REVISÃO DE LITERATURA

REVISITING THE S-INDEX FOR SOIL PHYSICAL QUALITY AND ITS USE IN BRAZIL[1]

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SUMMARY

The *S*-index was introduced in 2004 in a publication by A.R. Dexter. *S* was proposed as an indicator of soil physical quality. A critical value delimiting soils with rich and poor physical quality was proposed. At present, Brazil is world leader in citations of Dexter´s publication. In this publication the *S*-theory is mathematically revisited and extended. It is shown that *S* is mathematically correlated to bulk density and total porosity. As an absolute indicator, the value of *S* alone has proven to be incapable of predicting soil physical quality. The critical value does not always hold under boundary conditions described in the literature. This is to be expected because *S* is a static parameter, therefore implicitly unable to describe dynamic processes. As a relative indicator of soil physical quality, the *S*-index has no additional value over bulk density or total porosity. Therefore, in the opinion of the author, the fact that bulk density or total porosity are much more easily determined than the water retention curve for obtaining *S* disqualifies *S* as an advantageous indicator of relative soil physical quality. Among the several equations available for the fitting of water retention curves, the Groenevelt-Grant equation is preferable for use with *S* since one of its parameters and *S* are linearly correlated. Since efforts in soil physics research have the purpose of describing dynamic processes, it is the author´s opinion that these efforts should shift towards mechanistic soil physics as opposed to the search for empirical correlations like *S* which, at present, represents far more than its reasonable share of soil physics in Brazil.

Index terms: porosity, density, water retention curve, compaction.

RESUMO: *REVISITANDO O ÍNDICE* S *PARA QUALIDADE FÍSICA DO SOLO E SEU USO NO BRASIL*

O índice S *foi introduzido em 2004 numa publicação de A.R. Dexter. Esse índice foi proposto como um indicador da qualidade física do solo. Propôs-se um valor crítico para delimitar solos com qualidades físicas rica e pobre. Atualmente, o Brasil é líder mundial de*

citações do artigo de Dexter. Nessa publicação, a teoria do índice S *é matematicamente revisitada e estendida. Demonstra-se que* S *se correlaciona matematicamente com a densidade e a porosidade total do solo. Como indicador absoluto, o valor de* S *tem demonstrado ser incapaz de predizer a qualidade física do solo. O valor crítico não permite previsões confiáveis sob diversas condições de contorno descritas na literatura. Esse fato é esperado, uma vez que o* S *é um parâmetro estático, portanto implicitamente incapaz de descrever processos dinâmicos. Como indicador relativo da qualidade física do solo, o índice* S *não possui valor adicional em relação à densidade do solo ou à porosidade do solo. A determinação da densidade ou porosidade do solo é muito mais simples que a determinação de uma curva de retenção para obtenção do* S*, razão pela qual se desqualifica o* S *como um indicador interessante da qualidade física relativa do solo. Entre as várias equações disponíveis para o ajuste da curva de retenção, a de Groenevelt-Grant é preferível para uso em combinação com o* S*, uma vez que um de seus parâmetros se correlaciona linearmente com* S*. Tendo como finalidade a descrição de processos dinâmicos, os esforços de pesquisa em física do solo deveriam se deslocar na direção da física do solo mecanística, em detrimento da busca por correlações empíricas como* S*, que, atualmente, representa muito mais do que deveria na física do solo no Brasil.*

Termos de indexação: porosidade, densidade, curva de retenção de água, compactação.

INTRODUCTION

There is no single definition of soil quality. Sometimes it is defined as the ability of a specific kind of soil to perform ecological services or functions essential to people and the environment, like sustaining plant and animal productivity, maintaining or enhancing water and air quality, and supporting human health and habitation (Karlen et al., 1997). Soil physical quality, in the agricultural context, may then refer to mass and energy transfer and storage properties that permit water, dissolved nutrient, and air contents appropriate for maximizing crop development while minimizing environmental degradation, as well as adequate soil strength for maintaining structure and allowing root growth (Topp et al., 1997). A more wide-ranging concept is proposed by Garrigues et al. (2012) who discuss the internationally standardized life cycle assessment (LCA) method and its implications for evaluating soil quality.

Mass and energy transfer processes in the soil and their response to soil physical quality and functioning can be evaluated by less or more complex simulation models of hydrological, meteorological, agronomical or combined origin, like WEPP (Flanagan & Nearing, 1995), DSSAT (Jones et al., 2003) , SWAT (Neistsch et al., 2005) and SWAP (Kroes et al., 2008), among several others. These models allow evaluation of the sensitivity of involved processes to boundary conditions (Cancellieri et al., 1993; Brooks et al., 2001; Pedersen et al., 2004; Castaings et al., 2009). Specific techniques for performing sensitivity analysis in complex models were presented by Drechsler (1998).

In an attempt to avoid the need for complex models with a strong requirement for input parameters, many simple indicators of soil physical quality have been proposed and tested against datasets. Examples are aggregate stability (Jastrow et al., 1998; Saygin et al., 2012), serving as an indicator of soil recovery or degradation; soil bulk density (Reynolds et al., 2009), reflecting the ability of a soil to provide structural support, adequate water and solute movement, and soil aeration; organic carbon content and/or nutrient status (Gilley et al., 2001), indicators that integrate information on soil genesis and management, with implications for several other soil parameters; available water contents, TAW and RAW (Allen et al., 1998), that refer only to water availability; and the non-limiting or least-limiting water range (Topp et al., 1994; Da Silva et al., 1994), including aspects of water availability, aeration and rootability. Many other indicators involving parameters like slaking, soil crust, infiltration capacity, soil structure and macroporosity have also been proposed and tested (Rashidi et al., 2010). The use of these properties as indicators of soil quality is, implicitly, of empirical origin.

An indicator of soil physical quality which has gained attention recently is the S-index proposed and discussed by Dexter (2004a,b,c). S is defined as the absolute value of the slope of the water retention curve $\theta(\ln |h|)$ at its inflection point. Implicitly, S assumes a unimodal distribution of pore radii, not being applicable to the bimodal or multimodal soils which sometimes occur (Smettem & Kirkby, 1990; Durner, 1994; Carducci et al., 2011). S was hypothesized as a measure of soil microstructure, which would allow several important soil physical properties to be estimated directly from its value. In Part I (Dexter, 2004a), S is correlated to soil texture, density and organic matter content, and its consequences for root growth are discussed. In part II (Dexter, 2004b), S is applied to problems of agricultural soil mechanics. Part III (Dexter, 2004c) discusses the correlation between the unsaturated hydraulic conductivity at the inflection point with S.

Brazil is world leader in citations of Dexter (2004a). According to Google Scholar (consulted in August

2012), of a total of 164 citations of Dexter (2004a), 49 originated from Brazil, 23 from Poland (19 from A.R. Dexter himself), followed by France (16), Argentina (13), China (13), USA (12) and Spain (12). As the *S*-theory was developed using experience and evidence from soils from Northern Europe, the relatively high attention from Brazil is remarkable. Is there something about *S* that makes it especially applicable to Brazilian soils? Fidalski & Tormena (2007), Tormena et al. (2008), Freddi et al. (2009), Andrade & Stone (2009b), Pereira et al. (2011) and Santos et al. (2011), as well as other publications from Brazil, all referred to the empirical verification of the correlations between the *S*-index and other, more classical indicators of soil quality, mainly total porosity, macroporosity and bulk density.

While the *S*-theory is conceptually interesting, expectations would be too high upon supposing that any single indicator might be able to predict soil physical quality and substitute complex mechanistic eco-environmental models. It is our hypothesis that correlations between *S* and soil bulk density, porosity, and relative density are essentially inherent to the definition of *S* and do not require empirical investigation; it is the objective of this paper to sustain this hypothesis. Consequently, bulk density or porosity values contain the same quality of information for comparing the evolution of soil physical quality under agricultural or ecological management and they are much easier to perform than a determination of *S*.

THEORY

The van Genuchten soil water retention and hydraulic conductivity equation system

As the mathematical treatment of *S* has been carried out in the framework of the van Genuchten (1980) equation system, we first present the main mathematical statements and some further deductions.

The van Genuchten (1980) equation (VG) for $\Theta(h)$ is:

$$\Theta = \left[1 + \left(\alpha h\right)^{n}\right]^{-m} \qquad (1)$$

in which h is the absolute value of the pressure head; $\Theta = (\theta - \theta_r)/(\theta_s - \theta_r)$ is the effective saturation; θ, θ_r and θ_s are water content, residual water content and saturated water content, respectively; and α, n and m are fitting parameters, α having the inverse dimension of h. In this paper, all water contents indicated by θ (with or without subscripts) are expressed on a volume base ($m^3\,m^{-3}$). When defining *S*, Dexter (2004a) used the mass-based water content W ($kg\,kg^{-1}$), related to θ by:

$$\theta = W \frac{\rho_b}{\rho_a} \qquad (2)$$

where ρ_b and ρ_a are bulk soil density and water density, respectively. Note that the effective saturation Θ is the same for volume- or mass-based water content values.

Using equation 1 together with the theory presented by Mualem (1976), van Genuchten (1980) showed that, under the restriction:

$$m = 1 - \frac{1}{n} \; and \; n > 1 \qquad (3)$$

the hydraulic conductivity as a function of Θ is given in terms of the saturated hydraulic conductivity K_s, parameter m and parameter λ (often assumed to be 0.5) by:

$$K = K_s \Theta^{\lambda} \left[1 - \left(1 - \Theta^{\frac{1}{m}}\right)^{m}\right]^{2} \qquad (4)$$

Similarly, applying equation 1 together with a theory presented by Burdine (1953), and under the restriction:

$$m = 1 - \frac{2}{n} \; and \; n > 2 \qquad (5)$$

K as a function of Θ is given in terms of K_s, m and a parameter l (normally assumed to be 2) by:

$$K = K_s \Theta^{l} \left[1 - \left(1 - \Theta^{\frac{1}{m}}\right)^{m}\right] \qquad (6)$$

Equation 3 is often referred to as the Mualem restriction and equation 5 as the Burdine restriction. Other parameter constraints for the van Genuchten-Mualem equations were discussed by Fuentes et al. (1991) and Ippisch et al. (2006).

Derivative and inflection point of VG on a linear scale

On a linear scale, i.e., without any transformation, deriving equation 1 in relation to h yields:

$$\frac{d\Theta}{dh} = -mn\alpha^{n} h^{n-1} \left[1 + \left(\alpha h\right)^{n}\right]^{-m-1} \qquad (7)$$

The second derivative becomes:

$$\frac{d^2\Theta}{dh^2} = -mn\alpha^{n} h^{n-2} \left[1 + \left(\alpha h\right)^{n}\right]^{-m-2}$$
$$\left[(n-1)\left(1 + \left(\alpha h\right)^{n}\right) - n(m+1)\left(\alpha h\right)^{n}\right] \qquad (8)$$

The inflection point occurs at pressure head h_i:

$$\left.\frac{d^2\Theta}{dh^2}\right|_{h_i} = 0 \Rightarrow h_i = \frac{1}{\alpha}\left(\frac{n-1}{nm+1}\right)^{\frac{1}{n}} \qquad (9)$$

and the value of the first derivative (Equation 7) at the inflection point is:

$$\left(\frac{d\Theta}{dh}\right)_i = -mn\alpha \left(\frac{n-1}{nm+1}\right)^{1-\frac{1}{n}}\left[\frac{n(m+1)}{nm+1}\right]^{-m-1} \qquad (10)$$

Applying the Mualem restriction (Equation 3), these expressions become:

$$h_i = \frac{1}{\alpha}\left(\frac{n\text{-}1}{n}\right)^{\frac{1}{n}} \tag{11}$$

$$\left(\frac{d\Theta}{dh}\right)_i = (1\text{-}n)\,\alpha\left(1\text{-}\frac{1}{n}\right)^{1\text{-}\frac{1}{n}}\left(2\text{-}\frac{1}{n}\right)^{\frac{1}{n}\text{-}2} \tag{12}$$

or, in the case of the Burdine restriction (Equation 5):

$$h_i = \frac{1}{\alpha} \tag{13}$$

$$\left(\frac{d\Theta}{dh}\right)_i = 2^{\frac{2}{n}-2}(2-n)\alpha \tag{14}$$

Derivative and inflection point of VG on a log scale

For deriving h_i in a logarithmic representation of h, we define

$$f = \log_a h = \frac{\ln h}{\ln a} \Leftrightarrow h = a^f = \exp[f \ln a] \tag{15}$$

Consequently

$$dh = fa^{f-1}da \tag{16}$$

Equation 1 becomes

$$\Theta = \left[1 + (\alpha\,\exp[f\ln a])^n\right]^{-m} \tag{17}$$

and

$$\frac{d\Theta}{df} = -mn(\alpha h)^n\left[1+(\alpha h)^n\right]^{-m-1}\ln a \tag{18}$$

$$\frac{d^2\Theta}{df^2} = -mn^2(\alpha h)^n\left[1+(\alpha h)^n\right]^{-m-2}\left(1-m(\alpha h)^n\right)(\ln a)^2 \tag{19}$$

The logarithmic inflection point occurs at pressure head h_i:

$$h_i = \frac{1}{\alpha}\left(\frac{1}{m}\right)^{\frac{1}{n}} \tag{20}$$

Then:

$$\left(\frac{d\Theta}{df}\right)_i = -n\ln a\left[1+\frac{1}{m}\right]^{-m-1} \tag{21}$$

or, with the Mualem restriction (Equation 3):

$$h_i = \frac{1}{\alpha}\left(\frac{n}{n-1}\right)^{\frac{1}{n}} \tag{22}$$

$$\left(\frac{d\Theta}{df}\right)_i = -n\ln a\left[\frac{2n-1}{n-1}\right]^{\frac{1}{n}-2} \tag{23}$$

Applying the Burdine restriction (Equation 5):

$$h_i = \frac{1}{\alpha}\left(\frac{n}{n-2}\right)^{\frac{1}{n}} \tag{24}$$

$$\left(\frac{d\Theta}{df}\right)_i = -n\ln a\left[\frac{2n-2}{n-2}\right]^{\frac{2}{n}-2} \tag{25}$$

S - theory

Dexter (2004a) defined S as the absolute value of the slope of the curve expressing water content at a mass base (W) as a function of $\ln|h|$ at its inflection point, hence:

$$S = \left|\left(\frac{dW}{df}\right)_i\right|_{a=e} = \left|\frac{\rho_a}{\rho_b}\left(\frac{d\theta}{df}\right)_i\right|_{a=e} = (\theta_s - \theta_r)\frac{\rho_a}{\rho_b}\left|\left(\frac{d\Theta}{df}\right)_i\right|_{a=e} \tag{26}$$

Therefore, according to equation 21, with $a = e = \exp(1)$ and $\ln(a) = 1$:

$$S = \frac{\rho_a}{\rho_b}n(\theta_s - \theta_r)\left(1+\frac{1}{m}\right)^{-m-1} \tag{27}$$

For the Mualem restriction (analogous to equation 23, $n > 1$), the following expressions are obtained:

$$S = \frac{\rho_a}{\rho_b}n(\theta_s - \theta_r)\left(\frac{2n-1}{n-1}\right)^{\frac{1}{n}-2} = $$
$$= \frac{\rho_a}{\rho_b}\frac{1}{1-m}(\theta_s - \theta_r)\left(\frac{m}{1+m}\right)^{m+1} \tag{28}$$

$$\frac{\partial S}{\partial \theta_s} = -\frac{\partial S}{\partial \theta_r} = \frac{\rho_a}{\rho_b}n\left(\frac{2n-1}{n-1}\right)^{\frac{1}{n}-2} \tag{29}$$

$$\frac{\partial S}{\partial n} = \frac{\rho_a}{\rho_b}(\theta_s - \theta_r)\left(\frac{2n-1}{n-1}\right)^{\frac{1}{n}-2}\left(\frac{n}{n-1} - \ln\left[\left(\frac{2n-1}{n-1}\right)^{\frac{1}{n}}\right]\right) \tag{30}$$

From these equations it follows that:

$$\lim_{n\to\infty}\frac{\partial S}{\partial n} = \frac{\rho_a}{\rho_b}\frac{(\theta_s - \theta_r)}{4} \tag{31}$$

and

$$\lim_{n\to\infty}\frac{\partial S}{\partial \theta_s} = \frac{\rho_a}{\rho_b}\frac{n}{4} \to \infty \tag{32}$$

Alternatively, applying the Burdine restriction (Equation 5, for $n > 2$), from equation 25:

$$S = \frac{\rho_a}{\rho_b}n(\theta_s - \theta_r)\left[\frac{2n-2}{n-2}\right]^{\frac{2}{n}-2} = $$
$$= \frac{\rho_a}{\rho_b}\frac{2}{1-m}(\theta_s - \theta_r)\left[\frac{m}{1+m}\right]^{m+1} \tag{33}$$

$$\frac{\partial S}{\partial \theta_s} = -\frac{\partial S}{\partial \theta_r} = \frac{\rho_a}{\rho_b} n\left[\frac{2n-2}{n-2}\right]^{\frac{2}{n}-2} \tag{34}$$

$$\frac{\partial S}{\partial n} = \frac{\rho_a}{\rho_b}(\theta_s - \theta_r)\left(\frac{2n-2}{n-2}\right)^{\frac{2}{n}-2}\left(\frac{n}{n-2} - \ln\left[\left(\frac{2n-2}{n-2}\right)^{\frac{2}{n}}\right]\right) \tag{35}$$

Resulting in:

$$\lim_{n\to\infty}\frac{\partial S}{\partial n} = \frac{\rho_a}{\rho_b}\frac{(\theta_s - \theta_r)}{4} \tag{36}$$

and

$$\lim_{n\to\infty}\frac{\partial S}{\partial \theta_s} = \frac{\rho_a}{\rho_b}\frac{n}{4} \to \infty \tag{37}$$

S in Brooks-Corey soils

On proposing the S-index, Dexter (2004a) states that the slope of the retention curve "can be measured directly by hand from the curve (…) however, it is more convenient to fit the curve to a mathematical function and then to calculate the slope at the inflection point in terms of the parameters of the function". Dexter (2004a) discusses the S-theory based on the van Genuchten (1980) θ-h relation, and the S-index has been discussed in literature exclusively using this equation.

A frequently applied and mathematically simpler alternative to express the water retention curve was proposed by Brooks & Corey (1964):

$$\Theta = 1 \text{ for } h<h_b \tag{38}$$

$$\Theta = \left(\frac{h_b}{h}\right)^{\lambda} \text{ for } h \geq h_b$$

h_b and λ being fitting parameters. Substituting equation 15 to transform equation 38 to the logarithmic scale we obtain:

$$\Theta = 1 \text{ for } h<h_b \tag{39}$$

$$\Theta = h_b^{\lambda}\exp[-\lambda f \ln a] \text{ for } h \geq h_b$$

and

$$\frac{d\Theta}{df} = 0 \text{ for } h < h_b \tag{40}$$

$$\frac{d\Theta}{df} = -\lambda \ln a\left(\frac{h_b}{h}\right)^{\lambda} \text{ for } h \geq h_b$$

For the Brooks & Corey (1964) equation, the inflection point occurs at $h = h_b$ where $d\Theta/df$ is discontinuous, hence:

$$\left(\frac{d\Theta}{df}\right)_i = -\lambda \ln a \tag{41}$$

The combination of equation 40 with equation 26 results in the following expression for calculating S in Brooks-Corey type soils:

$$S = \lambda \frac{\rho_a}{\rho_b}(\theta_s - \theta_r) \tag{42}$$

S in Groenevelt-Grant soils

A mathematically versatile equation for fitting soil water retention curves was proposed by Groenevelt & Grant (2004):

$$\theta = \theta_s - (\theta_s - \theta_r)\exp\left[-\left(\frac{k}{h}\right)^r\right] \tag{43}$$

with k and r being fitting parameters, k having the same dimension as h. The goodness-of-fit of the model is shown to be very similar to fits to VG and allows estimation of unsaturated hydraulic conductivity using the Burdine (1953) or Mualem (1976) model (Grant et al., 2010). Transforming equation 43 to the logarithmic scale by substituting equation 15 yields

$$\theta = \theta_s - (\theta_s - \theta_r)\exp[-k^r\exp(-rf\ln a)] \tag{44}$$

The first derivative is

$$\frac{d\theta}{df} = -(\theta_s - \theta_r)r\ln a\left(\frac{k}{h}\right)^r\exp\left[-\left(\frac{k}{h}\right)^r\right] \tag{45}$$

and the second derivative becomes

$$\frac{d^2\theta}{df^2} = -\left[\left(\frac{k}{h}\right)^r - 1\right](\theta_s - \theta_r)r^2(\ln a)^2\left(\frac{k}{h}\right)^r\exp\left[-\left(\frac{k}{h}\right)^r\right] \tag{46}$$

from which it follows that the logarithmic inflection point occurs at

$$h_i = k \tag{47}$$

Combining equations 47, 45 and 26 results in the following expression for S in Groenevelt-Grant type soils:

$$S = \frac{r}{e}\frac{\rho_a}{\rho_b}(\theta_s - \theta_r) \tag{48}$$

DISCUSSION

Sensitivity of S to alterations in VG parameters

Equations 28 and 33 are graphically represented in figure 1 showing the relation between S and n with Mualem and Burdine restrictions. S is shown relative to $(\theta_s - \theta_r)\rho_a/\rho_b$, therefore, in order to obtain real S values the axis values should be multiplied by $(\theta_s - \theta_r)\rho_a/\rho_b$ which is between 0.2 and 0.5 for most soils. An increase in n results in higher values of S. This increase occurs at a rate tending to 0.25 for larger values of n, according to equations 31 and 36 (Figure 2).

S is also expected to increase with an increasing difference between θ_r and θ_s, as illustrated in figure 3 and in agreement with equations 29 and 34. According to equations 32 and 37, the rate tends to $n/4$ (Figure 4).

S versus porosity and bulk density

Saturated water content θ_s is equal to total porosity γ. Therefore, rewriting equation 29, we demonstrate the positive correlation between $|S|$ and γ (here assuming the Mualem restriction):

$$\partial S = \frac{\rho_a}{\rho_b} n \left(\frac{2n-1}{n-1}\right)^{\frac{1}{n}-2} \partial \gamma \qquad (49)$$

θ_s can also be expressed in terms of bulk density ρ_b and particle density ρ_p as

$$\theta_s = 1 - \frac{\rho_b}{\rho_p} \qquad (50)$$

Substituting equation 50 in 28 yields the following expression for S as a function of ρ_b, ρ_p and n, assuming the Mualem restriction:

$$S = \frac{\rho_a}{\rho_b} n \left(1 - \frac{\rho_b}{\rho_p} - \theta_r\right)\left(\frac{2n-1}{n-1}\right)^{\frac{1}{n}-2} \qquad (51)$$

from which the negative correlation between $|S|$ and ρ_b can be proven:

$$\partial S = -\frac{\rho_a}{\rho_b} \frac{n}{\rho_p} \left(\frac{2n-1}{n-1}\right)^{\frac{1}{n}-2} \partial \rho_b \qquad (52)$$

For a soil with $0.27\ \mathrm{kg\ kg^{-1}}$ clay and bulk densities in the range from 1350-1670 kg m^{-3}, Dexter (2004a) found $S = 0.1171 - 5.83 \cdot 10^{-5}\ \mathrm{d}\rho_b$, corresponding to $\mathrm{d}S = -5.83 \cdot 10^{-5}\ \mathrm{d}\rho_b$. Evaluating equation 52 with
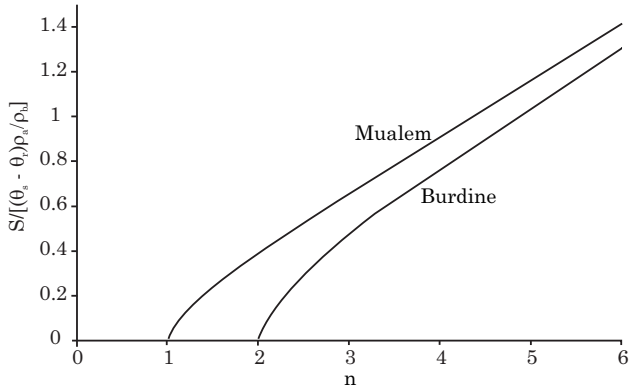

Figure 1. S relative to $(\theta_s - \theta_r)\rho_a/\rho_b$ as a function of van Genuchten n with Mualem and Burdine restrictions (graphical representation of equations 28 and 33).
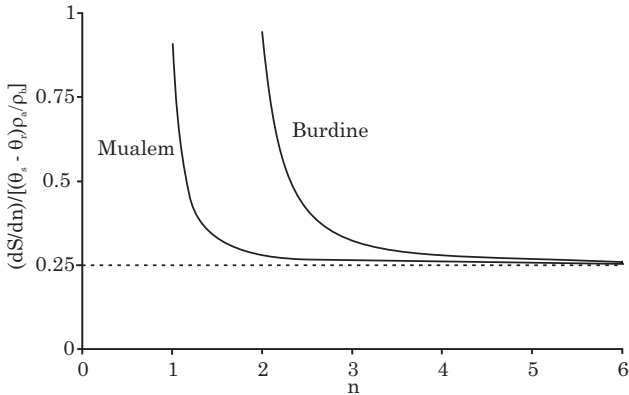

Figure 2. dS/dn relative to $(\theta_s - \theta_r)\rho_a/\rho_b$ as a function of van Genuchten n with Mualem and Burdine restrictions (graphical representation of equations 30 and 35).
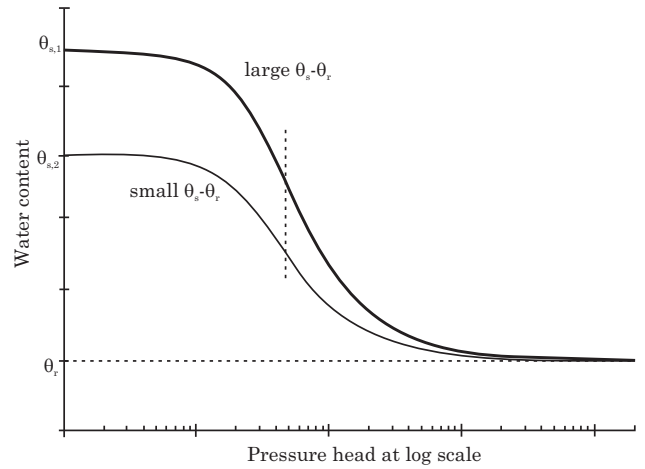

Figure 3. Water content as a function of pressure head at log scale, illustrating the effect of a small versus a large $\theta_s - \theta_r$ on the inclination of the curve at inflection point i.
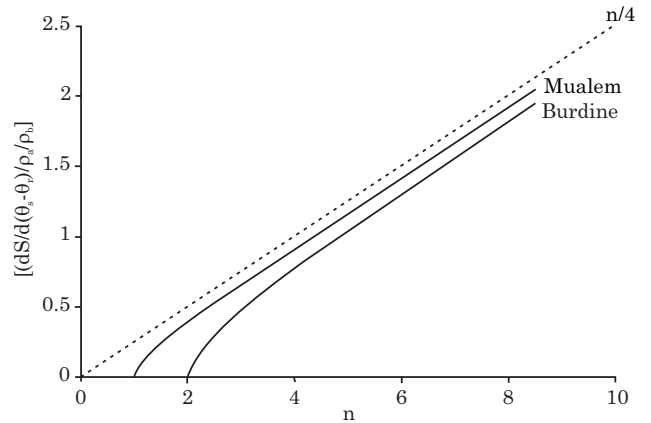

Figure 4. dS/d$(\theta_s - \theta_r)$ relative to ρ_a/ρ_b as a function of van Genuchten n with Mualem and Burdine restrictions (graphical representation of equations 29 and 34).

ρ_a = 1000 kg m^{-3}, ρ_p = 2800 kg m^{-3} and ρ_b = 1500 kg m^{-3}, for n = 1.5 we find dS = -6.0 ·10^{-5} dρ_b, of the same order of magnitude as the equation found by Dexter (2004a). For n = 2 and n = 3, these expressions become dS = -9.8 ·10^{-5} dρ_b and dS = -16.6 ·10^{-5} dρ_b, respectively. Equation 52 suggests a hyperbolic trend when plotting S versus ρ_b, similar to the trends shown by Dexter (2004a) in his figure 6.

S *versus* relative density

Relative density ρ_r can be used to express the state of relative soil compaction (Carter, 1990; Da Silva et al., 1997; Håkansson & Lipiec, 2000; Beutler et al., 2005) and is defined as

$$\rho_r = \frac{\rho_b}{\rho_m} \qquad (53)$$

where ρ_m is the maximum bulk density. ρ_m can be determined or estimated by a pedotransfer function (Marcolin & Klein, 2011). Combining equation 50 and 53, we obtain

$$\theta_s = 1 - \frac{\rho_m \rho_r}{\rho_p} \Leftrightarrow \rho_r = \frac{\rho_p \left(1 - \theta_s\right)}{\rho_m} \qquad (54)$$

Substituting equation 54 in 28 yields the following expression for S as a function of ρ_b, ρ_p and n, assuming the Mualem restriction:

$$S = \frac{\rho_a}{\rho_b} n \left(1 - \frac{\rho_m \rho_r}{\rho_p} - \theta_r\right) \left(\frac{2n-1}{n-1}\right)^{\frac{1}{n}-2} \qquad (55)$$

from which follows (assuming the Mualem restriction):

$$\partial S = - \frac{\rho_a}{\rho_b} n \frac{\rho_m}{\rho_p} \left(\frac{2n-1}{n-1}\right)^{\frac{1}{n}-2} \partial \rho_r \qquad (56)$$

Equation 56 shows a negative correlation to be implicitly expected between relative bulk density and $|S|$.

Comparison between models for soil water retention with respect to S

Equation 42 shows that S is directly proportional to one of the fitting parameters (λ) of the Brooks & Corey (1964) equation. Similarly, for Groenevelt-Grant type soils, equation 48 shows S to be directly proportional to fitting parameter r. In contrast, expressions for S using VG (equations 27, 28 or 33) are less straightforward. Therefore, if the objective is determining S, the Brooks-Corey or Groenevelt-Grant equation should be preferred over VG. Taking it as a disadvantage that the inflection point in the Brooks-Corey equation occurs at the discontinuity of the equation´s first derivative, Groenevelt-Grant seems to be the perfect equation for use in combination with S.

Is S an interesting indicator of soil physical quality?

One of the hypotheses of Dexter (2004a) is that "several important soil physical properties can be estimated directly from the value of S". Andrade & Stone (2009), analyzing existing information of more than 200 soil samples from the Brazilian *cerrado*, found good correlations between S and (macro)porosity and bulk density. Several other authors, including Dexter (2004a), Tormena et al. (2008) and Cunha et al. (2011), came to similar conclusions. These findings are plausible and easy to explain: in an agricultural scenario, machinery and/or animal trampling tend to destroy pores, mainly the larger pores that are more subject to collapsing. As a consequence, macroporosity and total porosity (as well as θ_s) decrease and bulk density increases. Cryptopores and micropores (and θ_r) are very little affected by the process, and there may even be a small increase in their content (Siegel-Issem et al., 2005; Pengthamkeerati et al, 2006; Beutler et al., 2007; Gontijo et al., 2008).

As shown by equation 52, but also by equations 27, 29, 34, 42 and 48, as well as in figure 3, whenever the difference between θ_s and θ_r decreases, the value of S also decreases. The correlations found may be considered as a mere reflection of this mathematical fact. Thus, it seems reasonable to conclude that, compared to simple soil bulk density, there is no additional value in the S index when it comes to detecting soil degradation or soil physical quality. Considering that it is much less laborious to determine soil total porosity or bulk density than it is to determine an entire water retention curve to obtain S, S should be disqualified as a useful indicator of relative soil physical quality. In other words, whenever we aim to detect changes in soil pore space that reflect modifications in soil physical quality, it is equally fine, yet much simpler, to determine total porosity or bulk density than it is to determine the S index.

Another question arises. Can the value of S be used, on its own, to predict the physical quality of a soil? In other words, can S be considered to be an absolute indicator of soil quality? Dexter (2004a) states that "the slope, S, at the inflection point is a measure of soil microstructure that can be used as an index of soil physical quality", suggesting a limiting (absolute) value of 0.035 to distinguish between "good" and "bad" soil physical quality. The author added that "individual soils may differ significantly in behaviour from these typical values and trends", which means that no conclusions can be drawn about the physical quality of a soil just by knowing its S value. Cunha et al. (2011) determined S in a soil from Brazil (Latossolo Vermelho distrófico - Oxisol) with common bean under conventional tillage and no-tillage. S values were all below 0.035, and many were below 0.020, whereas bulk density was not in the range normally considered as critical. On the contrary, Varandas (2011) found S values at an order of magnitude higher than those described by Dexter (2004a) - from 0.02 to 0.15 - in several soils (Latossolo, Neossolo, Nitossolo) from the State of São Paulo, Brazil, under several agricultural and other uses, some of the soils being physically degraded. These two examples corroborate the

observation about "individual soils" by Dexter (2004a) and show that S is not an absolute indicator of soil physical quality. It is, therefore, questionable whether anything can be inferred based on the value of S alone, even if this is common practice in many publications (Calonego & Rosolem, 2011; Cavalieri et al., 2011)

Evaluation of soil quality depends on understanding the insertion of soil in the landscape-soil-plant-atmosphere system; therefore, it depends on knowledge of how the system functions and the underlying physical, chemical and biological processes. We mentioned in the Introduction that process-based models capable of simulating these processes applied to agronomy, hydrology, ecology and meteorology are being developed by specific research groups and are available to the scientific community. As stated by Vezzani & Mielniczuk (2009), it is more important to identify how to obtain soil (physical) quality than to identify parameters to measure it. Models can play an important role in this. However, static indexes like S will never be able to present systematic correlations. Souza & Reichardt (1996) came to an analogous conclusion regarding the use of static, pressure-head based indicators for something as complex and dynamic as field capacity. They recommended not using these indicators, but rather searching for a process-based understanding. We agree and propose a shift of research efforts towards mechanistic soil physics as opposed to the search for empirical correlations like S which, at present, represents far more than its reasonable share of soil physics in Brazil.

CONCLUSIONS AND REMARKS

1. S is mathematically correlated to bulk density and total porosity. Therefore, as a relative indicator of soil physical quality, the S-index has no additional value over bulk density or total porosity. The fact that bulk density or total porosity are much more easily determined than the water retention curve for obtaining S disqualifies S as an advantageous indicator of relative soil physical quality;

2. As an absolute indicator, the value of S alone has proven to be incapable of predicting soil physical quality. A limiting or threshold value like the frequently used $S = 0.035$ does not hold under several boundary conditions described in the literature.

We showed that the attention given to S in Brazilian research is incompatible with the information it really represents. Research efforts should shift towards mechanistic soil physics as opposed to the search for empirical correlations like S that, at present, represents far more than its reasonable share of soil physics in Brazil. We observed that S is a static parameter, therefore implicitly unable to describe dynamic processes. If the objective is to systematically determine S, the Groenevelt-Grant water retention equation is preferable to the van Genuchten equation since one of its fitting parameters is linearly correlated to S.

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