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Rigorous time domain responses of polarizable media II

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Abstract
We present and test in detail with synthetic data a method which may be used to retrieve the parameters describing the induced polarization properties of media which fit the generally accepted frequency dependent formula of Cole and Cole (1941) (CC model). We use time domain data and rigorous formulae obtained from the exact solution of the problem found in a previous note (Caputo, 1996). The observed data considered here are the theoretical responses of the medium to box inputs of given duration in media defined with different parameters; however, as is usually done, only the discharge data are used (Patella *et al.*, 1987). The curve at the beginning of the discharge is studied in some detail. The method is successful in identifying the parameters when the data fit the CC model; if the medium is not exactly of the CC type the method may also help identify how the medium departs from the CC model. The Laplace Transform of the discharge for a box type input data is also given.

Key words *induced polarization – Cole-Cole model – constitutive equations*

1. Introduction

This note, as the title indicates, follows and completes a previous note (Caputo, 1996) investigating a model of induced polarization which, with the introduction of fractional order derivatives in the relation between electric field E and induction D, fits the usually accepted frequency dependent formula of Cole and Cole (1941). The relation is

$$D + \tau^z D^{(z)} = \varepsilon_0 E + \varepsilon_\infty \tau^z E^{(z)} \qquad (1.1)$$

where z is the order of fractional differentiation. The method retrieves the parameters ε_0, ε_∞, τ, z describing the induced polarization phenomena of the medium using time domain observations.

In this note in order to illustrate the method of retrieval of the values of the parameters ε_0, ε_∞, τ, z we shall use the response to a box input of unit amplitude and duration T (Caputo, 1993, 1996)

$$D_{b1}(t) = \varepsilon_\infty + B(\sin \pi z/\pi z) \int_0^\infty (1 - \exp(-u^{1/z} t/\tau)) \cdot du/(u^2 + 2u\cos \pi z + 1) \quad \text{for } 0 < t < T \qquad (1.2)$$

$$D_{b2}(t) = B(\sin \pi z/\pi z) \int_0^\infty (\exp(-u^{1/z}(t-T)/\tau) \cdot du/(u^2 + 2u\cos \pi z + 1) - B(\sin \pi z/\pi z) \cdot \int_0^\infty \exp(-u^{1/z} t/\tau)\, du/(u^2 + 2u\cos \pi z + 1) \quad \text{for } T < t,$$

$$B = \varepsilon_0 - \varepsilon_\infty .$$

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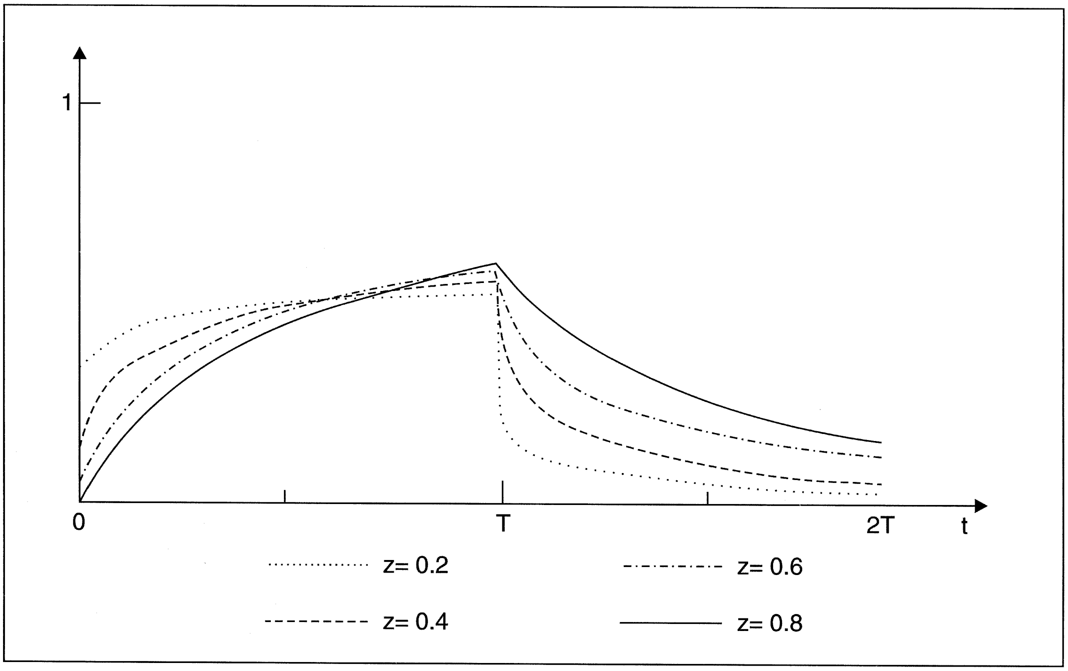

Fig. 1a. Induction in a medium with constitutive eq. (1.1) and caused by a box of unit amplitude and duration T. The time is in units of the relaxation time τ. The curves are for $z = 0.2$ (dotted curve), $z = 0.4$ (dashed curve), $z = 0.6$ (dotted dashed curve), $z = 0.8$ (solid curve). The constant term ε_∞, in the time interval $0 < t < T$, is to be added. The ordinate is in units of $(\varepsilon_0 - \varepsilon_\infty)(\sin \pi z)/\pi z$.

The formula (1.1), used to obtain (1.2), is the time domain equivalent of the CC formula as shown by Caputo and Mainardi (1971) and Pelton *et al.* (1978).

The formulation of Caputo and Mainardi (1971) introduces one more free parameter as factor of D in the left hand member of (1.1) which also discusses the case in which the left hand member of (1.1) is simply $\tau^z D^{(z)}$. In conformity with the literature, however, we use formulation (1.1).

In (1.2) the value of the second integral of $D_{b2}(t)$ is always smaller than the first; in particular, when $T \gg \tau$, this integral is much smaller than the first. However the contribution of this integral reaches its largest value in $t = T$ and may be relevant in the neighbourhood of T. $D_{b1}(t)$ and $D_{b2}(t)$ are shown in fig. 1a for several values of z.

Of interest in the analysis of experimental data are the values of $D_{b2}(t)$ in the neighbourhood of $t = T$. The first integral in $D_{b2}(t)$, in $t = T$ gives B; while the values of the second integral in $t = T$, in units of B, are given in fig. 1b as a function of T/τ, for several values of z. It is verified in fig. 1b that the values of $D_{b2}(t = T)$ may be relevant also when $T \gg \tau$ but only when z is small.

For the knowledge of the theoretical behaviour of $D_{b2}(t)$ in the neighbourhood of T, it is important to compute the derivative of $D_{b2}(t)$ with respect to time.

It is seen in the Appendix that when $0 < z < 1$ the discharge curve is finite, continuous and monotonically decreasing for $t \geq T$ while its time derivative is finite and continuous only for $t > T$. The derivative monotonically decreases when t approaches T; in $t = T$ it is infi-

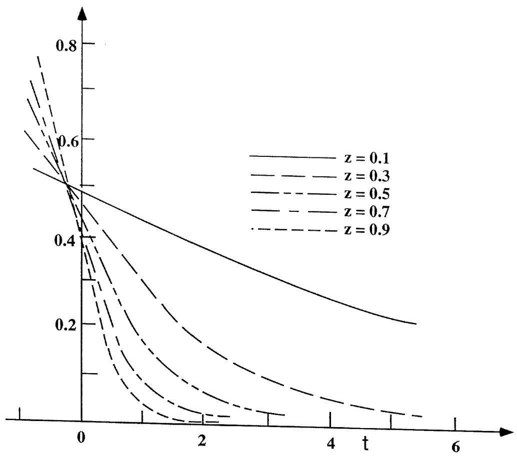

Fig. 1b. Values of the second integral appearing in $D_{b2}(t)$ (formula (1.2)), for $t = T$, as function of T measured in units of the relaxation time τ and for several values of z. In the ordinate the values of the function are given in units of B.

nite. The same applies to the charge curve $D_{b1}(t)$ in the neighbourhood of $t = 0$; the derivative is finite, continuous and monotonically decreases with t for any $t > 0$ but it is infinite for $t = 0$. The discharge curve for $0 < z < 1$ is then tangent to the ordinate axis in $t = T$ while the charge curve is tangent to the ordinate axis in $t = 0$.

When $z > 1$ the time derivative is not infinite in $t = T$ and in $t = 0$.

2. The method

In order to find the values of the parameters B, z, and τ resulting from the fitting of the theoretical curves to the observed ones we must recall that theoretically we have

$$\lim_{t\to\infty} D_{b1}(t) = \varepsilon_0, \qquad D_{b1}(\infty) - D_{b1}(0) = B,$$

$$D_{b1}(T) - D_{b2}(T) = \varepsilon_\infty, \qquad D_{b1}(0) = \varepsilon_\infty \tag{2.1}$$

If $T/\tau \gg 1$, which is not difficult to obtain since T is selected by the experimenter, that is when T is sufficiently large to give the asymptotic value of the response to the charge stage, then from the first and the third of (2.1) one may assume that

$$D_{b1}(T) = \varepsilon_0$$

$$D_{b2}(T) = B = \varepsilon_0 - \varepsilon_\infty \tag{2.2}$$

which may be used to control the values obtained from the fitting of the Theoretical Curve (TC) to the Curve of the Observed Data (COD).

In the case when $\varepsilon_\infty = 0$ the discontinuity at $t = T$ concerns only the first order derivative since from (2.1) we obtain $D_{b1}(T) - D_{b2}(T) = \varepsilon_\infty = 0$; moreover $D_{b1}(0) = \varepsilon_\infty = 0$.

In practice, IP experts use the observed data for $t \geq T$ only (Patella *et al.*, 1987); with the same data in the time domain one may retrieve the theoretical values of ε_0, ε_∞, τ, z and B using the following method (Caputo, 1996).

A double set of TC for $z = l\Delta z$ and $\tau = m\Delta\tau$, with l and m integers, is computed from the second of (1.2) for $t \geq T$; the TC are normalized to their maximum value (the initial value $D_{b2}(T_+)$) and the values defining the points of each curve are then stored in the memory of the computer.

At this stage an automatic search is made with the following procedure in order to find which TC has the closest match to the observed one.

For this purpose a point in the grid is selected, $z = l\Delta z$ and $\tau = m\Delta\tau$, and the Mean Square Deviation (MSD) computed between the assumed TC and the curve of the observed data (COD) normalized to its maximum value, the initial value after the end of the box corresponding to $D_{b2}(T_+)$. Then the computer finds which of the 8 possible directions of the grid around the point selected has the largest decrease of the MSD between the TC and the COD curves. The procedure is then automatically repeated untill a relative minimum of the MSD is reached.

One may reasonably increase the number of TC of the set matching the COD by taking into account the experimental errors. In fact one may estimate the Mean Square Error (MSE) of the experimental curve and, during the search of the minimum of the MSD, obtain a number of TC which have MSD ≤ MSE. In principle one should consider as acceptable all the TC which satisfy the relation MSD ≤ MSE.

To obtain a tentative initial value of τ we may approximate the discharge data, normalized to its maximum value, to the simple exponential $C\exp(-(t-T)/\varsigma)$ and assume $\tau = \varsigma$.

When B, z and τ are found then, from the second of (1.2) we compute $D_{b2}(T)$; then the given value of $D_{b1}(T)$, gives ε_∞ which is the discontinuity in $t = T$. The discontinuity in $t = T$ does not affect the fitting to the theoretical curve since the first datum used is with $t = T + \Delta t$.

The method of finding with a guided walk all the theoretical curves with MSD ≤ MSE, compatible with the errors of the data, and tentatively assuming them as physically acceptable (known as the Hedgehog method) has been succesfully applied in geophysics especially in the studies of the Earth's surface waves (*e.g.*, Gasperini and Caputo 1979) where, instead of the 2D space (that of the grid $z = l\Delta z$ and $\tau = m\Delta\tau$), a space with a larger number of dimensions is used where the models of the thickness and velocity of the layers forming the astenosphere and lithosphere are represented. The discussion of the results, in general, is on the set of solutions, the models of the lithosphere and of the asthenosphere, which are compatible with the estimated errors of the data. The problem of non uniqueness of the solution due to the inevitable errors in the data or simply to the inversion is extensively illustrated in the work of Backus and Gilbert (1968) and, more recently, in that of Cook (1997).

The topological non uniqueness of the solutions was verified for the first time by Gasperini and Caputo (1979) when investigating the structure of the crust and upper mantle in the Tyrrhenian Sea using the dispersion of the surface waves; they found two independent sets of acceptable solutions in topologically disconnected regions of the parameter's space.

In our case, this problem is considered for the minimum of the MSD and, therefore, for the possibility that other sets of TC with MSD ≤ MSE exist which belong in a domain of the grid $z = l\Delta z$ and $\tau = m\Delta\tau$ not connected with the domain of the grid already found.

The advantage of the method discussed in this note is that it also discloses the possible cases when the parameters determined are in a point of relative minimum, it is the priviledge of the experimenter, as well documented in Patella *et al.* (1991), to foresee which of the curves selected by the method are the most appropriate to model the medium under study. As we mentioned already the number of acceptable solutions depends on the errors of the data. The larger errors imply a wider range of

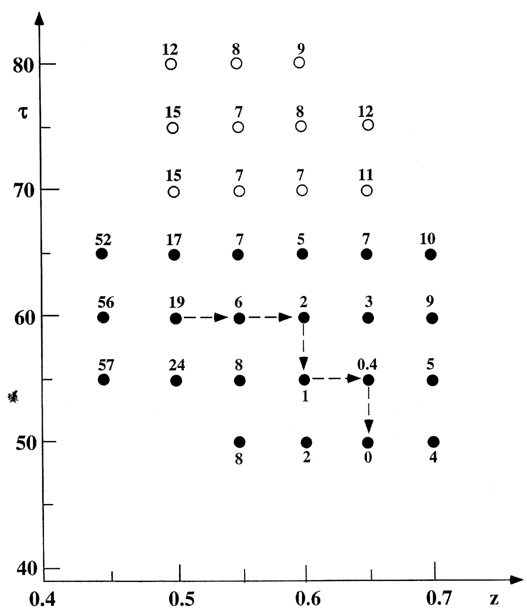

Fig. 2. Guided walk from the initial values of the parameters τ and z towards the values which represent the data. The numbers near the points of the square grid are the Mean Square Deviation (MSD) of the curve defined by the point selected. The MSD is in units of 10^{-4} computed for 8 values of t. Beginning from the curve represented by the point (60, 0.5) it is seen that, of the curves represented by the points of the grid surrounding it, the curve with the least mean square deviation is that represented by the point (60, 0.55). Beginning from the latter point it is seen that, of the curves represented by the points of the grid surrounding it, that with the least MSD is (60, 0.6). Then one goes to the point (55, 0.6), to the point (55, 0.65) and finally to the point (50, 0.65) whose curve has zero MSD.

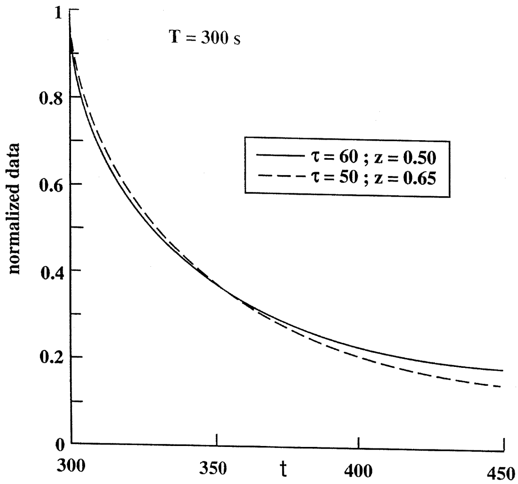

Fig. 3. Curves defined by $\tau = 60$, $z = 0.50$ (solid line) and $\tau = 50$, $z = 0.65$ (dashed line).The decay curves represented by coordinates of the points of fig. 2 along the path indicated by the arrows are located between the two curves presented in the figure. The curves are normalized to their initial value at $t = T$. The time in abscissa is measured in units of the relaxation time τ.

solutions compatible with the data. This fact may not be ignored when performing the inversion (*e.g.*, Backus and Gilbert, 1968; Cook, 1997).

If the input E is not exactly a box and, for instance its rise and decay times are not nil, then formulae (1.2) are not rigorously valid. To take this into account one may then compute analytically the response curve to the actual input obtaining formulae similar to (1.2) and then proceed as previously suggested. In this case however the number of unknowns is larger but the method would still be valid.

Figure 2 gives an example of the retrieval of parameters B, z and τ from the synthetic data obtained from the second of (1.2) assuming $B = 1$, $T = 300$ s, $z = 0.65$ and $\tau = 50$ s; we used steps $\Delta\tau = 5$ s and $\Delta z = 0.05$. The estimate of the tentative initial value of τ is made averaging the values obtained approximating the data with two separate exponentials in the time intervals 0 s, 20 s and 20 s, 100 s respectively, finding the average value $\tau = 60$ s; as initial value of z we assumed 0.5 which is the medium value of the range 0,1 where the value of z is generally found (Cole and Cole, 1941).

The guided walk from the point $z = 0.5$, $\tau = 60$ is seen in fig. 2 which also gives the MSD of the TC, corresponding to the point, relative to the given data. The arrows indicate the path followed along the full circles.

In practice, to be certain that the discontinuity at $t = 300$ s does not influence the fitting, the first datum to use is for $t = 300.001$ s, as was done in this example where, however the ambiguity would not exist since the datum is synthetic. When the values of B, τ and z are known then the value computed for $t = T$, that is $D_{b2}(T_+)$, and $D_{b1}(T_-)$, known experimentally, give ε_∞.

To show the convergence of the method fig. 3 presents two of the curves represented by the

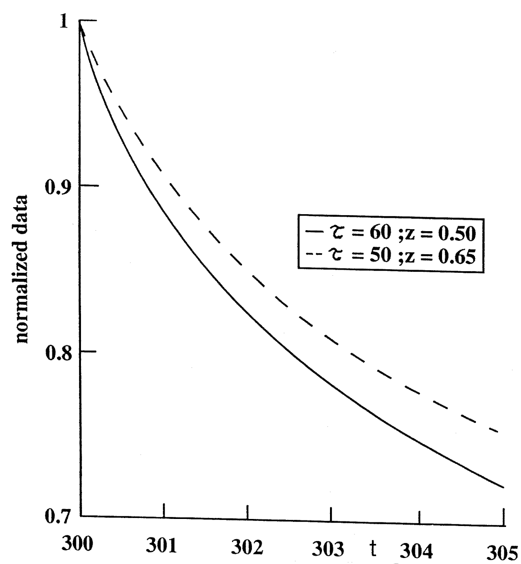

Fig. 4. As in fig. 3 showing the fine structure of the curves near the point $t = T$. The time in the abscissa is in units of the relaxation time. The curves would show graphically that they are tangent to the ordinate axis in $t = T$ only for very small values of the time measured in units of the relaxation time. For $z = 0.1$ one should show the values for $(t - T)/\tau$ smaller than 0.0001.

points in the path indicated by the arrows of fig. 2 normalized to their initial values. Namely, the curves represented by the points (60, 0.55), (60, 0.60), (55, 0.60), (55, 0.65) are located between the curves defined by the points (60, 0.50) (solid) and the curve used to produce the data corresponding to the point (50, 0.65) (dashed), both shown in fig. 3. Figure 4 shows the fine structure of the curves of fig. 3.

As a check we followed another guided walk beginning from the point (75, 0.55) and, as shown in fig. 2, the arrows would now explore other points (those indicated with open circles in fig. 2), but we arrived at the same final point (50, 0.65).

A second example studies the case when the synthetic data are obtained with $z = 0.45$ and $\tau = 75$. The search of the minimum in the plane τ, z is illustrated in fig. 5 which presents near each point the MSD between the TC and the COD curves; there are no other minima than that in the point of the COD curve. In this case, the search is not guided as in the previous case shown in fig. 2 but we have considered all z and τ in a range of possible values. The absolute minimum is in the values used to originate the data $z = 0.45$, $\tau = 75$.

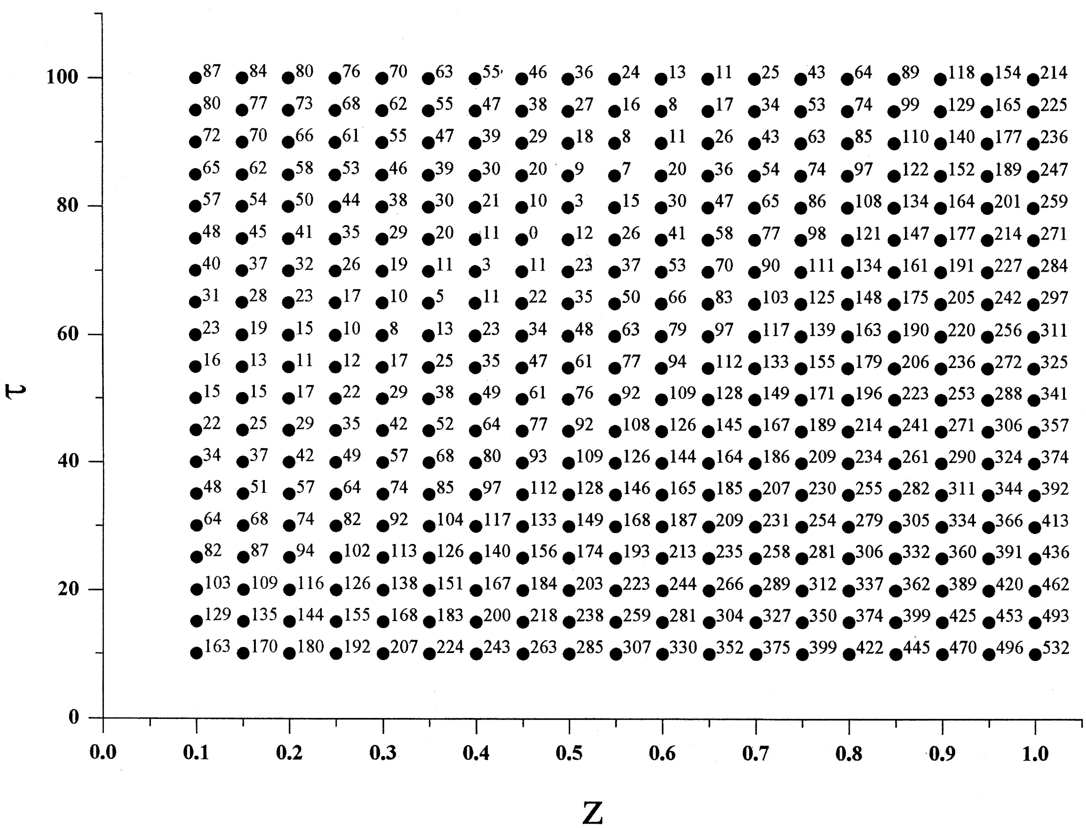

Fig. 5. The MSD of the curves defined by the values of the parameters τ, z are given near each point. In this case the search is not guided as in fig. 2 but we have considered all z and τ in a range of possible values. The absolute minimum is in the values used to originate the data $z = 0.45$, $\tau = 75$. There are no other relative minima. The MSD is in units of 10^{-4} computed for 14 values of t.

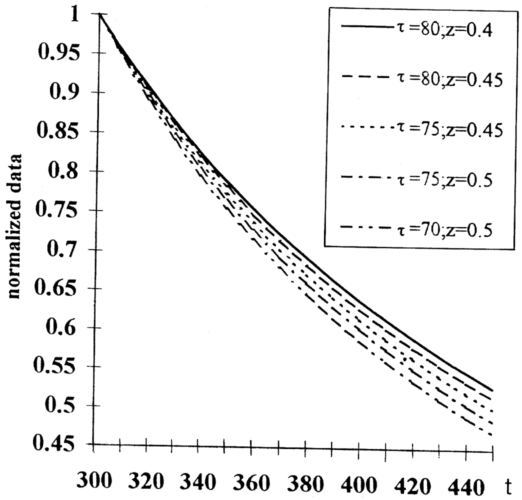

Fig. 6. The synthetic data are obtained with $z = 0.45$ and $\tau = 75$ (dashed line). Some of the 8 curves surrounding that of the synthetic data are so close to others that it is not possible to separate them graphically. However in this specific case all the curves of the set are located between the curves $z = 0.4$, $\tau = 80$ (solid line) and $z = 0.5$, $\tau = 70$ (double dot and dashed line) which give the largest MSD.

The 8 curves corresponding to the points surrounding the point $z = 0.45$, $\tau = 75$ and converging to the COD are shown in fig. 6.

The accuracy of the parameters retrieved from the discharge curves with the method discussed here is of the same order of magnitude as the order of the error of the observations. Concerning the determination of the discontinuity at time $t = T$, the error depends on the resolution of the data. In the case discussed above ($z = 0.45$, $\tau = 75$), when the readings are taken at *ms* intervals near $t = T$, the error in the determination of the discontinuity at $t = T$ is less than 0.001 B.

3. Retrieval of *IP* parameters from frequency data

As we mentioned, the analysis of the relaxation curve $D_{b2}(t)$ is often made in the frequency domain (Patella *et al.*, 1987). In order to use the frequency domain form of $D_{b2}(t)$ we first find its Laplace Transform (LT). Theoretically the LT of the relaxation is obtained from $D_{b2}(t)$ assuming the time origin in $t = T$ and assuming also $t' = t - T$ with $0 \leq t' < \infty$. When $0 < z < 1$ one finds, using the formulae of Caputo (1984),

$$LT(D_{b2}(t')) =$$

$$= LT(B \sin \pi z / \pi z) \int_0^\infty (\exp(-u^{1/z} t'/\tau) +$$

$$-\exp(-u^{1/z}(t' + T)/\tau))\, du/(u^2 + 2u \cos \pi z + 1) =$$

$$= B[p^{z-1}/(\tau^{-z} + p^z) - LT(\sin \pi z/\pi z) \int_0^\infty \cdot \tag{3.1}$$

$$\cdot (\exp(-u^{1/z}(t' + T)/\tau))\, du/(u^2 + 2u \cos \pi z + 1)]$$

where the integral in the last term of (3.1) is a decreasing function of t'. For any given t' the value of the integral is also a decreasing function of time; both decreasing functions are asymptotically nil. Taking into account the contribution represented by the LT of this integral we find

$$LT(D_{b2}(t')) =$$

$$= B[p^{z-1}/(\tau^{-z} + p^z) - (\sin \pi z/\pi z) \int_0^\infty (\exp(-u^{1/z} T/\tau)) \cdot \tag{3.2}$$

$$\cdot du/(p + u^{1/z}/\tau)(u^2 + 2u \cos \pi z + 1)].$$

The expression (3.2) is the LT of the discharge curve in CC media and may be compared with the LT of the experimental discharge curve, for instance the LT of the approximation of the discharge data with three exponentials used by Patella *et al.* (1987). The comparison of the LT of the discharge data with the theoretical LT representation of the CC model, given by (3.2), is another possible path to follow to recognize whether the medium studied is of the CC type. However, in this note, we shall limit ourselves to the study in the time domain which follows and concludes the preceding note (Caputo, 1996).

4. Conclusions

The new method to retrieve CC parameters from the time domain observation using to the Discharge Data (DD) of a box-like input was here tested with synthetic data and shown to be applicable to synthetic data and therefore to a variety of substances of the type of CC.

The method determines the set of parameters of the CC formula which represents the DD with the minimum MSD from the data; given the accuracy of the DD, the method also determines sets of parameters, whose MSD is smaller or equal to the MSE of the DD, which are physically compatible with the given DD.

These sets of parameters surround the point which gives the minimum standard deviation from the data. With reference to fig. 2, if the minimum standard deviation of the data were to render acceptable the curves with MSD < 10^{-4}, then among the sets of the physically acceptable parameters, is also that represented by the point (50, 0.65) to be considered with the associated values of ε_0 and ε_∞.

The method then discusses the variety of sets of parameters which represent the IP phenomenon of a medium which obeys the CC formula.

It is also verified in the examples given that the percentual variation of z gives a much larger variation of the MSD than the corresponding variation in τ.

In the retrieval of the CC parameters using the frequency domain data, the accuracy of the inversion decreases with decreasing width of the range covered by the experimental values used. Then, since the range of frequencies used in the complex-resistivity frequency method, in the laboratory and field experiments, is necessarily limited, the accuracy of the CC parameters obtained with the frequency domain data is also limited accordingly.

However, the time domain data also have limits due to the sampling rate and the truncation at the end of the registration.

The truncation limits the lowest frequency identifiable and the resolution of the spectrum; these limitations, however, may be reduced almost at will provided the record is sufficiently long.

The sampling rate limits the highest frequency identifiable in the spectrum; this limitation, due to the sampling capability of the equipment used for the registration, with the instrumentation currently available may be a problem only in extreme cases.

As a final comment, we note that when the values of z and τ are very small, the variation of the values of CC formula, as a function of the frequency, is very small which limits the accuracy of the determination of the CC parameters; then the complex resistivity frequency domain method introduced by Van Voorhis *et al.* (1973), used to retrieve the set of parameters of CC formula, would not give as accurate results as the time domain methods (Pelton *et al.*, 1978; Patella *et al.*, 1987; Caputo 1996).

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Appendix

The derivative with respect to t of the response to a box charge of duration T, for $0 < t < T$, is

$$D'_{b1}(t) = B(\sin \pi z / \pi z) \int_0^\infty (u^{1/z}/\tau) \exp(-u^{1/z} t/\tau)\, du/(u^2 + 2u \cos \pi z + 1) \tag{A.1}$$

which is positive, finite, continuous and monotonically decreasing with t for any $t > 0$ and for any value of $z > 0$. For $t = 0$ it is

$$D'_{b1}(t) = B(\sin \pi z/\pi z) \int_0^\infty (-u^{1/z}/\tau)\, du/(u^2 + 2u \cos \pi z + 1)$$

which diverges when $0 < z < 1$ and converges for $z > 1$.
The derivative with respect to t of the discharge curve $D_{b2}(t)$, for $T < t$ is

$$D'_{b2}(t) = B(\sin \pi z / \pi z) \int_0^\infty (-u^{1/z}/\tau) \exp(-u^{1/z}(t - T)/\tau)\, du/(u^2 + 2u \cos \pi z + 1) +$$

$$- B(\sin \pi z/\pi z) \int_0^\infty (-u^{1/z}/\tau) \exp(-u^{1/z} t/\tau)\, du/(u^2 + 2u \cos \pi z + 1)$$

and with $t = T + s$ we find

$$D'_{b2}(t) = B(\sin \pi z / \pi z) \int_0^\infty (-u^{1/z}/\tau) \exp(-u^{1/z} s/\tau)(1 - \exp(-u^{1/z} T/\tau))\, du/(u^2 + 2u \cos \pi z + 1)$$

which is negative, continuous and monotonically increases with s for any $s > 0$ ($t > T$) and for any $z > 0$. For $s = 0$ ($t = T$) it is

$$D'_{b2}(t) = B(\sin \pi z/\pi z) \int_0^\infty (-u^{1/z}/\tau)(1 - \exp(-u^{1/z} T/\tau))\, du / (u^2 + 2u \cos \pi z + 1)$$

which diverges for $0 < z < 1$ and converges for $z > 1$.