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soilphysics: An R package for calculating soil water availability to plants by different soil physical indices

R.P. de Lima [a,*], A.R. da Silva [b], A.P. da Silva [a], T.P. Leão [c], M.R. Mosaddeghi [d]

[a] Department of Soil Sciences, University of Sao Paulo – ESALQ, Av. Padua Dias, 11, CEP 13418-900 Piracicaba, SP, Brazil
[b] Agronomy Department, Goiano Federal Institute, Geraldo Silva Nascimento Road, km 2.5, CEP 75790-000 Urutai, GO, Brazil
[c] Universidade de Brasília–UnB, Faculdade de Agronomia e Medicina Veterinária, Campus Universitário Darcy Ribeiro Asa Norte, CEP 70910-900 Brasília-Distrito Federal, Brazil
[d] Department of Soil Science, College of Agriculture, Isfahan University of Technology, Isfahan 84156-83111, Iran

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ABSTRACT

Soil available water is an important factor for plant growth. It has been estimated by different soil physical indices, such as the least limiting water range (LLWR), integral water capacity (IWC) and integral energy (E_I). Moreover, salinity is an important limitation for soil water availability to plants. Despite the advances in the quantification of LLWR, IWC and E_I, a comprehensive description of the computational methods, including data management, curve fitting procedures and graphing techniques, is still lacking. The salinity effect on these quantities has still not been implemented in a computer package. In this paper, we present an R package *soilphysics* and its implementations to determine LLWR, IWC and E_I. We described the theory behind each implementation, illustrated the functionalities and validated the outcomes of *soilphysics* with other software packages for LLWR, IWC and E_I calculations (an Excel® algorithm and SAWCal). The salinity effect on soil available water was also employed in the package. The outcomes are basically the same as other software available, with small differences (<4%). The package *soilphysics* takes advantage of all the power of R for dealing with extensive algorithms and for building high-quality graphics. It is currently available from the CRAN website (http://cran.r-project.org/web/packages/soilphysics/index.html).

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1. Introduction

The concept of soil available water (SAW) for plants was stated by Veihmeyer and Hendrickson (1927, 1931) in its simplest form as the water content available between field capacity (FC) and wilting point (WP). The concept aims to estimate, by a soil physical index, the water available for plant growth.

Letey (1985) elaborated the concept of SAW by considering some soil physical factors that could restrict plants growth in addition to SAW, such as aeration and penetration resistance. He suggested the term non-limiting water range (NLWR) for which the limiting effects of aeration, penetration resistance and matric head are non-limiting. Then, Silva et al. (1994) quantitatively developed the concept introduced by Letey (1985), and renamed it the least limiting water range (LLWR).

The LLWR is an important index for the evaluation of soil physical quality and soil available water, as it allows the integration of three main plant growth-limiting factors (i.e. penetration resistance, aeration and soil water potential) into a single parameter (Silva et al., 1994; Leão et al., 2005; Leão and da Silva, 2004; Guedes Filho et al., 2013), which is related to the bulk density variation.

Groenevelt et al. (2001) introduced the integral water capacity (IWC) to determine the SAW. In order to calculate SAW by the IWC approach, continuous weighting functions accounting for various soil physical restrictions are multiplied by the differential water capacity ($C(h)$) and the effective values of $C(h)$ are integrated over the full matric head (h) range (Asgarzadeh et al., 2014). Groenevelt et al. (2001) presented the IWC theory and considered four limiting factors at wet and dry ranges. At the wet range, they considered rapid drainage by gravity and lack of sufficient aeration. At the dry range, the low hydraulic conductivity and root penetrability were considered. The weighting functions were constructed as functions of the matric head so that they ranged between zero and unity at appropriate limits (Asgarzadeh et al., 2014).

In addition to limiting factors used by Groenevelt et al. (2001) and Asgarzadeh et al. (2014) for calculating the IWC, Groenevelt et al. (2004) proposed a weighting function to account for the

* Corresponding author.
E-mail addresses: renato_agro_@hotmail.com (R.P. de Lima), anderson.silva@ifgoiano.edu.br (A.R. da Silva), apisilva@usp.br (A.P. da Silva), tleao@unb.br (T.P. Leão), mosaddeghi@cc.iut.ac.ir (M.R. Mosaddeghi).

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Nomenclature

a, b, c	parameters of Silva model, with a, b ($m^3\ m^{-3}\ cm^{-1}$)
a, c	parameters of Ross model, with a ($m^3\ m^{-3}\ cm^{-1}$)
b_0, b_1, b_2	parameters of Busscher model , with b_0 (MPa $m^3\ m^{-3}$ - Mg m^{-3})
b_1, b_2	parameters of PR power model for LLWR, with b_0 (MPa $m^3\ m^{-3}$)
a, b	parameters of PR power model for IWC, with a (MPa cm^{-1})
ρ	bulk density (Mg m^{-3})
ρ_p	particle density (Mg m^{-3})
h	matric head (cm)
FC	field capacity ($m^3\ m^{-3}$)
WP	wilting point ($m^3\ m^{-3}$)
θ_{FC}	volumetric water content at field capacity ($m^3\ m^{-3}$)
θ_{WP}	volumetric water content at wilting point ($m^3\ m^{-3}$)
θ_{PR}	volumetric water content at critical penetration resistance ($m^3\ m^{-3}$)
θ_A	critical volumetric air content ($m^3\ m^{-3}$)
PR	soil penetration resistance (MPa)
θ	volumetric water content ($m^3\ m^{-3}$)
θ_s	saturated water content ($m^3\ m^{-3}$)
θ_r	residual water content ($m^3\ m^{-3}$)
n	shape parameter of van Genuchten (1980) model (dimensionless)
α	scaling parameter of van Genuchten (1980) model (cm^{-1})
d	parameter of the power function for low soil hydraulic conductivity
$K_r(h)$	relative hydraulic conductivity (dimensionless)
$C(h)$	differential water capacity (first derivative of van Genuchten model, cm^{-1})
$E(h)$	effective differential water capacity (cm^{-1})
LLWR	least limiting water range ($m^3\ m^{-3}$)
IWC	integral water capacity ($m^3\ m^{-3}$)
E_I	integral energy (J kg^{-1})
m	number of soil physical limiting factors
Π	symbol of product (i.e. multiplying function)
ω	weighting function of a limiting factor
h_{os}	osmotic head of the saturated soil extract (cm)
EC_e	electrical conductivity of the saturated soil extract (dS m^{-1})
$\boldsymbol{\beta}$	vector of nonlinear parameters
σ^2	error variance of the regression model
$\mathbf{x}$	vector of explanatory variables
y	observation of the regression analysis
N	number of observations
p	number of fitting parameters

effect of salinity on the water available for plants. Salinity can significantly decrease the SAW through the osmotic effect.

The energy required for plants to remove a defined amount of water from the soil is also considered as an index of soil water availability. Minasny and McBratney (2003) introduced the integral energy (E_I) concept to quantify the energy required of a plant to take up an unit amount of water from the soil at a given water content or matric head range (Asgarzadeh et al., 2014). This concept was extended for the LLWR and IWC (Asgarzadeh et al., 2011, 2014) to quantify the energy required to extract water in the LLWR and IWC ranges.

Many researchers have used the LLWR and IWC approaches to evaluate soil physical quality (e.g. Asgarzadeh et al., 2010, 2014; Guedes Filho et al., 2013). These researchers considered the LLWR and IWC as important indicators of SAW for plant growth.

According to Leão et al. (2005) and Asgarzadeh et al. (2014), despite advances in the quantification of the LLWR, IWC and E_I, a detailed description of the computational methodology for calculating these indexes from soil properties data, including data management, curve fitting procedures, and graphing techniques, is still lacking. In addition, salinity effect on these quantities has not been included in a user-friendly computer package so far. Leão and da Silva (2004) and Leão et al. (2005) proposed a simplified algorithm for calculation of the LLWR using the spreadsheet software Microsoft Excel® and Statistical Analysis System (SAS), respectively. Asgarzadeh et al. (2014) proposed a software called SAWCal (Soil Available Water Calculator) to calculate LLWR, IWC, and E_I. These algorithms and softwares are important tools for determination and popularization of soil physical indices.

The software R (R Core Team, 2015) is a distribution-free computing environment that receives contributions from researchers and experts in various fields of science worldwide. However, the packages destined for soil science are scarce (Omuto and Gumbe, 2009) and there is still no package that can deal with LLWR, IWC, and E_I for the users of the R software.

In this paper, a computer program is presented which is available as an R package called *soilphysics*. With *soilphysics*, it is possible to determine the LLWR, IWC and E_I by two simple functions, respectively. In addition to limiting factors used by Groenevelt et al. (2001) and Asgarzadeh et al. (2014) for calculation of the IWC, we included salinity effect (i.e. salinity weighting function) proposed by Groenevelt et al. (2004) as an option for users. The package produces graphics with high quality, included as outputs, when *soilphysics* is run. This package is a new interface for the calculations of plant available water quantities using R language. The package *soilphysics* is distribution-free and is available at CRAN (http://cran.r-project.org/).

2. Theory

2.1. Least limiting water range (LLWR)

The LLWR concept was introduced by Silva et al. (1994) as the integration of three main plant growth-limiting factors (i.e. soil penetration resistance, aeration and water potential) into a single parameter. The changes in the LLWR as a function of bulk density are considered (Guedes Filho et al., 2013). According to Silva et al. (1994), the LLWR can be described as follows:

(i) The soil water retention curve is determined as the relationship between the volumetric water content and matric head, as proposed by Ross et al. (1991), Eq. (1), or following the adaptation presented by Silva et al. (1994), Eq. (2):

$$\theta = ah^c \tag{1}$$

$$\theta = \exp(a + b\rho)h^c \tag{2}$$

where θ is the soil volumetric water content ($m^3\ m^{-3}$); ρ is the bulk density (Mg m^{-3}); h is the matric head (i.e. cm); and a, b, and c are model-fitting parameters.

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