LINKING SOIL PROPERTIES TO PERMITTIVITY DATA: BEYOND THE REFRACTIVE INDEX MODEL

ALESSANDRO BROVELLI[1] AND GIORGIO CASSIANI[2]

[1] *Dipartimento di Scienze dell'Ambiente e del Territorio, University of Milano-Bicocca, P.zza della Scienza 1, 20126 Milano, Italy.*

[2] *Dipartimento di Scienze Geologiche e Geotecnologie, University of Milano-Bicocca, P.zza della Scienza 4, 20126 Milano, Italy.*

ABSTRACT

The availability of reliable constitutive models linking the bulk electric properties of porous media to their inner structure is a key requirement for useful quantitative applications of non invasive methods. In this paper we focus on the use of dielectric measurements for (time-lapse) monitoring of fluid saturation changes in porous materials, e.g. via Time Domain Reflectometry (TDR) or ground penetrating radar (GPR). A number of empirical, semi-empirical and theoretical relationships have been proposed, linking the bulk dielectric constant with volumetric water content. Among the most popular are mixing models that involve some form of weighted average of the dielectric constants of the components. One such model, named CRIM (complex refractive index model) has found extensive application in recent years. In this paper we first analyze the characteristics of the CRIM by means of theoretical considerations. Next, we use pore-scale modelling and experimental results to show other characteristics of the CRIM, and in particular the dependence of its parameters on dielectric properties of the components, as well as on porosity. We then proceed to assess the robustness of the identification of CRIM parameters in presence of synthetic data error, concluding that CRIM parameters cannot, in general, be independently identified on the basis of bulk dielectric constant versus moisture content data. A novel theoretical model for the dielectric response of saturated porous media is proposed in the second section. The new constitutive relationship incorporates the theoretical link with Archie's law as well as a combination of the well established Hashin and Shtrikman bounds. The proposed model is shown to be able to match both experimental and pore-scale modelling data with no use of ad-hoc fitting parameters.

1. INTRODUCTION

The development of reliable models for the prediction of effective porous media permittivity is a task of great importance in geophysics. In the recent years, electromagnetic methods, such as ground penetrating radar (GPR), time domain reflectometry (TDR) and electrical resistivity tomography (ERT) have been adopted for a large number of applications, ranging from the study of contaminated soils, to hydrogeology, civil engineering, etc (for reviews see e.g. Rubin and Hubbard, 2005; Vereecken et al., 2006). The main advantage of such tools is that they allow fast, field-scale and non invasive surveys. One of the limitations is the lack of general constitutive relationships, that are required to translate the measured data into useful subsurface information, such as moisture content, solute concentration, petrophysical and geotechnical properties of the porous medium, etc.

Most of the existing models are based on the assumption of a simple geometry of the porous medium, such as the assumption of grains with a simple, well-defined shape (spherical, ellipsoidal, plate-like, etc.), while a number of other relationships involve some fitting parameters which are not easily and clearly related to the micro-geometrical properties of the medium (e.g. Guèguen and Palciauskas, 1994; Chelidze and Gueguen,1999).

2. THE CRIM EQUATION: PARAMETER ESTIMATION AND SENSITIVITY

In hydrogeophysics, large application has found in the recent years the complex refractive index model (CRIM) (Roth et al., 1990), a weighted average of the permittivity of the phases composing the medium. For a three-phase porous medium, the CRIM equation reads

$$\varepsilon_b^\alpha = (1-\phi)\varepsilon_s^\alpha + \theta\varepsilon_w^\alpha + (\phi-\theta)\varepsilon_n^\alpha \tag{1}$$

where ε_b is the effective (bulk) permittivity of the medium, ε_s, ε_w, ε_n are the permittivities of the solid matrix, the aqueous phase and the non-aqueous (NAPL) phase, respectively, ϕ is the porosity, θ the volumetric moisture content. Conversion of field bulk permittivity data into the relevant information (e.g. water content) usually requires the calibration of both the matrix permittivity and the exponent α. The matrix permittivity depends on the mineralogical composition of the solid grains and is usually found around 5 for silica sands with a low content of clay and organic carbon, while the exponent α is not easily related to the soil properties; it is usually set equal to 0.5 or is treated as a fitting parameter. Several studies, both theoretical (Birchak et al.,1974; Zackri et al. 1998) and experimental (Dobson et al., 1985; Roth at al. 1990; Jacobsen and Schjonning, 1995; Persson and Berndtsson, 2002; Ajo-Franklin et al., 2004) investigate the physical meaning of α and the values this parameter may assume in natural porous media. A general conclusion is that a constant value close to 0.5 appears to be suitable for a two-phase system (water saturated media), while α varies in the range 0.3-0.7 in porous media containing three or more phases (water, NAPL, etc.).

2.1 Theoretical considerations and pore-scale modelling

Archie's law (Archie, 1942) is a semi-empirical relationship that describes the electrical conductivity of porous media with a non-conductive solid matrix:

$$\sigma_b = \frac{\sigma_w}{F} = \frac{\sigma_w}{\phi^{-m}} \tag{2}$$

where σ_b, σ_w are the bulk and the water electrical conductivity, respectively, F is the formation factor and *m* is Archie's cementation exponent, which depends only on the micro-geometrical properties of the porous medium (e.g. connectivity, tortuosity, etc.).

Due to the formal analogy between the governing equations, the dielectric constant ε in the high frequency limit and the electrical conductivity σ are equivalent (e.g. Guèguen and Palciauskas, 1994); consequently, Archie's law may be used to compute the bulk permittivity of a saturated medium in the situation of negligible matrix permittivity.

For a fully saturated porous medium ($\phi = \theta$), eq. (1) reduces to

$$\varepsilon_b^\alpha = (1-\phi)\varepsilon_s^\alpha + \phi\varepsilon_w^\alpha \tag{3}$$

and from the above considerations, equating eq. (2) and eq. (3) it is possible to link the CRIM relationship to Archie's law, obtaining (Brovelli and Cassiani, submitted):

$$\frac{\sigma_b}{\sigma_w} = \phi^m = \phi^{1/\alpha} = \left(\frac{\varepsilon_b}{\varepsilon_w}\right)_{\varepsilon_s=0} \tag{4}$$

the CRIM exponent α is equivalent to m^{-1} in the zero matrix permittivity condition; thus the parameter α depends on the porous medium microstructure. Hence we can conclude that in general α is not a constant (e.g. equal to 0.5) but should be related to the structural properties of the porous medium (Brovelli and Cassiani, submitted).

Next, we studied the possible dependence of the parameter α on the matrix permittivity. Brovelli et al., (2005) presented a pore-scale model developed to compute the bulk electrical properties (conductivity and permittivity) of porous media. The model solves numerically the electrical continuity equation within a digital representation of a porous medium. Each digital sample is composed by a solid matrix, an aqueous phase and possibly a non-aqueous phase. Further details on the approach and model validation can be found in the literature (Brovelli et al., 2005, Dalla et al., 2004). Bulk permittivity values of a simulated random packing of spheres were computed, using matrix permittivity values in the range 1-80. The medium porosity was 0.39 and water permittivity was set equal to 80.

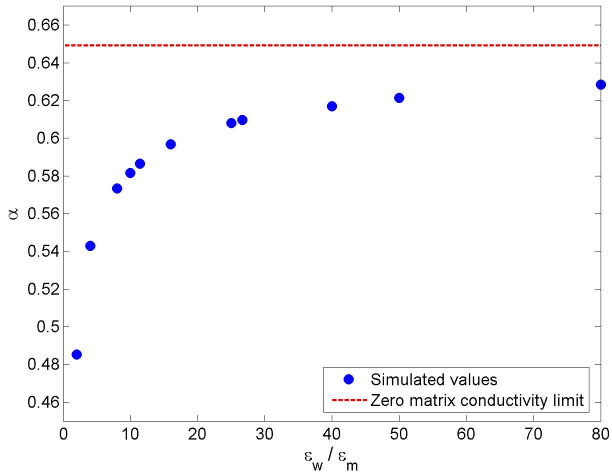

FIGURE 1. Dependence of the exponent α on the matrix permittivity.

Figure 1 reports the simulated results, together with the theoretical limit $\alpha = m^{-1}$. The value of m was independently computed from electrical conductivity simulations on the same packing. A clear dependence of α on the matrix permittivity can be observed; once again we have a clear indication that the CRIM exponent is not constant, but varies as a function of both the structure of the porous medium and the permittivity of the phases.

2.2 Parameter correlation

Following the results obtained in the previous section, we studied the robustness of the regression analysis used to estimate the couple of parameter (α, ε_s). The following procedure was adopted (e.g. Cassiani et al., 2005):

1. A synthetic dataset is generated using the CRIM.
2. Gaussian random error is added to the data.
3. A new couple (α^e, ε_s^e) is estimated, via least-square regression analysis.
4. An approximated confidence interval is computed using the following formula (Draper and Smith, 1998):

$$S(\alpha, \varepsilon_s) = S(\hat{\alpha}, \hat{\varepsilon}_s)\left\{1 + \frac{2}{n-2} F(2, n-2, 1-\beta)\right\} \tag{5}$$

where β is an arbitrary confidence level, chosen as 5% for this study. S is the sum-of squares error objective function, n is the number of observation points (number of data in the synthetic dataset, i.e. number of different saturation values), F(.) is the Fisher distribution function.

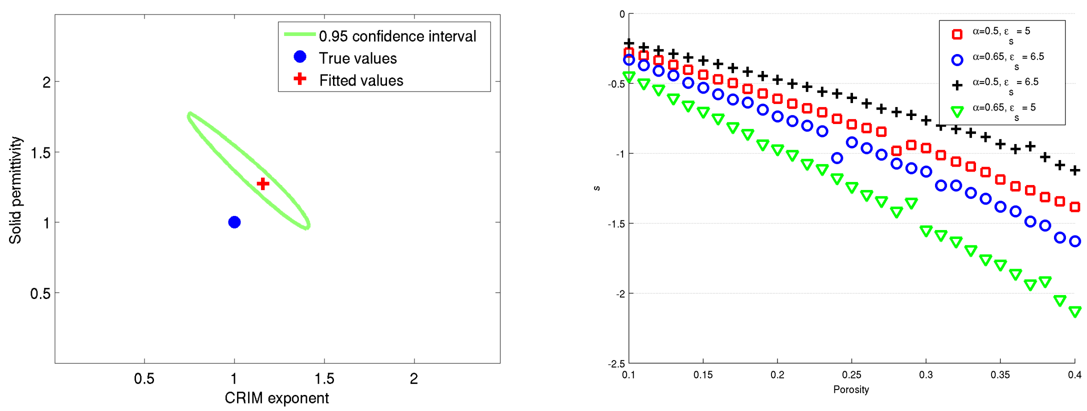

FIGURE 2. Robustness of the regression analysis. (a) The true and estimated parameters (α, ε_s) and the confidence ellipse (b) the correlation index *s* as a function of porosity. Note that *s* = -1 means perfect inverse correlation between the parameters.

A possible index for the parameter correlation can be computed from the slope *s* of a line fitted on the confidence contour (Cassiani et al., 2005): a value of $|s| = 1$ indicates perfect correlation, while as $|s| \to 0$ or $|s| \to \infty$ the parameters are becoming completely independent. We studied the parameter correlation as a function of porosity using 4 different initial couples of parameters (α, ε_s); for each value of porosity 50 different synthetic datasets were generated, and the mean value of the correlation index was computed. Results are reported in fig. 2; on the left side, a typical confidence contour is shown, having the shape of an elongated ellipsoid. On the right side of fig. 2 the correlation index *s* is reported. It can be easily observed that high or complete inverse correlation exists between the parameters in the whole porosity range. We can then conclude that matrix permittivity and exponent α can not be independently estimated.

3. DEVELOPMENT AND VALIDATION OF A NEW CONSTITUTIVE LAW

From the foregoing discussion, we have concluded that the CRIM equation does not allow to independently identify the key parameters (α, ε_s); moreover, the exponent α depends on both the medium geometry and the phase permittivities, but the relationship is not identifiable. In this section we develop a new constitutive equation that ideally should (1) be physically based and (2) contains only parameters that can be independently identified.

The Hashin-Shtrikman (HS) bounds (Hashin and Shtrikman, 1962) are exact bounds for the transport properties of granular media, developed using a variational approach. The general formulation of the HS bounds for a two-phase medium is

$$\varepsilon_{HS} = \varepsilon_1 + \frac{\phi}{(\varepsilon_2 - \varepsilon_1)^{-1} + \frac{1-\phi}{3\varepsilon_1}} \tag{6}$$

where ε_1, ε_2 are the phase permittivities. Equation 6 is an upper bound for permittivity in the case $\varepsilon_1 > \varepsilon_2$, while it is a lower bound if $\varepsilon_1 < \varepsilon_2$. Once ε_1, ε_2 are fixed, the 'true' bulk conductivity is somewhere between the upper (*HSU*) and lower (*HSL*) bound, and thus can be computed from a linear combination of the above bounds,

$$\varepsilon_b = \varphi\varepsilon_{HSU} + (1-\varphi)\varepsilon_{HSL} \tag{7}$$

where φ is a weight that can be derived using Archie's law (eq. 2) as an additional constrain, obtaining,

$$\varphi = \frac{\varepsilon_w}{\varepsilon_{HSU}\phi^{-m}} \tag{8}$$

Rearranging eq. (7) and eq. (8), the final form of the new constitutive law reads:

$$\varepsilon_b = \frac{\varepsilon_w}{\phi^{-m}} + \varepsilon_{HSL} - \frac{\varepsilon_{HSL}}{\varepsilon_{HSU}}\frac{\varepsilon_w}{\phi^{-m}} \tag{9}$$

A more detailed description of how eq. (9) is recovered can be found in Brovelli and Cassiani, (submitted), together with a wider discussion on the properties of the permittivity bounds.

3.1 Validation with simulated and experimental data

The proposed relationship was validated using permittivity simulations conducted with the pore-scale model presented by Brovelli et al., (2005); all the sphere packing parameters (porosity, cementation factor) were independently computed. Figure 3b reports the comparison; the new law agrees well with the simulations.

Following successful validation with simulated data, we compared eq. (9) with experimental measurements reported in the literature. Sen et al., (1981) presents bulk permittivity measurements on glass beads as a function of porosity for three different fluids (water, air, methanol) having different permittivities. Both the solid matrix permittivity and the cementation factor were independently measured (fig. 4a).

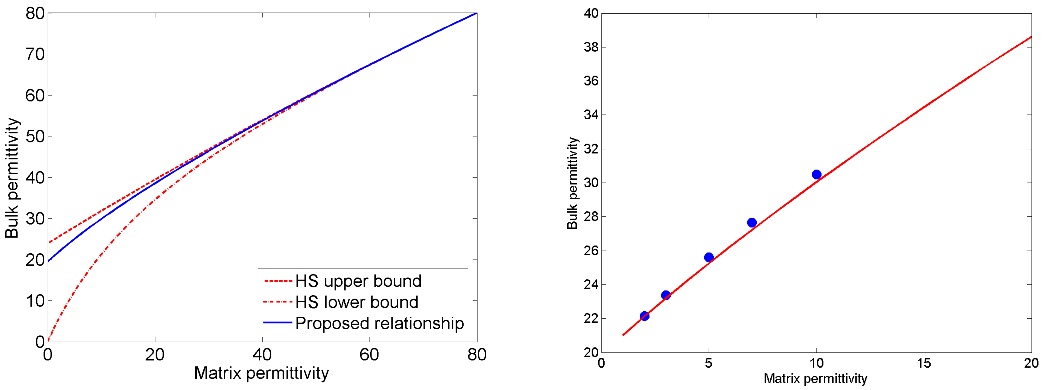

FIGURE 3. On the left side Hashin-Shtrikman bounds (red dashed lines) and the proposed relationship, eq. (9) (solid blue line). On the right side, the new constitutive law (red line) compared with simulated results (blue dots).

The second dataset we used (Robinson and Friedman, 2003) reports bulk permittivities for several natural porous media, measured using saturating fluids with different dielectric constant. The solid matrix permittivity was independently measured as well as the porosity, but the actual value of the Archie cementation factor is unknown and was calibrated fitting eq. (9) on the data. Results and comparison with this second dataset are reported in fig. 5b.

The proposed constitutive law shows an excellent agreement with both datasets; particularly, the shape of the function closely reproduces the observed behaviours, even without any tuneable parameter. Moreover, the estimated values for the cementation factor perfectly stay within the ranges reported for natural porous media (e.g. Rubin and Hubbard, 2005, tab 4.1).

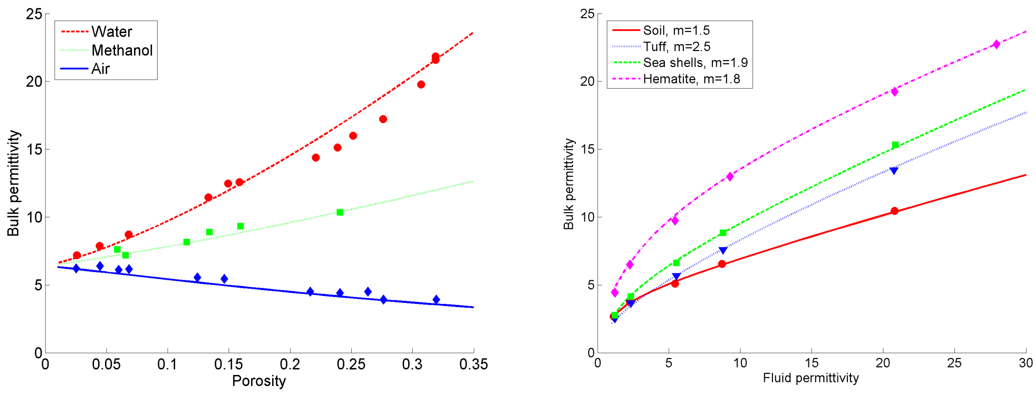

FIGURE 4. (a) Comparison with the experimental dataset by Sen et al., (1981). The cementation factor is independently measured. (b) Comparison with the Robinson and Friedman, (2003) data. The cementation factor is estimated.

4. CONCLUSIONS

In this paper we have first analyzed the characteristics of a classical mixing model for bulk permittivity of multiphase media, usually referred to as CRIM. As a result of the analysis above, we drew some general conclusions:

The two key CRIM parameters (α, ε_s) are inversely correlated. This results from the shape of the confidence interval, which is an elongated ellipsoid with axes not parallel to the (α, ε_s) axes.

The exponent α is a function of both the geometrical properties of the porous medium, being linked to Archie's cementation exponent *m*, as well as the ratio between the matrix and fluid phase permittivities.

The CRIM model is therefore satisfactory neither in terms of parameter meaning nor as a purely empirical tool to represent laboratory data.

Next, we developed an alternative constitutive model that is physically based and involves only parameters that can be easily measured independently. The physical basis of the model rests upon the Hashin and Shtrikman, (1962) lower and upper bounds for bulk permittivity. These bounds are combined in a weighted average, with a weighting coefficient that is physically linked to Archie's cementation exponent, for which it is possible to derive independent estimates, e.g. via DC resistivity measurements. The novel model compares in an excellent manner against both pore scale modeling tests and experimental results. If Archie's exponent *m* is known from other sources, the new model is totally defined, i.e. there is no fitting parameter, and it still can fit experimental data in an excellent manner.

Some theoretical aspects of the proposed model have not been fully investigated to date; particularly, the weighting factor is derived in the zero matrix permittivity limit, and thus the actual formulation of the weight is independent from the matrix conductivity. However the excellent capability of the proposed model to reproduce both pore scale modeling results and actual laboratory data with no need for fitting parameters warrants attention and should lead to further research to tackle the unresolved issues.

5. ACKNOWLEDGEMENTS

This work was partly supported by the Consorzio Interuniversitario CINECA and by the Italian Ministry of Education, University and Research (MIUR) FIRB grant RBAU01TAL5. The authors would like to acknowledge D. A. Robinson for providing some of the experimental datasets.

REFERENCES

Archie, G. E., (1942) The electrical resistivity log as an aid in determining some reservoir characteristics, Trans. Amer. Inst. Mining Metallurgical and Petroleum Engineers, 146, 54-62.

Birchak, J. R., C. G. Gardner, J. E. Hipp, and J. M. Victor (1974), High dielectric constant microwave probes for sensing soil moisture. Proceedings of the IEEE, Vol. 62, N. 1, 93-98.

Brovelli, A., G. Cassiani, E. Dalla, F. Bergamini, and D. Pitea (2005), Electrical properties of partially saturated sandstones: Novel computational approach with hydrogeophysical applications, Water Resour. Res., 41, W08411, doi:10.1029/2004WR003628.

Brovelli, A. and G. Cassiani, Effective permittivity of porous media: a critical analysis of the Complex Refractive Index Model (CRIM) and the development of an alternative law. Submitted to Journal of Geophysical Research – Solid Earth.

Cassiani, G., L. F. Burbery and M. Giustiniani (2005), A note on in situ estimates of sorption using push-pull tests, Water Resour. Res., 41, W03005, doi: 10.1029/2004WR003382.

Chelidze, T. L., and Y. Gueguen (1999a), Electrical spectroscopy of porous rocks: a review. I. Theoretical models. Geophys. J. Int, 137, 1-15.

Dalla, E., G. Cassiani, A. Brovelli, and D. Pitea (2004), Electrical conductivity of unsaturated porous media: Pore-scale model and comparison with laboratory data, (2004) Geophys. Res. Lett., 31, L05609, doi: 10.1029/2003GL019170.

Dobson, M. C., F. T. Ulaby, M. T. Hallikainen, and M. A. El-Rayes (1985) Microwave dielectric behaviour of wet soils, II Dielectric mixing models, IEEE Trans. Geosci. Remote Sens., GE-23, 35-46.

Draper, N. R., and H. Smith (1998), Applied Regression Analysis, 3rd ed., John Wiley, Hoboken, N. J.

Gueguen, Y. and V. Palciauskas (1994), Introduction to the physics of rocks. Princeton University Press

Jacobsen, O.H. and P. Schjonning, (1995) Comparison of TDR calibration function for soil water determination, in Proceeding of the Symposium: Time-Domain Reflectometry applications in soil science, SP Rep. 11, vol. 3, pp 25-33.

Persson, M. and R. Berndtsson (2002) Measuring nonaqueous phase liquid saturation in sil using time domain reflectometry, Water Resour. Res., 38(5), 1064, doi:10.1029/2001WR000523.

Hashin, Z. and S. Shtrikman (1962) A variational approach to the theory of the effective magnetic permeability of multiphase materials, J. App. Phys, 33 (10), 3125-3131

Robinson, D. A. and S. P. Friedman (2003), A method for measuring the solid particle permittivity or electrical conductivity of rocks, sediments, and granular materials. J. Geophys. Res., 108(B2), 2076, doi: 10.1029/2001JB000691.

Roth, K., R. Schulin, H. Fluher and W. Attinger (1990), Calibration of time domain reflectometry for water content measurement using a composite dielectric approach, Water Resour. Res., Vol. 26, N. 10, 2267-2273.

Rubin, Y., and Hubbard, S.S., Eds., 2005. Hydrogeophysics: Springer.

Sen, P. N., C. Scala and M. H. Cohen(1981) A self-similar model for sedimentary rocks with application to the dielectric constant of fused glass beads, Geophys., Vol. 46, N. 5, 781-795.

Vereecken, H., A.M. Binley, G. Cassiani, A. Revil and K. Titov (eds), 2006, Applied Hydrogeophysics, Springer.

Zakri, T., J.-P. Laurent, and M. Vauclin (1998), Theoretical evidence for 'Lichtenecker's mixture formulae' based on effective medium theory. J. Phys. D: Appl. Phys., 31, 1589-1594.