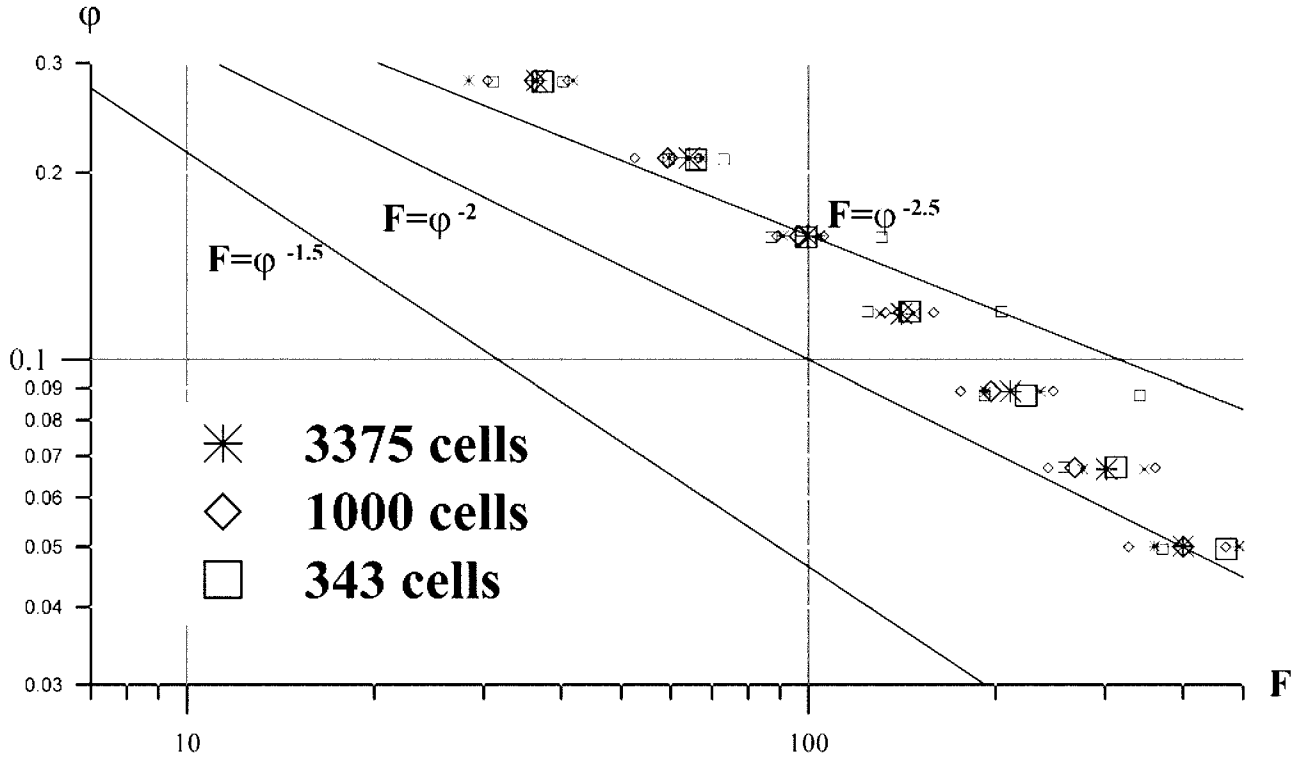


Figure 1. Median and quartile values of the formation factor when changing the number of cells (MoM calculations).

will be considered. The intensity of each source depends on the total field E and thus all the sources are coupled together. Equation (5) is identical to that derived in low frequency EM [Raiche, 1974; Hohmann, 1975; Caetermann et al., 1979; Tabbagh, 1985] and (4) is specific of the static case.

[17] To solve the coupled equations (4) and (5), for secondary fields (E_s, H_s) the potential vector A is defined by:

$$H_s = \frac{1}{\mu_0} \nabla \times A \tag{6}$$

Substitution of (6) into (5) results in:

$$E_s = \frac{1}{\mu_0 \sigma_0} \nabla \times (\nabla \times A) - \frac{J}{\sigma_0} \tag{7}$$

From equation (4), one obtains: $E_s = -\nabla U$, and by introducing the Lorentz gauge, $\nabla \cdot A - \mu_0 \sigma_0 U = 0$,

$$\begin{aligned} \nabla \cdot A - \mu_0 \sigma_0 U &= 0, \\ \nabla^2 A &= -\mu_0 J \end{aligned} \tag{8}$$

[18] The solution of equation (8) which is the potential vector created by the heterogeneity at a point r can thus be expressed as the following integral:

$$A(r) = -\mu_0 \iiint_V J(r') \tilde{G}(r - r') d\tau' \tag{9}$$

where V is the volume of the heterogeneity and \tilde{G} is the dyadic Green tensor (with $\tilde{G}(r - r') = G(r - r') \delta$ where δ is the dyadic unity tensor, $G(r - r') = \frac{1}{4\pi|r - r'|}$ inside a homogeneous medium). From equations (7) and (9), the secondary field inside the heterogeneity is obtained:

$$E_s(r) = -\frac{1}{\sigma_0} \iiint_V J(r') \nabla \times [\nabla \times \tilde{G}(r - r')] d\tau' - \frac{J}{\sigma_0} \tag{10}$$

and outside one has:

$$E_s(r) = -\frac{1}{\sigma_0} \iiint_V J(r') \nabla \times [\nabla \times \tilde{G}(r - r')] d\tau' \tag{11}$$

[19] To convert integral equation (10) into a set of algebraic equations, we divide the volume of the body (or of the bodies) into N cubic cells and assume that the total electrical field and conductivity are constant in each cell. Then, the integral (10) can be approximated by a finite summation:

$$\begin{aligned} E(r) - E_p(r) &= -\sum_{n=1}^N \left(\frac{\sigma_b^n - \sigma_0}{\sigma_0} \right) \iiint_{V_n} \nabla \times [\nabla \times \tilde{G}(r - r')] d\tau' E^n \\ &\quad - \left(\frac{\sigma_b(r) - \sigma_0}{\sigma_0} \right) E(r) \end{aligned} \tag{12}$$

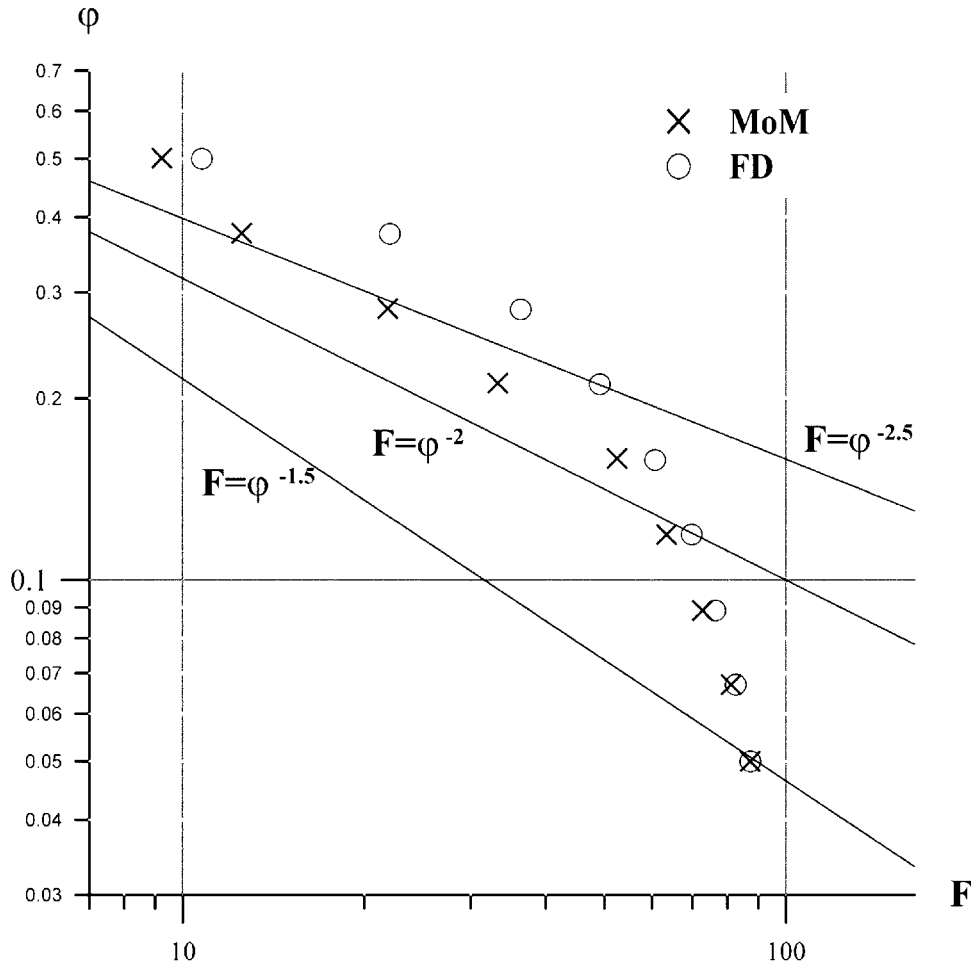


Figure 2. Relationship between formation factor and porosity for a random distribution of water cells, MoM calculation (crosses), FD calculation (circles).

[20] In more concise notation, the total electric field at the center of cell m (of which the center is located at \mathbf{r}) is given by:

$$\mathbf{E}_s^m = - \sum_{n=1}^N \left(\frac{\sigma_b^n - \sigma_0}{\sigma_0} \right) \Gamma_{mn} \cdot \mathbf{E}^n - \left(\frac{\sigma_b^m - \sigma_0}{\sigma_0} \right) \mathbf{E}^m \quad (13)$$

with the integral $\Gamma_{mn} = \int \int \int_{V_n} \nabla \times [\nabla \times \tilde{\mathbf{G}}(\mathbf{r} - \mathbf{r}')] d\tau'$ which is numerically computed.

[21] Therefore, from equation (13), a system of $3N$ linear equations with $3N$ unknowns which are the three components of the total electrical field in the center of each elementary cell (i.e. E_x , E_y and E_z) can be written in matrix form:

$$\mathbf{E}_p = \mathbf{a}_{EE} \cdot \mathbf{E} \quad (14)$$

[22] In the matrix \mathbf{a}_{EE} , each term represents the coupling between one component of the electric field in one cell to one component of the electrical field in another (or the same) cell. When \mathbf{J} is known, the effect of the heterogeneities at a point outside the volume is calculated by a simple integration (11) of the effect of each secondary source.

[23] The MoM we apply hereafter does not contain physical approximations in the calculation, in addition it can allow a clear definition of the different assumptions: (i)

by assuming $\mathbf{E} = \mathbf{E}_p$, the Born's approximation, the effects of each cell are simply added which corresponds to the simple mixing law, (ii) considering only the diagonal coefficients of the matrix and neglecting the others, the so-called "localized nonlinear approximation", corresponds to the assumption used for inclusions in effective medium models [Maxwell-Garnett, 1904].

[24] In the presentation of the results, one defines the bulk conductivity as the conductivity of an equivalent homogeneous material to generate the same external effect as is seen from the heterogeneous material.

3. Modeling Using the Finite Difference Method

[25] The finite difference (FD) approximation can be used to model the response of direct current (DC) measurements to 3D conductivity distribution of the ground [Dey and Morrison, 1979]. FD is widely used in physical properties modeling because it generally allows both sufficient accuracy (typically 5%) and speed of the calculation. Then, several authors have changed the original algorithm in order to increase its accuracy—for example with more appropriate boundary conditions [Zhang et al., 1995]—or to decrease the time calculation—with adequate linear system solving [Zhang et al., 1995; Spitzer, 1995].

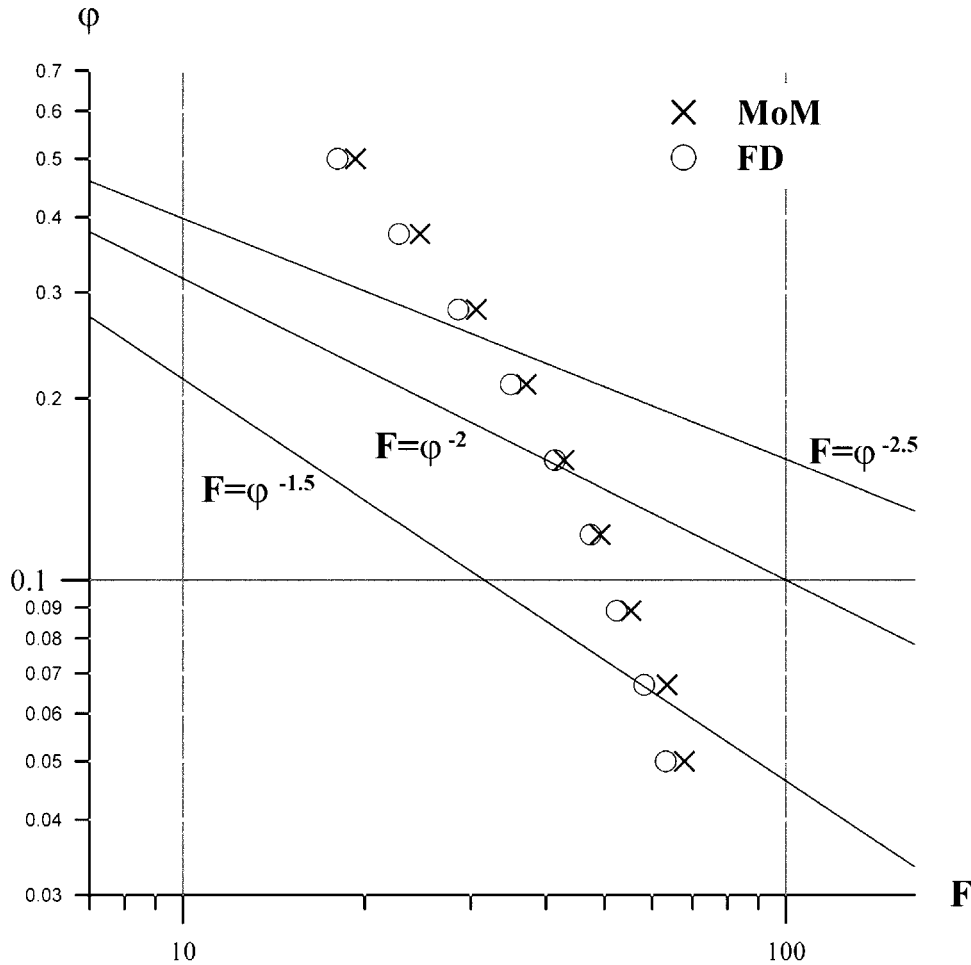


Figure 3. Relationship between formation factor and porosity for elongated volumes of water, MoM calculation (crosses), FD calculation (circles).

[26] The DC forward problem consists in solving the following equation:

$$\nabla \cdot (\sigma(\mathbf{r})\nabla U(\mathbf{r})) = I\delta(\mathbf{r} - \mathbf{r}_S) \quad (15)$$

where σ is the conductivity distribution, U the potential function, I the intensity of the source and \mathbf{r}_S the source location.

[27] Our 3D modeling algorithm, based on the FD approximation, used the Dey and Morrison grid geometry. With this scheme of discretization, the equation is transformed in the following linear system:

$$\mathbf{C} \cdot \mathbf{v} = \mathbf{i} \quad (16)$$

where \mathbf{C} is the capacitance matrix, \mathbf{v} the vector containing the potential at the nodes and \mathbf{i} the source vector. The \mathbf{C} matrix is a sparse matrix, which only contains 7 nonzero terms in a row. The terms of the \mathbf{C} matrix only depend on the grid geometry and on the conductivity distribution.

[28] This fact allows the use of a very efficient way of storage called row-indexed compact storage [Press et al., 1992]. Moreover, to solve the system, the conjugate gra-

dients or more generally the biconjugate gradients procedure is well adapted. This method consists in the minimization of the function:

$$f(\mathbf{v}) = \frac{1}{2} \mathbf{v}^T \cdot \mathbf{C} \cdot \mathbf{v} - \mathbf{i}^T \cdot \mathbf{v}, \quad (17)$$

where the matrix \mathbf{C} is in general nonsymmetric and nonpositive.

[29] To model bulk conductivity, we consider a cubic volume divided in small elementary cells attributed either to solid or to water. Sources are placed on the whole surface of two sides (left-right, front-back, or top-bottom) of the cubic volume. Then, the potential difference between both sides of the volume is calculated for the homogeneous (rock without water $\rightarrow \Delta U_0$) and heterogeneous (rock with water $\rightarrow \Delta U$) cases.

[30] Thus, we have the following equations:

$$\Delta U_0 = \frac{I \cdot l}{\sigma_0 \cdot S} \quad \text{and} \quad \Delta U = \frac{I \cdot l}{\sigma \cdot S} \quad (18)$$

where l is the side of the cubic volume and S the surface of a side of the cubic volume. Finally, the apparent

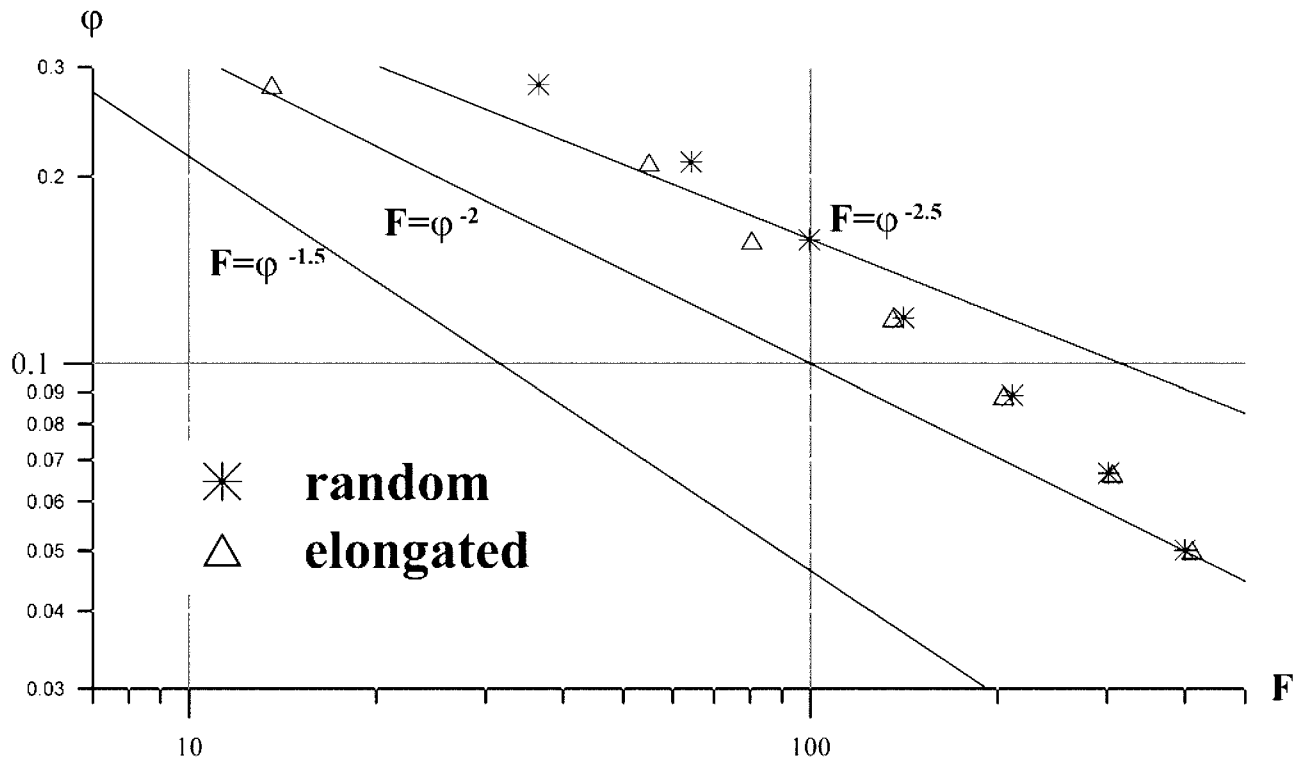


Figure 4. Differences in formation factor values between randomly located water cells and elongated volumes of water (MoM calculations for $\sigma_s = 10^{-11} \text{ S.m}^{-1}$).

conductivity of the cubic volume can be defined by the following term:

$$\sigma = \sigma_0 \frac{\Delta U_0}{\Delta U} \tag{19}$$

4. Clean Rocks

[31] The application of Maxwell-equation based modeling tends toward to answer two questions: (i) are the theoretical results in agreement with experiment based Archie’s law? and (ii) is there any other information that can be obtained from this theoretical approach and that was not already observed in experiments? In order to evaluate the reliability of numerical calculations we compare, when possible, the MoM and FD results. As they correspond to two totally independent principles and numerical processes, the agreement between both confirms the absence of error in numerical codes and the differences that remain between the results sets the limits of numerical approaches.

[32] One considers a two-phase model where solid and water cubic elementary cells are randomly mixed in a cubic volume, the number of water cells being proportional to φ and the number of solid cells to $(1 - \varphi)$. The random character of the elementary cell distribution is achieved by considering the median of 27 different trials of the cell positions. This solution allows to obtain coherent results even with a quite small number of cells. In Figure 1 are presented the MoM results obtained with 343, 1000, 3375 cells for a $10^{-11} \text{ S m}^{-1}$ solid conductivity and a 0.05 S m^{-1}

water conductivity, which respectively correspond to that of a pure silicate mineral and that of a common fresh water in the vadose zone. After this comparison we adopted a 1000 cells volume.

[33] In Figure 2 are presented the results for a 0.05 S m^{-1} water conductivity and a $5 \cdot 10^{-4} \text{ S m}^{-1}$ solid conductivity, this last value was chosen to avoid difficulties generated by too high a resistivity contrast in FD calculations (but a discussion of the best value to consider for solid fraction resistivity is out of the scope of the present paper). Except for high porosities, the agreement between the two calculation methods is good. The curve $\varphi(F)$ present a curvature and its slope decreases as the formation factor increases, this decrease is due to the limitation introduced by the solid resistivity value which limits to 100 the maximum value of F (this limit corresponds to the ratio of 0.05 S m^{-1} water conductivity value over $5 \cdot 10^{-4} \text{ S m}^{-1}$ solid conductivity value). The existence of this curvature, here established from theoretical modeling, merits to be underlined while it would be difficult to obtain experimentally because it is not possible to change the porosity of a rock sample without changing also other parameters (for example, the pore lattice structure). Nevertheless the present results are not in disagreement with Archie’s law, at the two ends of the usual rock porosity range: a 0.21 porosity value corresponds (with the MoM method) to $F = 33$ the exponent is thus -2.28 and for a 0.066 porosity value one has $F = 81$ which corresponds to -1.62 exponent.

[34] To test a different pore arrangement, one considers elongated volumes of water of which length increases as the porosity increases. One first starts with a deal of randomly

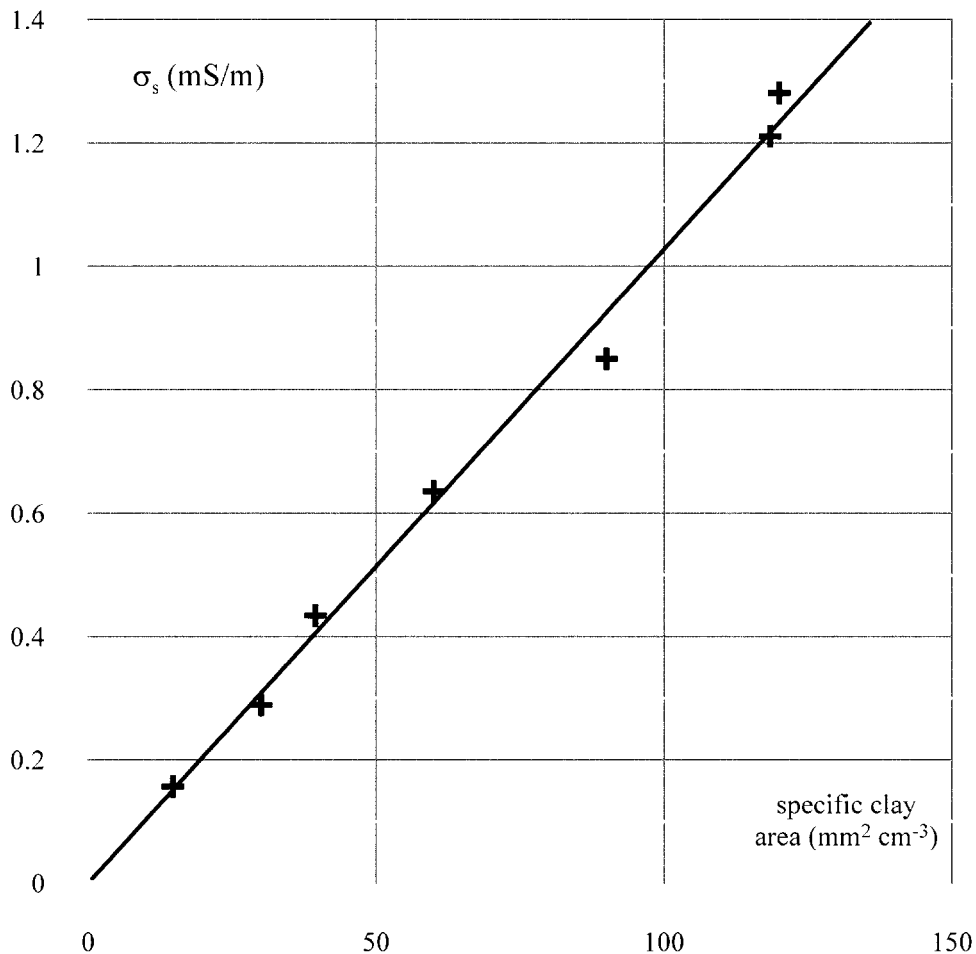


Figure 5. Relationship between surface conductivity and specific clay area for a random distribution of clay platelets inside water volumes (MoM calculation). The line is obtained by a statistical linear regression.

distributed water cells corresponding to $\varphi = 0.05$ and then the porosity was increased by locating other water cells beside them in x, y or z directions where they replace solid cells. In Figure 3 are presented the medians of the results for 27 original trials using MoM (crosses) and FD (circles). The agreement between both methods is here better, for the middle porosity range the values of F is again comprise between $F = \varphi^{-1.5}$ and $F = \varphi^{-2.5}$. The lower values of F may correspond to a better connectivity. When considering the MoM results for a $10^{-11} \text{ S m}^{-1}$ solid conductivity the F values are also slightly different (Figure 4).

[35] The microscopic arrangement of cells do have a non negligible influence over the bulk conductivity even is this effect is more limited than for the relative dielectric permittivity case [Tabbagh *et al.*, 2000].

5. Media With Clay

[36] The presence of clay considerably modifies the bulk conductivity of natural media and thus the interpretation that can be proposed for conductivity data. The clay mineralogy, the clay content and the mode of distribution in the formation have different effects over the conductivity.

They drastically change its in-phase value and generate an out of phase induced polarization response. In this part, we focus on media with clay for which electrical in-phase conductivity follows the empirical addition law (equation (2)) established by *Waxman and Smits* [1968] for shaly reservoir rocks and validated by *Rhoades et al.* [1976] for clayey soils. These media show three features:

1. Clay content is limited, typically lower than 10 wt%.
2. However, the macroscopic conductivity is drastically changed by the presence of clay.
3. Clay is distributed in a dispersed way. In these media, clay exists as small particles inside the pore space between coarser solid grains and/or may adhere and coat sand grains. Therefore, the comparison with empirical addition law is restricted to particular water-solid-clay systems that exist especially in shaly sedimentary rocks and soils.

[37] Considering the particular mode of clay distribution, clay cells are modeled with a special type of cells (which we call platelets hereafter) within the water volumes in MoM method. One dimension (for example w) is small compared the two others (for example u and v). The counter ion displacement being parallel to the (u, v) surface and blocked in the w direction, the electrical conductivity tensor corre-

sponding to these cells have diagonal terms such that $\sigma_w = 0$ and $\sigma_u = \sigma_v = 0.2 \text{ S m}^{-1}$ which is a value commonly used in applied geophysics [Parasnis, 1997].

[38] The location and geometrical arrangement of the clay platelets can be very complex and variable; in the present work, we choose to limit the study to the case where both the orientation and the location of the platelets inside water volume is random, which implies that statistically one third is parallel to x , one third to y and one third to z . Consequently the modeling process is organized with the following steps:

- One fixes the macroporosity at a given value, for example 0.30, and calculates the apparent conductivity, σ_1 , of the cube without clay.

- One places inside water volumes clay platelets with random orientation and arrangement and calculate the new apparent conductivity, σ_2 .

- One deduces the clay contribution to the conductivity, $\sigma_s = \sigma_2 - \sigma_1$.

This process is repeated with different clay contents corresponding to different total platelet surface, in order to get the relationship between σ_s and the specific clay area. This relationship is presented in Figure 5; it is linear, which is in perfect correspondence with the *Waxman and Smits* [1968] empirical law.

6. Conclusion

[39] The approaches developed here to model the relationship between electrical conductivity and water and clay contents are based on numerical solutions of Maxwell's equations written at the microscopic scale. They can take into account: (i) the EM coupling between the different components without assumptions and thus constitute physics-based methods, (ii) the water and clay volumetric distributions and their effect over the bulk electrical conductivity.

[40] The results presented here confirm those of the different other modeling techniques already applied and match empirical laws. Numerical values of the formation factor are, in the middle porosity range, in agreement with Archie's law for the two considered different distributions of water cells. The electrical conductivity due to the clay contribution is shown to be proportional to specific clay area.

[41] In case of clean media, the case where the water phase does not correspond to microscopic isotropic volumes, differs from the case with a random distribution of cubic water volumes, but getting significant information about the microscopic arrangement of water and solid volumes from the macroscopic conductivity will be more difficult than with permittivity.

[42] Considering media with clay, one must emphasized that, even if the present modeling results are in agreement with published experimental results expressed by the empirical addition law, both refers to a particular group of geomaterials, the media where clay content is limited and where clay particles are dispersed inside the pore. The calculations do not take into account overall diversity of water-rock-clay systems and especially the time dependent phenomena. Others compacted clayey media with different clay platelet mineralogy and arrangement inside the pores and with higher clay content could be also studied by the same

numerical tools in future works, but these studies will have to be supported by extensive experimental data sets that do not exist yet.

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