Int. Agrophysics, 2004, 18, 181-187

INTERNATIONAL
**Agrophysics**
www.ipan.lublin.pl/int-agrophysics

# Effect of aggregate size on the water content estimated with time domain reflectance (TDR)

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*Received February 18, 2004; accepted April 29, 2004*

Abstract. Time domain reflectance (TDR) gives reliable estimates of the water content of structure-less soil. The effect of soil structure on the performance of TDR has received relatively little attention in comparison with the development of new calibration models and also the use of TDR for simultaneously measuring water content and the electrical conductivity of the pore water. In this paper we report on the effect of aggregate size on the reliability of water content determined from TDR measurements. The experiments that we report are relevant to loose seed-beds. We show that as aggregate size increases TDR progressively under-estimates the volumetric water content when a standard calibration function is used. We suggest a simple rule of thumb to avoid large errors in the TDR estimated water content.

Keywords: TDR calibration, aggregated soil

## INTRODUCTION

The work of Topp and colleagues (Topp *et al*., 1980; 1982; 1984; 1996; Topp and Davis, 1985) has led to time domain reflectance (TDR) becoming one of the more important methods that is currently used to measure soil water content. Progress has been made in a number of different aspects related to the use of TDR. This include the development of improved transmission lines (Zegelin *et al*., 1989) and the use of TDR for making simultaneous measurements of water content and pore water electrical conductivity (Dasberg and Dalton, 1985; Dirksen and Dasberg, 1983; Nadler *et al*., 1991). In this paper we will consider the calibration of TDR in aggregated soil. Much effort has been directed into the development of improved calibration functions (Dirksen and Dasberg, 1983; Hilhorst, 2001; Roth *et al*., 1990; Whalley, 1993; White *et al*., 1994; Yu *et al*., 1994). The simplest calibration of TDR is based on the following linear expression:

$$\sqrt{\varepsilon_a} = \theta\left(\sqrt{\varepsilon_{aw}} - 1\right) + \frac{\rho_b}{\rho_s}\left(\sqrt{\varepsilon_{as}} - 1\right) + 1, \qquad (1)$$

where: $\varepsilon_a$ is the dielectric constant estimated from TDR measurement, $\varepsilon_{aw}$ is the apparent dielectric constant of water, $\varepsilon_{as}$ is the apparent dielectric constant of solid particles, $\rho_s$ is the density of solids, $\rho_b$ is bulk density of the soil and $\theta$ is the volumetric water content (Alharthi and Lange, 1987; Annan, 1977; Whalley, 1993; 1994; White *et al*., 1994). The adjective apparent is used to qualify dielectric constant because the travel time measured by TDR instruments cannot simply be used to calculate the real component of the dielectric constant, but if the loss tangent is small ($\tan\delta = \varepsilon''/\varepsilon'$, where $\varepsilon'$ is the real part of the dielectric constant and $\varepsilon''$ is the imaginary part of the dielectric constant) then $\varepsilon_a$ is approximately equal to $\varepsilon'$ (Topp *et al*., 1982; Whalley, 1993; 1994; White *et al*., 1994). Equation (1) provides a simple linear calibration which has parameters which are in principal calculable. In practice the fits to experimental data yield parameters which are different from those that might be expected (Whalley, 1993; White *et al*., 1994). Thus, we may view Eq. (1) as empirical and write it in general terms:

$$\sqrt{\varepsilon_a} = a + b\rho_b + c\theta, \qquad (2)$$

where *a*, *b* and *c* are fitted parameters. Equation (2) can be improved statistically by including additional quadratic parameters to describe bulk density (Malicki *et al*., 1996). Although, many issues related to dielectric constant of moist soil remain to be resolved (Hilhorst *et al*., 2001) the simple ideas that underpin Eq. (1) have led to widespread adoption of simple linear calibrations, which can be used to interpret TDR data (Topp *et al*., 1996).

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The use of TDR in aggregated soil remains a problem that has received little attention. The overwhelming majority of work has focussed on structure-less and often repacked soil. This is perhaps surprising since it is well documented that poor contact between the soil and TDR transmission line can lead to errors in TDR estimated water content (Annan, 1977; Knight, 1969). In this paper we make TDR measurements in soil which consists of different sizes of aggregates. We test the performance of published calibration functions either with published or fitted parameters. A simple calibration that includes aggregate size is presented.

## MATERIALS AND METHODS

An Evesham clay (King, 1969) was used for the experiments reported in this paper. The parent material of this soil is chalky boulder clay. It contains 72.5% clay, 17% silt and 10.5% sand. The soil was chosen because it occurs naturally in stable aggregates. The soil from the field was air dried and then sieved into four size fractions (9.5-5, 5-2.8, 2.8-1.4 and <1.4 mm). The gravimetric water content of air dry soil was similar for each of the fractions and approximately 0.075 g $g^{-1}$. The soil aggregates were divided into 3 sub-samples. Water was added to two of these sub-samples to obtain soil with a gravimetric water content of 0.15 and 0.25 g $g^{-1}$. The wetter soil became plastic and was not used.

To make TDR measurements the soil was packed into a wooden box (24 x 15 x 15 cm) and a three wire transmission line (Zegelin *et al*., 1989) was inserted into the soil through holes in a plastic cover at one end of the box. The transmission line was made from brass rods 3.2 mm in diameter and 9.5 cm long. A Teckronix 1502C cable tester was used to make the TDR measurements. The value of $\sqrt{\varepsilon_a}$ was determined by comparing the transmission time in moist soil with that in water (Roth, 1990). Thus:

$$\sqrt{\varepsilon_a} = \left(\frac{l}{l_w}\right)\sqrt{\varepsilon_{aw}}\ , \tag{3}$$

where: $l$ is in the length of the transmission line measured in moist soil from time delay with TDR and similarly $l_w$ is its length measured in water.

To obtain a range of bulk densities two methods of packing were used to fill the wooden box. For the three larger aggregate sizes (9.5-5, 5-2.8 and 2.8-1.4 mm) the box was either loosely packed or it was filled by tapping the box. The fine fraction (< 1.4 mm) was either filled loosely or it was compressed. The value $\sqrt{\varepsilon_a}$ for each of the treatments (4 aggregate sizes x 2 gravimetric water contents x 2 packing methods) was measured in a random order with at least 4 independent replicates for each treatment. The bulk density and volumetric water content of the soil was determined from the weight of wet soil needed to fill the wooden box.

The data will be used to test different calibration models for predicting the volumetric water content of structured soil with TDR.

## RESULTS AND DISCUSSION

Analysis of variance (using Minitab, 3081 Enterprise Drive, State College, PA16801-3008, USA) showed that packing method, aggregate size and water content all had a significant effect on the bulk density ($p < 0.001$). In addition there was a significant interaction ($p < 0.001$) between packing method and aggregate size on bulk density. The bulk density ranged from 0.85 to 1.22 g $cm^{-3}$. The calibration functions that we used to relate $\sqrt{\varepsilon_a}$ to water content are listed in Table 1. Equations (5) and (7) were used with published coefficients. Equations (6), (8)-(10) where fitted to our experimental data with the Marquardt-Levenberg algorithm. In Fig. 1 fitted (Eqs (6), (8)-(10)) or predicted water content (Eqs (5) and (7)) is plotted against the known water content. In Fig. 2 the mean residual water content $\left(\theta_{\text{TDR}} - \theta_{\text{Known}}\right)$ is plotted against aggregate size.

Table 2 lists the residual sums of squares after applying Eqs (5)-(10) to the measured data. Equation (10) is a significant improvement on the others as seen by the F-test (Table 2). The trends in residuals using Eq. (10) indicate a dependence on s that is almost completely removed by including a term linear in s in Eq. (9) (Fig. 2).

Agreement between model and measured data can also be tested using a lack of fit test LOFIT (Whitmore, 1991:.

$$LOFIT = \frac{\sum_{j=1}^{N} n_j\left(\overline{y_j} - x_j\right)^2}{N} \cdot \frac{\sum_{j=1}^{N} (n_j - 1)}{\sum_{j=1}^{N}\sum_{i=1}^{n_j} \{(y_{ij} - x_j) - (\overline{y_j} - x_j)\}^2}, \tag{4}$$

where: $N$ is the number of occasions on which measurements were made minus the degrees of freedom taken by each model (8, 6, 8, 3, 5, 4 respectively, see Table 3), $n_j$ is the number of replicate measurements made on the jth data set, $x_j$ is the mean of the $i$ replicate measurements made for that set, $y_{ij}$ is each replicate measurement and $x_j$ is the corresponding value given by the model. The smaller this statistic is, the better the model; a value of zero indicates perfect agreement. An F test is used to establish the significance of LOFIT using $N$ and $\Sigma(n_j\text{-}1)$ degrees of freedom for the greater and lesser variances respectively. Even Eq. (10) is found to be significantly different from the data in conventional terms using this test (Table 3). Nonetheless it gave the most satisfactory fit to the data given the variability in the data themselves. Support for this assertion comes from an examination of the likelihood ratios of the models given this set of data (Edwards, 1972). Likelihood overwhelmingly favours Eq. (10).

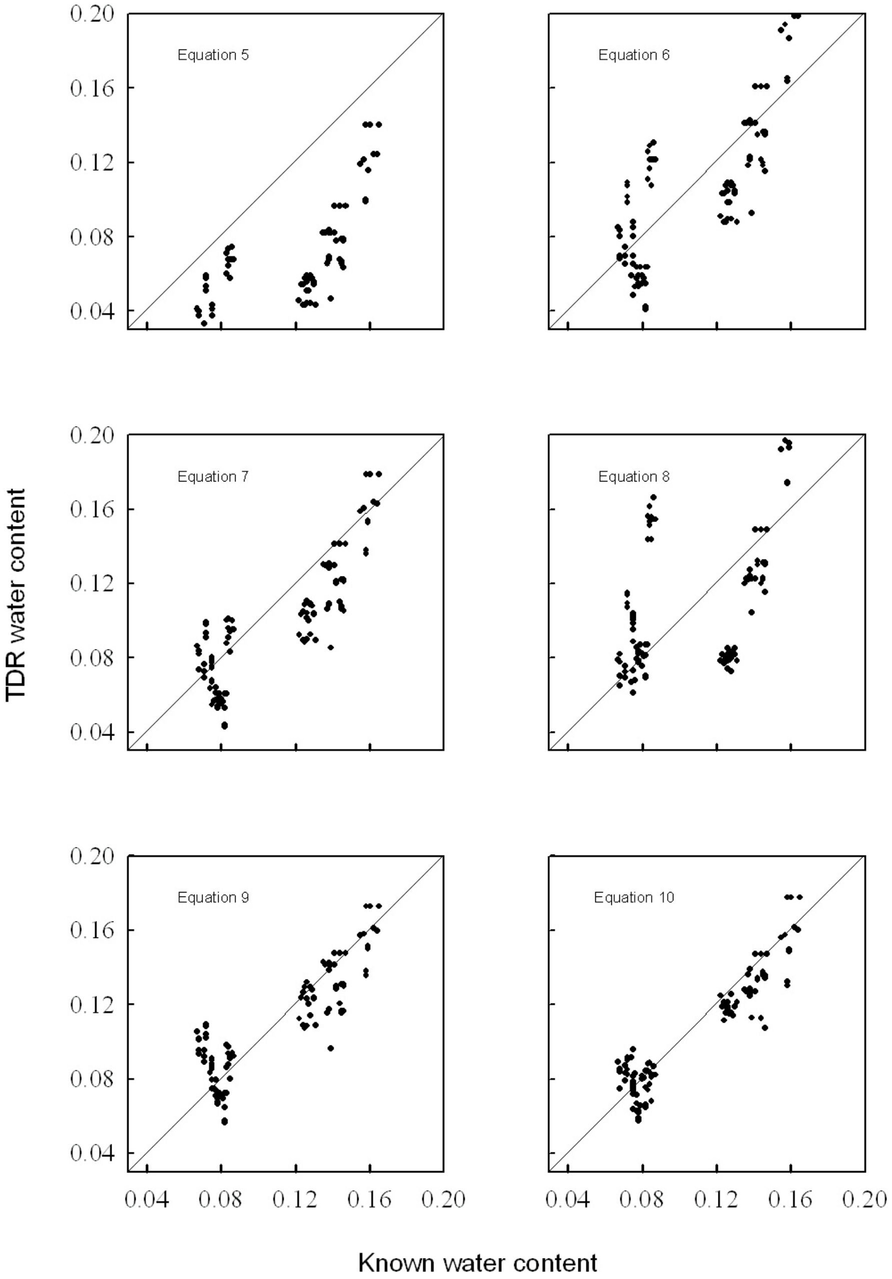
**Table 1.** Calibration functions used to relate $\sqrt{\varepsilon_a}$ to volumetric water content

| Calibration function | Equation No. | Comments |
|---|---|---|
| $\theta = \left(\sqrt{\varepsilon_a} - 1.451\right) / 8.979$ | 5 | White *et al.* (1994) |
| $\theta = \left(\sqrt{\varepsilon_a} - 1.26\right) / 6.59$ | 6 | Same form as Eq. (5) fitted to our experimental data |
| $\theta = \dfrac{\sqrt{\varepsilon_a} - 0.819 - 0.168\rho - 0.159\rho^2}{7.17 - 1.18\rho}$ | 7 | Malicki *et al.* (1996) |
| $\theta = \dfrac{\sqrt{\varepsilon_a} - 5.399 + 8.041\rho - 3.622\rho^2}{17.89 - 9.045\rho}$ | 8 | Same form as Eq. (7) but fitted to our experimental data |
| $\theta = \dfrac{\sqrt{\varepsilon_a} + 0.4365 - 1.357\rho}{9.566}$ | 9 | Inverse of Eq. (2) fitted to our experimental data |
| $\theta = \dfrac{\sqrt{\varepsilon_a} - 0.4631 - 0.8428\rho + 0.04275s}{7.598}$ | 10 | Similar to Eq. (9), but with aggregate size included and fitted to our experimental data |

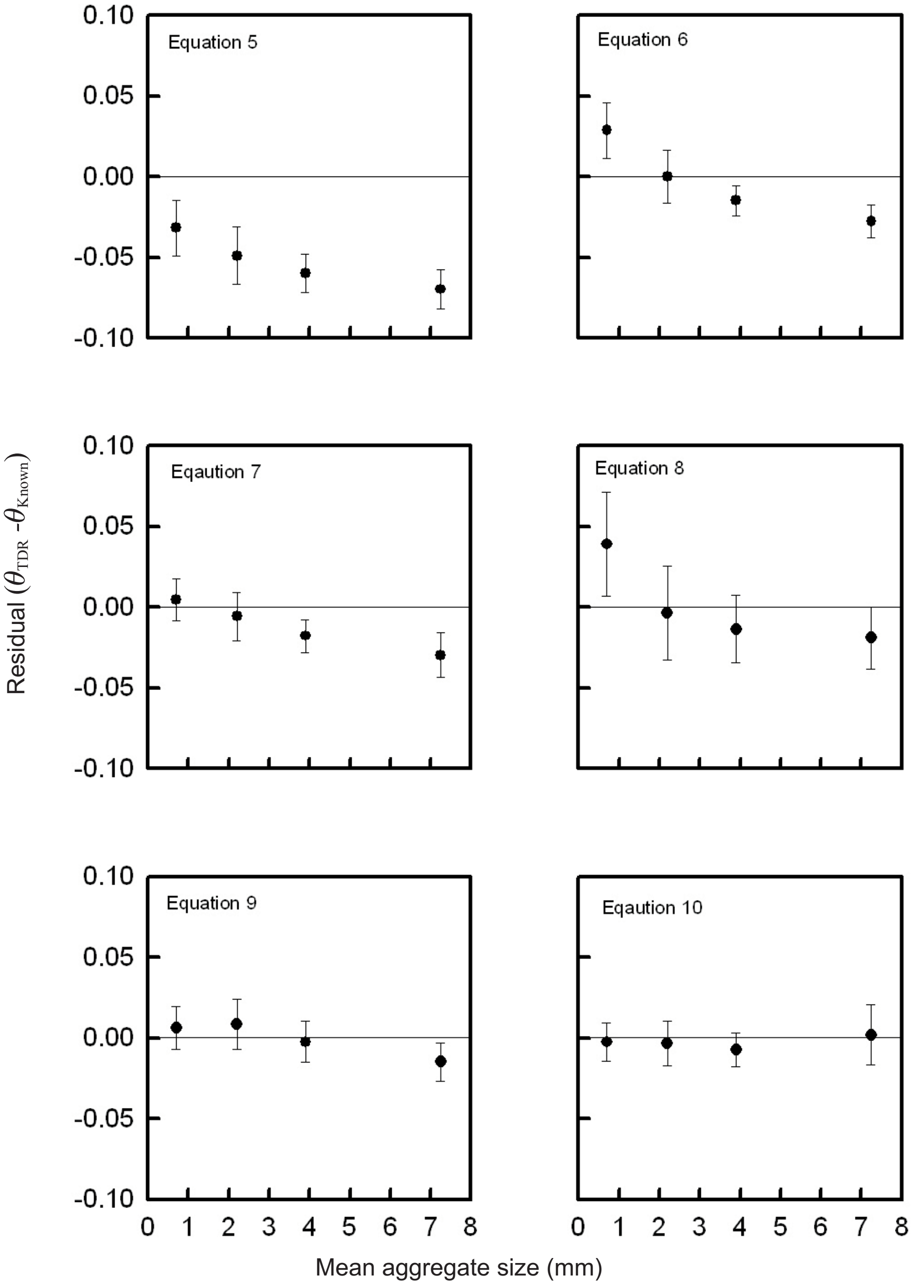
If the calibration function of Topp *et al.* (1980) and White *et al.* (1994) is used then the error in the TDR estimate increases rapidly with aggregate size. We used a linear function (Eq. (5)) with coefficients consistent with the polynomial of White *et al.* (1994). The under-estimate of water content by TDR when aggregate sizes are small is almost certainly due to a high bound water content in the heavy clay soil that we used (Dirksen and Dasberg, 1993). When this calibration function was fitted to the experimental data (Eq. (6)) the residual still showed a strong trend with aggregate size although the mean residual was very small (-0.002 g cm$^{-3}$). The calibration of curve of Malicki *et al.* (1996) (Eq. (7)), when used with their published coefficients, gave good agreement for aggregate sizes smaller than 2.2 mm. There was still a trend to under-estimate water content with increasing aggregate size, but inspection of residuals (Fig. 2) suggests that in this case the published coefficients of Malicki *et al.* (1996) give better results than fitting a simple linear calibration function to experimental data. When the calibration of Malicki *et al.* (1996) was fitted to our experimental data (Eq. (8)), the fitting procedure that we used changed the mean residual from -0.01 to 0.004 g cm$^{-3}$ but the sum of squared residuals increased. It appears that the calibration proposed by Malicki *et al.* (1996) provides a useful field calibration that can take into account some of the effect of aggregate size from considering soil bulk density alone. When a simple function (Eq. (9)) based on a mixing model in which $\sqrt{\varepsilon_a}$ is linear function of both water content and soil bulk density was fitted to our data we obtained a calibration with a relatively small trend in residual with aggregate size. However, including mean aggregate size in the calibration function (Eq. (10)) eliminated the trend in residual with aggregate size. Perhaps the most surprising result is the extent to which including the dry bulk density of soil in the calibration function appears to compensate for the effect of aggregate size.

In most circumstances, the *a priori* knowledge of soil physical characteristics that can be used in TDR calibration functions would at best be limited to bulk density. Inspection of Figs 1 and 2 would suggest that in this case either the calibration of Malicki *et al.* (1996) or the simpler calibration based on a mixing model (Whalley, 1993; White *et al.*, 1994) would be the best calibrations to use. In the absence of soil bulk density data then fitting a linear calibration would be advisable, although it should be recognised that there will be a trend in residuals with aggregate size. The use of a calibration that includes aggregate size as a parameter is not a practical proposition. The experiments that we have conducted in this work may perhaps be considered to be worst case scenarios because our soils were sieved to obtain a relatively narrow size range of aggregates. In a natural seed-bed it is likely that a wide range of aggregates sizes will occur together and even if there are large aggregates present then it will be likely that smaller aggregates will fill the space around the transmission line.

For a continuous gap around the transmission line element (Alharthi, 1987) it was shown that the error in estimating the dielectric constant of the bulk soil was related to the ratio of the radius of the transmission line element to the radius of the continuous gap, as well as the spacing between the transmission line elements. Whalley (1993) found that the theory of Annan (1987) gave reasonable estimates of the effect of a continuous gap on the performance of a 3 wire unbalanced transmission lines when



immersed in water. In this work we used only one size of transmission line element, but it is reasonable to make some general recommendations by comparing the aggregate size with the size of the transmission line element. From inspection of Figs 1 and 2 we suggest as a rule of thumb, that if published calibration functions for TDR are to be used then the aggregate size should be smaller than the radius of the transmission line element. In our work the radius was 1.6 mm and the finest aggregate fraction was less the 1.4 mm. When the largest aggregate sizes are similar in size to the diameter of the transmission line element, errors in the TDR estimates water content should be expected. This corresponds to the size fraction from 1.4 to 2.8 mm in this work. Our results suggests that, even for aggregates of this size, the published calibration of Malicki *et al.* (1996) will work well provided the soil bulk density is known. When soil aggregates are more than twice the diameter of the transmission line element, the estimates of water content



obtained from TDR measurements are likely to be very unreliable. However, as we have suggested above for most soils it is likely that the space between larger aggregates will be filled by smaller aggregates and the contact between soil and transmission line will be better than in our work. Thus we may view the suggested rule of thumb as precautionary. Knight *et al.* (1997) concluded that discontinuous pockets of air adjacent to transmission line elements would not have a significant impact on the TDR measurement. In this work the estimates of water content in the soils with the largest aggregates are approximately 80% of those estimates for soil with the smallest aggregates. This under-estimate is small in comparison with that which can occur when there is a continuous gap between the transmission line element and the soil or porous material (Whalley, 1993; Whalley *et al.*, 2001). This comparison supports the conclusion of Knight *et al.* (1997) from numerical analysis, that errors in TDR measurements due to discontinuous gaps adjacent to transmission line elements would not be large.

**Table 2.** Residual sums of squares (RSS), mean squares and a comparison of the mean squares of each model with Eq. (10)

| Calibration model | RSS | df[1] | Mean square | F relative to Eq. (10) |
|---|---|---|---|---|
| 5 | .3139 | 105 | 0.003108 | 20.00 p[2]<0.001 |
| 6 | .08400 | 103 | 0.0008235 | 5.30 p[2]<0.001 |
| 7 | .04503 | 105 | 0.0004330 | 2.79 p[2]<0.01 |
| 8 | .1377 | 102 | 0.001377 | 8.87 p[2]< 0.001 |
| 9 | .02670 | 100 | 0.0002644 | 1.70 p[2]<0.05 |
| 10 | .01553 | 101 | 0.0001553 | - |

[1]degrees of freedom, [2]probability of a value as large occurring by chance alone.

**Table 3.** Agreement between model and measurement

| Calibration model | LOFIT | df Lofit |
|---|---|---|
| 5 | 498 p[1]>0.999 | 8 |
| 6 | 147 p[1]>0.999 | 6 |
| 7 | 51.7 p[1]>0.999 | 8 |
| 8 | 39.1 p[1]>0.999 | 3 |
| 9 | 14.8 p[1]>0.999 | 5 |
| 10 | 4.11 p[1]>0.999 | 4 |

[1]With 97 degrees of freedom for pure error p is the probability that the lack of fit found could not have arisen by chance alone.

It should be noted that in this work the soil water contents were relatively low. We did not use higher water contents because sieved aggregates broke down and the size class of aggregates became undefined. However, the problem that we have examined has several important practical applications. These include studies of water relations in aggregated seed-beds and measuring the water content of swelling and shrinking clays.

## CONCLUSIONS

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## ACKNOWLEDGMENTS

Silsoe Research Institute is grant aided by the Biotechnology and Biological Science Research Council. ??PKS ?? (what is it?) (full name) was supported by a British Council training award.

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