Computers and Electronics in Agriculture 120 (2016) 63–71

Contents lists available at ScienceDirect

Computers and Electronics in Agriculture

journal homepage: www.elsevier.com/locate/compag

Original papers

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

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ARTICLE INFO

Article history:
Received 23 June 2015
Received in revised form 20 September 2015
Accepted 1 November 2015
Available online 3 December 2015

Keywords:
Soil available water
Least limiting water range
Integral water capacity
Integral energy
Salinity

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).

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

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http://dx.doi.org/10.1016/j.compag.2015.11.003
0168-1699/

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.

(ii) The soil penetration resistance curve can be obtained from the volumetric water content ($m^3\,m^{-3}$), modeled using a power model, Eq. (3), or using the function proposed by Busscher (1990) as a function of volumetric water content and bulk density, Eq. (4):

$$\mathrm{PR} = b_0\theta^{b_1} \tag{3}$$

$$\mathrm{PR} = b_0\theta^{b_1}\rho^{b_2} \tag{4}$$

where PR is soil penetration resistance (MPa), and b_0, b_1, and b_2 are model-fitting parameters.

(iii) The water contents ($m^3\,m^{-3}$) at field capacity (θ_{FC}) and at wilting point (θ_{WP}) can be calculated using the soil water retention curve model (Eq. (2)) by the Eqs. (5) and (6), respectively:

$$\theta_{FC} = \exp(a + b\rho)h_{FC}^{c} \tag{5}$$

$$\theta_{WP} = \exp(a + b\rho)h_{WP}^{c} \tag{6}$$

The water content ($m^3\,m^{-3}$) at which soil penetration resistance reaches the critical value of 2.0 MPa (i.e. θ_{PR}) can be calculated by the soil penetration resistance model, Eq. (3) and (4), using:

$$\theta_{PR} = \left(\frac{\mathrm{PR}}{b_0}\right)^{\frac{1}{b_1}} \tag{7}$$

$$\theta_{PR} = \left(\frac{\mathrm{PR}}{b_0\rho^{b_2}}\right)^{\frac{1}{b_1}} \tag{8}$$

The water content ($m^3\,m^{-3}$) at which the volumetric air content is equal to 0.10 $m^3\,m^{-3}$, denoted by θ_A, can be calculated with Eq. (9), where ρ_p is the particle density:

$$\theta_A = \left(1 - \frac{\rho}{\rho_p}\right) - 0.1 \tag{9}$$

After fitting these models, θ_A, θ_{PR}, θ_{FC} and θ_{WP} are given as functions of the soil bulk density.

2.2. Integral water capacity (IWC)

The calculation procedure of IWC, as proposed by Groenevelt et al. (2001), was presented by Asgarzadeh et al. (2014) in a simplified form, based upon the soil water retention (Eq. (10)) and relative hydraulic conductivity (Eq. (11)) equations of van Genuchten (1980) and Mualem (1976), respectively.

$$\theta(h) = \theta_r + (\theta_s - \theta_r)\left[1 + (\alpha h)^n\right]^{\left[\frac{1}{n}-1\right]} \tag{10}$$

$$K_r(h) = \left[1 - (\alpha h)^{n-1}\left[1 + (\alpha h)^n\right]^{\left[\frac{1}{n}-1\right]}\right]^2\left[1 + (\alpha h)^n\right]^{\left[\frac{1-n}{2n}\right]} \tag{11}$$

where θ and h are the volumetric water content ($m^3\,m^{-3}$) and matric head (cm), respectively; θ_s and θ_r are the saturated and residual water contents ($m^3\,m^{-3}$), respectively, and α (cm^{-1}) and n are fitting parameters; $K_r(h)$ is the relative hydraulic conductivity.

The IWC calculation requires the differential water capacity function ($C(h)$, cm^{-1}), which is the first derivate of the van Genuchten (1980) equation (i.e. $|d\theta/dh|$, Eq. (12)) and corresponds to the slope of the soil water retention curve:

$$C(h) = (\theta_s - \theta_r)(n-1)h^{-1}(\alpha h)^n\left[1 + (\alpha h)^n\right]^{\left[\frac{1-2n}{n}\right]} \tag{12}$$

A continuous function of soil resistance penetration is also needed to calculate IWC. It can be defined by a simple power model (Asgarzadeh et al., 2014):

$$\mathrm{PR}(h) = ah^b \tag{13}$$

where PR(h) is the soil penetration resistance (MPa), h (cm) is the matric head and a and b are empirical fitting parameters (Groenevelt et al., 2001; Asgarzadeh et al., 2014).

Finally, the IWC can be calculated using the following equation (Groenevelt et al., 2001; Asgarzadeh et al., 2014):

$$\mathrm{IWC} = \int_0^{\infty}\left(\prod_{i=1}^{m}\omega_i(h)\right)C(h)dh \tag{14}$$

The modeled soil water retention curve is used to generate 1000 discrete data points for each (i = 1,2,...,m) integration portion (Eq. (14)), considering the h range of 0–15,000 cm. The integration is evaluated numerically by means of the trapezoidal method (Spiegel, 1990). Weighting functions, $\omega_i(h)$, account for various limiting soil physical properties (1 to m) as a function of h. The symbol Π indicates that different weighting functions are *multiplicative*. The values of $\omega_i(h)$ are considered zero when there is complete restriction to water uptake by plants and is being increased continuously to 1 where there is no restriction to water uptake by plants (Groenevelt et al., 2001; Asgarzadeh et al., 2014). The weighting function for soil hydraulic conductivity, $\omega_K(h)$, at the wet range is calculated as follows (Groenevelt et al., 2001; Asgarzadeh et al., 2014):

$$\omega_K(h) = \left[\frac{K_{r(330)}}{K_r(h)}\right]^{0.08} \tag{15}$$

where $\omega_K(h)$ is 1 at h of 330 cm and decreases as h decreases, but it is assumed that it never reaches 0, even when the soil is saturated.

The values of the weighting function for soil aeration, $\omega_a(h)$, at the wet range are set to 0 and 1 at volumetric air contents of 0.1 and 0.15 $m^3\,m^{-3}$, respectively, and are calculated for intermediate values using the following equations:

$$\omega_a(h) = A\log\left(\frac{h}{h_{10}}\right) \tag{16}$$

$$A = \frac{1}{\log\left[\frac{h_{15}}{h_{10}}\right]} \tag{17}$$

where h_{10} and h_{15} are h values at volumetric air contents of 0.10 and 0.15 $m^3\,m^{-3}$, respectively, and inferred from the soil water retention function.

Restriction of PR (i.e. $\omega_R(h)$) at the dry range is assumed to start from 1.5 MPa and to be completed at 2.5 MPa (Groenevelt et al., 2001; Asgarzadeh et al., 2014). Based on Eq. (13), it is calculated as follows:

$$\omega_R(h) = 2.5 - (ah^b) \tag{18}$$

Restriction of low soil hydraulic conductivity, $\omega_{Kdry}(h)$, in the dry range starts from h = 12,000 cm, increasing with h. It is calculated using the following equation:

$$\omega_{Kdry}(h) = \left[\frac{12{,}000}{h}\right]^{-d} \tag{19}$$

where the power d is the fitting empirical parameter of the function:

$$K_r(h) = Ch^d \tag{20}$$

According to Groenevelt et al. (2001), $\omega_{Kdry}(h)$ is relevant at the h range of 12,000–15,000 cm, therefore, Eq. (20) is fitted in this range to the $K_r(h)$ data generated from Eq. (11) in order to obtain the estimate of d. According to Groenevelt et al. (2001) and Asgarzadeh et al. (2014), the calculation of IWC is limited to h of 15,000 cm because negligible water is released from the majority of soils at greater values of h.

Since salinity (e.g. saline water or saline soils) can significantly decrease the SAW through the osmotic effect, Groenevelt et al. (2004) proposed another weighting function, $\omega_o(h)$, accounting for the effect of salinity on the water available to plants. Based on the fact that the differential water capacity indicates the rate of soil water release and, as consequence, salinity increases upon drying, Groenevelt et al. (2004) introduced the following function for salinity limitation:

$$\omega_o(h, h_{os}) = \left[1 + h_{os}\left(\frac{\theta_s}{\theta^2}\right)C(h)\right]^{-1} \tag{21}$$

where $\omega_o(h,h_{os})$ is the weighting function for salinity restriction expressed as a function of the matric head (h) and osmotic head at saturation (h_{os}); θ_s is the volumetric water content at saturation, θ is the volumetric water content and $C(h)$ is the differential water capacity (Groenevelt et al., 2004), as defined by Eq. (12). According to Groenevelt et al. (2004), h_{os} is not easy to be measured directly, however, an approximate indirect relationship exists between h_{os} (m) and the electrical conductivity of saturated soil extract (EC_e, dS m^{-1}), according to USDA Handbook, No. 60 (Richards, 1953):

$$h_{o_s} = 3.6EC_e \tag{22}$$

Therefore, in order to consider the weighting function of salinity effect on IWC according to the method proposed by Groenevelt et al. (2004), the soil water retention curve, $\theta(h)$, or its derivative, $C(h)$, and EC_e, are required as inputs (see Eqs. (21) and (22)).

2.3. Integral energy (E_I)

Soil water retention function is integrated over the corresponding available water range to calculate the E_I values (Asgarzadeh et al., 2011, 2014). The E_I (J kg^{-1}) for the available water values (i.e. IWC) is calculated using the modified and generalized equation of Minasny and McBratney (2003), as presented by Asgarzadeh et al. (2011, 2014):

$$E_I = \frac{1}{10SAW}\int_{h_i}^{h_f} h\left(\prod_{i=1}^{n}\omega_i(h)\right)C(h)dh \tag{23}$$

where h_i and h_f are boundary matric heads (cm) at the wet (initial) and dry (final) ends, respectively, SAW (m^3 m^{-3}) is the volumetric soil available water that can be calculated by different approaches; the other symbols were previously defined. The constant 10 is used to convert the units of E_I from cm to J kg^{-1}. The values of h_i and h_f for IWC are found by determining when one of the values for $\omega_i(h)$ at the wet and dry ends becomes zero, respectively (see Asgarzadeh et al., 2011, 2014). The soil water retention function is used to generate 1000 discrete data in the h range 0–15,000 cm and the integration shown in Eq. (23) is done numerically by trapezoidal method (Spiegel, 1990).

3. The R package *soilphysics*

soilphysics is an easy-to-use R package which contains several functions relating to soil physics. The theory of LLWR and IWC was implemented into two functions: `llwr()` and `iwc()`, respectively. Users are required to pass simple input arguments. The outputs were designed to be concise and both functions provide didactic graphical solutions.

4. Function architecture

4.1. Function `llwr()`

The function `llwr()` needs the inputs required by the LLWR theory (Silva et al., 1994), which are essentially soil physical quantities, as follows:

```
llwr(theta, h, Bd, Pr,
  particle.density, air,
  critical.PR, h.FC, h.WP,
  water.model = c(''Silva'', ''Ross''),
  Pr.model = c(''Busscher'', ''noBd''),
  pars.water = NULL, pars.Pr = NULL,
  graph = TRUE, graph2 = TRUE,
  xlab = expression(Bulk~Density~(Mg~m^{-3})),
  ylab = expression(theta~(m^{3}~m^{-3})),
  main = ''Least Limiting Water Range'', ...)
```

The user has two main options to determine LLWR: (a) when the parameters of each model (Eq. (1) or Eq. (2), and Eq. (3) or Eq. (4)) need to be estimated, and b) when the user already knows the estimates. The latter requires passing the arguments `pars.water` and `pars.Pr`, which are optional; if it is left as "NULL" (default), then `llwr()` calculates nonlinear least squares estimates via Newton–Raphson algorithm. Users can choose the water retention model (Eqs. (1) and (2)) and soil penetration resistance model (Eqs. (3) and (4)) using the argument `water.model` and `Pr.model`, respectively. It must be either "`Silva`" (default, Silva et al., 1994) or "`Ross`" (Ross et al., 1991), when for water retention model, and "`Busscher`" (default, Busscher, 1990) or "`noBd`" (power model), when for soil penetration resistance model. The specification of all arguments is available in the *soilphysics* manual (R Core Team, 2015). Nevertheless, the easiest way of using `llwr()` basically requires a $n \times 4$ numeric matrix (n rows and four columns) or four vectors of length n containing the values of soil water content (`theta`), matric head (`h`), dry bulk density (`Bd`) and soil penetration resistance (`Pr`) on n observations. When there is no bulk density variation, a single value of bulk density (`Bd`) can be passed; in addition, `llwr()` requires the particle density value (`particle.density`), the value of the limiting volumetric air content (`air`), the critical value of the soil penetration resistance (`critical.PR`), the value of the matric head at the field capacity (`h.FC`) and the value of the matric head at the wilting point (`h.WP`). These values have been used as 2.65 Mg m^{-3}, 0.1 m^3 m^{-3}, 2.0 MPa, 100 or 330 cm and 15,000 cm, respectively (Silva et al., 1994; Leão et al., 2005; Guedes Filho et al., 2013). Finally, the arguments `''graph''`, `''graph2''`, `"xlab"`, `''ylab''`, `''main''` and `''...''` are optional.

4.2. Function `iwc()`

The inputs required on the function `iwc()` are all based on the IWC theory (Groenevelt et al., 2001, 2004; Asgarzadeh et al., 2014), as follows:

```
iwc(theta_R, theta_S, alpha, n, a, b, hos = 0,
  graph = TRUE,
  xlab = ''Matric head (cm)'',
  ylab = ''Water content'', ...)
```

Basically, arguments consist of the parameters θ_r (`theta_R`), θ_s (`theta_S`), α (`alpha`) and n (`n`) of the van Genuchten (1980) model for water retention curve (Eq. (10)), the parameters a (`a`) and b (`b`) of the power model for soil penetration resistance curve (Eq. (13)), and the osmotic head of the saturated soil extract, h_{os}, (`hos`), (Groenevelt et al., 2004). If the argument "`hos = 0`" is left to be 0 (as default), it means that the salinity limitation is ignored. For more details about the specification of each argument, consult the *soilphysics* manual (R Core Team, 2015).

5. Calculations performed in *soilphysics*

5.1. Determining `llwr()`

soilphysics uses Eqs. (1)–(9) for determining LLWR. Parameters are estimated using a self-start Newton–Raphson algorithm for non-linear fitting. After convergence, *soilphysics* outputs the summary and the statistical significance of the estimates for the water retention and penetration resistance curves. If convergence is not achieved, a warning message is printed on console.

The statistical significance for coefficients of both the water retention (Eqs. (1) or (2)) and the penetration resistance (Eqs. (3) or (4)) models is calculated through the non-linear least squares method. The residuals are considered to be normally distributed with mean zero and variance σ^2. Likewise, the vector of estimates, $\hat{\boldsymbol{\beta}}$, is considered to be, asymptotically, normally distributed with mean $\boldsymbol{\beta}$ and covariance $\mathbf{H}^{-1}(\hat{\boldsymbol{\beta}})\sigma^2$, where $\mathbf{H}$ is the Hessian matrix and σ^2 is the error variance, estimated by:

$$\hat{\sigma}^2 = \frac{1}{N-p}\sum_{i=1}^{n}\left[y_i - f(\mathbf{x}_i, \hat{\boldsymbol{\beta}})\right]^2 \tag{24}$$

where y_i corresponds to the i-th ($i = 1,2,\ldots,N$) observation being modeled, $\mathbf{x}_i$ is the i-th vector of explanatory variables and p is the number of parameters. Then, p-value associated with each parameter in $\boldsymbol{\beta}$ is calculated by means of the t-Student variable with $N-p$ degrees of freedom.

5.2. Coefficient of determination

The pseudo-coefficient of determination (R^2) is calculated by:

$$R^2 = 1 - \frac{(N-p)\hat{\sigma}^2}{\sum_{i=1}^{n}[y_i - \bar{y}]^2} \tag{25}$$

The adjusted value (for N and p) of R^2 is calculated by:

$$R^2_{adj} = 1 - \frac{N(1-R^2)}{N-p} \tag{26}$$

5.3. The shaded area

The shaded area presented on the graphical solution of the LLWR is obtained by:

$$\begin{aligned} A &= \int_{\rho\in\Omega} \min\left[f_{\theta_A}(\rho), f_{\mathrm{FC}}(\rho)\right]d\rho - \int_{\rho\in\Omega}\max\left[f_{\mathrm{PR}}(\rho), f_{\mathrm{WP}}(\rho)\right]d\rho \\ &= \int_{\rho\in\Omega}\min\left[\left(1-\frac{\rho}{\rho_p}\right) - \theta_A,\ \exp(a+b\rho)h_{\mathrm{FC}}^c\right]d\rho \\ &\quad - \int_{\rho\in\Omega}\max\left[\left(\frac{\mathrm{PR}}{b_0\rho^{b_2}}\right)^{\frac{1}{b_1}},\ \exp(a+b\rho)h_{\mathrm{WP}}^c\right]d\rho \end{aligned} \tag{27}$$

where ρ is the bulk density, Ω defines the range of bulk density over which the LLWR lies, ρ_p is the value of particle density, θ_A is the value of critical volumetric air content, a, b and c are the parameters of the water retention model, h_{FC} and h_{WP} are the values of matric heads at the field capacity and wilting point, respectively, PR is the critical value of soil penetration resistance, b_0, b_1 and b_2 are the parameters of the soil penetration resistance model. Eq. (27) is evaluated numerically, by the means of the trapezoidal method.

5.4. Determining `iwc()`

soilphysics uses Eqs. (10)–(21) for calculating IWC and Eq. (23) for determining E_I, according to Groenevelt et al. (2001, 2004) (for salinity effect) and Asgarzadeh et al. (2014).

6. Examples

6.1. Illustrating LLWR

As an example, we used a data set also used by Leão and da Silva (2004) (Table 1). They used a simplified Excel® algorithm for determining LLWR of a silt loam soil. This data set is available in *soilphysics* under the name `skp1994`. The columns BD, W, PR and h correspond to the values of dry bulk density, soil water content, soil penetration resistance and matric head, numeric vectors to be passed for the arguments `Bb`, `theta`, `Pr` and `h`, respectively. According to Leão and da Silva (2004), the particle density is 2.65 Mg m^{-3}, the critical value of the soil volumetric air content is 0.1 m^3 m^{-3}, the critical value of the soil penetration resistance is 2.0 MPa, and the matric heads at field capacity and wilting point are 100 and 15,000 cm, respectively. For modeling the soil water retention and soil penetration resistance curves, Leão and da Silva (2004) used the models suggested by Silva et al. (1994) and Busscher (1990), respectively, where bulk density is required in both models. In part of the data set (first 7 rows) shown in Table 1, the matric head is given in cm. In the examples shown in this paper, also available from *soilphysics*, values of bulk density, water content, soil penetration resistance and matric head are given in Mg m^{-3}, m^3 m^{-3}, MPa and cm, respectively, although it does not prevent the user to use other units. Nonetheless, one must be certain that units match, so that values can be consistently calculated. To see more about usual units for calculating LLWR and IWC, consult Leão and da Silva (2004), Groenevelt et al. (2001, 2004) and Asgarzadeh et al. (2014).

The LLWR is determined by the following command lines:

```
llwr(theta = W, h = h, Bd = BD, Pr = PR,
  particle.density = 2.65, air = 0.1,
  critical.PR = 2.0, h.FC = 100, h.WP = 15000)
```

After running the code above, the estimates of the parameters of the water retention model (default, Silva et al., 1994) and the penetration resistance model (default, Busscher, 1990) as well as their

Table 1
Part of the data set (first 7 rows) used by Leão and da Silva (2004) and available in *soilphysics* to exemplify the inputs of `llwr()` function, where BD, W, PR and h are bulk density, volumetric water content, soil penetration resistance and matric head, respectively.

BD (Mg m^{-3})	W (m^3 m^{-3})	PR (MPa)	h (cm)
1.35	0.43	0.23	20
1.53	0.41	1.16	20
1.36	0.45	0.20	20
1.46	0.43	0.38	20
1.53	0.40	0.42	20
1.44	0.43	0.37	20
1.47	0.41	1.03	20
...	...	...	...

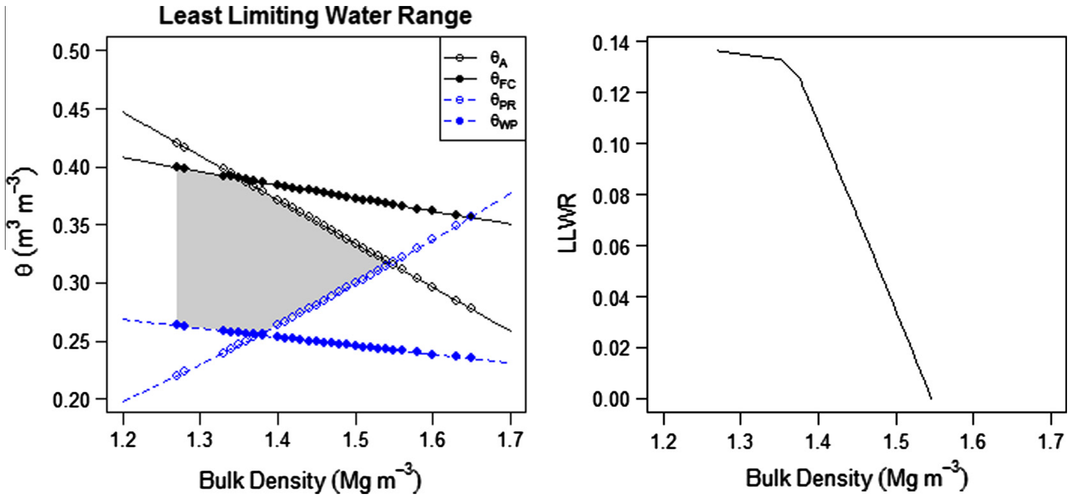

Fig. 1. Output from `llwr()` function in the *soilphysics*: graphical presentation for upper and lower limits and LLWR ($m^3\ m^{-3}$) as a function of bulk density. Data set extracted from Leão and da Silva (2004).

standard errors, t values and statistical significance are printed on console. We present the estimates obtained for this example in the Section 7. Finally, a graph containing the LLWR limits (Fig. 1) is created. The function contains an algorithm to paint (in gray) the interval (i.e. LLWR), as bounded by θ_{FC} or θ_A, and θ_{WP} or θ_{PR}. The shaded area is also calculated by `llwr()`.

6.2. Illustrating LLWR using a single value of bulk density

A similar code is presented in this section to exemplify the calculation of LLWR in the case where there is no bulk density variation. For this reason, power models are considered to estimate the parameters of the water retention and the soil penetration resistance curves, as suggested by Ross (1991) and Asgarzadeh et al. (2014). When a single value of bulk density is passed to the argument `Bd`, the functions presented in Eqs. (1) and (3) are automatically fitted.

```
llwr(theta = W, h = h, Bd = 1.5, Pr = PR,
  particle.density = 2.65, air = 0.1,
  critical.PR = 2.0, h.FC = 100, h.WP = 15000)
```

After running the code above, the estimates of the parameters of the water retention model (Ross et al., 1991) and penetration resistance model (power model) are given, as well as their statistical significance. The value of LLWR can be displayed on console and a graph illustrates its limits (Fig. 2).

6.3. Illustrating IWC

For illustrating the calculation of IWC in *soilphysics*, we used the example (i.e. the parameter estimates) available in Asgarzadeh et al. (2014). We divided the calculations into two parts: without and with salinity effect, as presented in the following codes:

```
iwc(theta_R = 0.166, theta_S = 0.569, alpha = 0.029,
  n = 1.308, a = 0.203, b = 0.256) # without salinity effect
```

```
iwc(theta_R = 0.166, theta_S = 0.569, alpha = 0.029,
n = 1.308, a = 0.203, b = 0.256, hos = 200) # with salinity
  effect
```

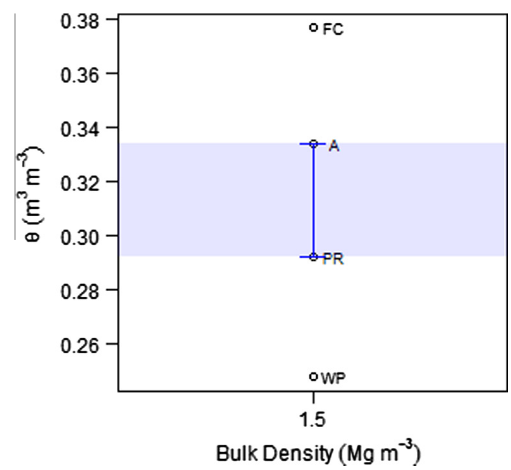

Fig. 2. Output of the function `llwr()`: graphical representation of the limits of LLWR for a single value of soil bulk density, equal to 1.5 Mg m^{-3}. Data set extracted from Leão and da Silva (2004). Where FC, A, PR and WP are the limiting volumetric water contents at field capacity, critical volumetric air content, critical soil penetration resistance and wilting point, respectively.

The salinity effect is not considered in SAWCal (Asgarzadeh et al., 2014) yet, but we used an EC_e of 0.56 dS m^{-1}, available from Groenevelt et al. (2004) in this example. Thus, using Eq. (20), the h_{os} value corresponding to $EC_e = 0.56$ dS m^{-1} is 2 m (i.e. $h_{os} = 3.6 \times 0.56 = 2.0$ m). The function `iwc()` requires the h_{os} value in cm, so the value 200 cm (after converting m to cm) must be passed to the argument "`hos`", as showed in the second code (with salinity effect).

A summary table containing the values of IWC and E_I will be displayed on the R console. A graphical representation of the differential water capacity, $C(h)$, and the effective differential water capacity, $E(h)$, by considering the limitations of high hydraulic conductivity and low soil aeration (in the wet range) and the restrictions of low hydraulic conductivity and high soil penetration resistance (in the dry range) are also plotted. Fig. 3 shows the result for the first code, i.e., ignoring the salinity effect. In Fig. 4, the same functions are presented under the salinity limitation (h_{os} = 200 cm)

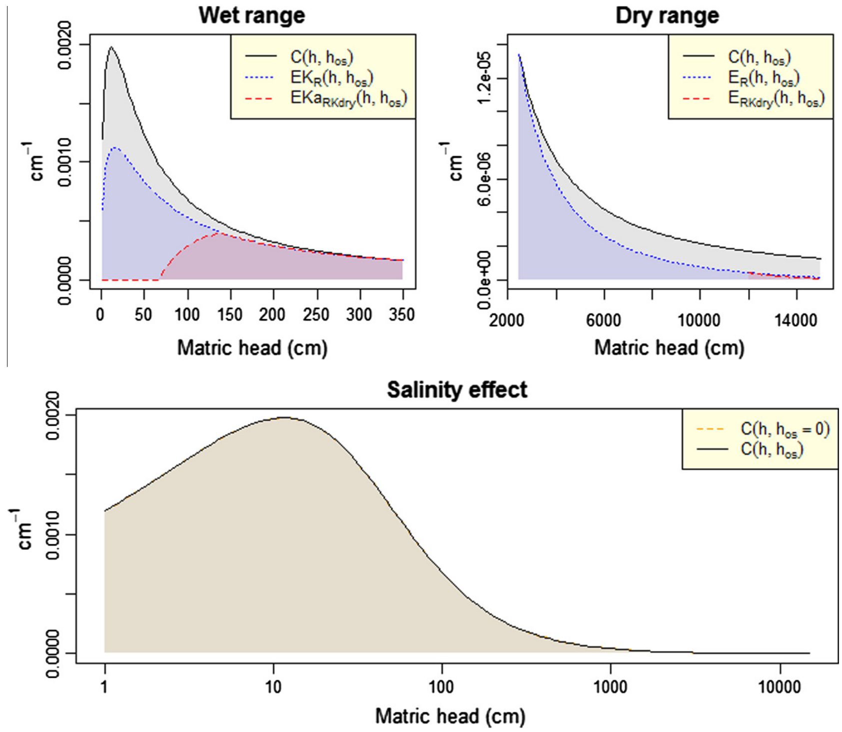

Fig. 3. Output from `iwc()` function without considering salinity effect in the *soilphysics*. Graphical presentation of differential water capacity ($C(h, h_{os})$) and effective differential water capacity ($E(h, h_{os})$) for the wet and dry ranges as a function of matric head (h). Parameters are extracted from the example in Asgarzadeh et al. (2014).

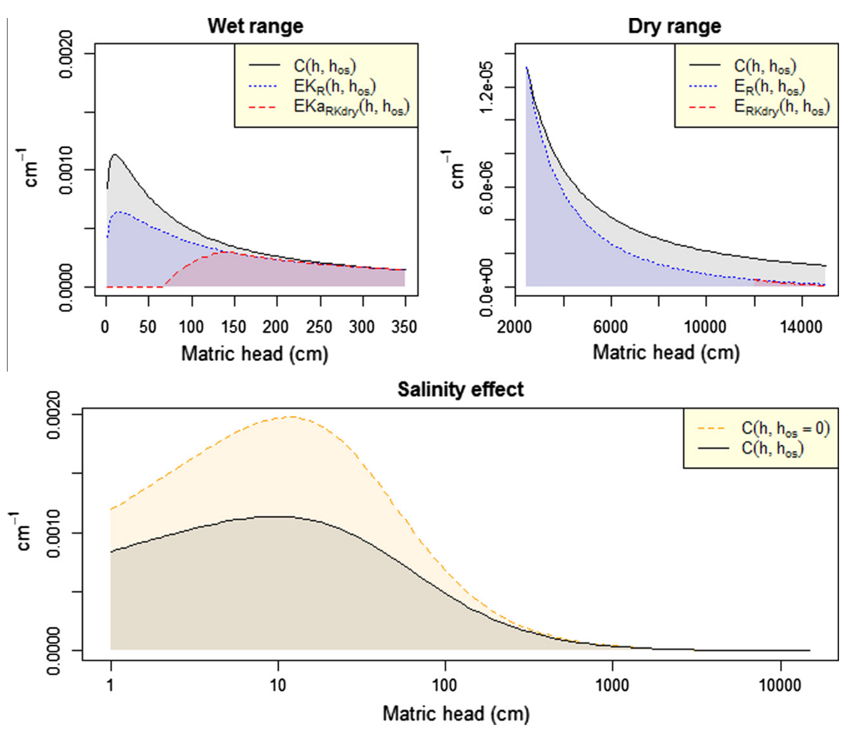

Fig. 4. Output from `iwc()` function with considering salinity effect in the *soilphysics*. Graphical presentation of differential water capacity ($C(h, h_{os})$) and effective differential water capacity ($E(h, h_{os})$) for the wet and dry ranges as a function of matric head (h). Parameters are extracted from the example in Asgarzadeh et al. (2014) with h_{os} = 200 cm (EC = 0.56 dS m^{-1}, Groenevelt et al., 2004).

Table 2
Comparisons between fitted[a] parameters of soil water retention (Eq. (2); Silva et al., 1994) and penetration resistance (Eq. (4); Busscher, 1990) models and coefficient of determination (R^2) as calculated by *soilphysics* and Leão and da Silva (2004) algorithm.

Model	Program	*a*	*b*	*c*	R^2
Soil water retention curve	*soilphysics* (`llwr`)	−0.92	−0.30	−0.08	0.89
	Leão and da Silva (2004)	−0.92	−0.30	−0.08	0.89
		d	*e*	*f*	
Soil penetration resistance curve	*soilphysics* (`llwr`)	0.08	−1.66	3.08	0.67
	Leão and da Silva (2004)	0.08	−1.61	3.06	0.66

[a] In order to compare estimates, matric head data were transformed into MPa, as used by Leão and da Silva (2004).

Table 3
Comparisons of IWC and E_I calculations by SAWCal, MS Excel and *soilphysics*, all based on van Genuchten (1980) model for water retention curve, power model for penetration resistance curve (see Asgarzadeh et al., 2014), and EC_e values from Groenevelt et al. (2004), with h_{os} calculated using Eq. (22) and converted to cm (USDA Handbook, No. 60, Richards, 1953). IWC is calculated for h_{os} = 200 and 800 cm, using the parameters from the examples 1 and 2, respectively, for the results with considering salinity effect.

	Example	Input parameters						
		van Genuchten model				Power model		–
		θ_s ($m^3\ m^{-3}$)	θ_r ($m^3\ m^{-3}$)	α (cm^{-1})	*n* –	*a* ($MPa\ cm^{-1}$)	*b*	EC_s ($dS\ m^{-1}$)
	1	0.569	0.166	0.029	1.308	0.203	0.256	0.56
	2	0.482	0.016	0.047	1.298	0.203	0.255	2.22

Program	Example	IWC ($m^3\ m^{-3}$)	E_I ($J\ kg^{-1}$)	h_{os} (cm)
		Results without considering salinity effect		
SAWCal	1	0.1888	130.8	0
`iwc()`		0.1896	136.0	0
SAWCal	2	0.2327	111.4	0
`iwc()`		0.2333	116.4	0
		Results with considering salinity effect		
MS Excel	1	0.1684	141.0	200
`iwc()`		0.1689	147.8	200
MS Excel	2	0.1088	180.0	800
`iwc()`		0.1094	186.7	800

7. Results and comparisons

7.1. LLWR by `llwr()`

We compared the results calculated by `llwr()` function with those obtained using the Excel® algorithm presented by Leão and da Silva (2004). Results are shown in Table 2. Both algorithms have promoted the same values, with negligible differences.

7.2. IWC by `iwc()`

We also compared the results calculated by `iwc()` function with those obtained through SAWCal (Asgarzadeh et al., 2014) for the examples without considering salinity effect (Table 3). The results of both software (SAWCal and *soilphysics*) are essentially the same, again with only negligible differences (Table 3). However, there is no software available for comparing the results obtained by *soilphysics* when dealing with salinity effect.

8. Availability of *soilphysics*

soilphysics is freely available as an R (R Core Team, 2015) package from the Comprehensive R Archive Network (http://CRAN.R-project.org/package=soilphysics). Thus, users first need to download a recent version of R, which is also available from CRAN.

9. Conclusions

We have developed a user-friendly R package, called *soilphysics*, which has two functions related to available soil water, `llwr()` and `iwc()`, for determination of the least limiting water range (LLWR), the integral water capacity (IWC) and the integral energy (E_I). In addition, we included an option for the user to calculate IWC by considering salinity effect on the soil available water.

We compared the LLWR, IWC and E_I calculations by *soilphysics* with those obtained using a published MS Excel® spreadsheet and the software SAWCal. The results are essentially the same, with negligible differences (<4%).

The functionalities presented should help to popularize the application of plant-available water indices in agriculture and soil science. The package *soilphysics* is freely distributed and it is currently available from http://cran.r-project.org/web/packages/soilphysics/index.html.

Acknowledgements

We thank the Coordination for Improvement of Higher Level Personnel (CAPES, Brazil) for granting scholarships, and the Goiano Federal Institute (Brazil) for the financial support, as well as to the referees of this paper for their thoughtful reviews.

Appendix A. Supplementary material

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.compag.2015.11.003.

References

Asgarzadeh, H., Mosaddeghi, M.R., Mahboubi, A.A., Nosrati, A., Dexter, A.R., 2010. Soil water availability for plants as quantified by conventional available water, least limiting water range and integral water capacity. Plant Soil 335, 229–244.

Asgarzadeh, H., Mosaddeghi, M.R., Mahboubi, A.A., Nosrati, A., Dexter, A.R., 2011. Integral energy of conventional available water, least limiting water range and integral water capacity for better characterization of water availability and soil physical quality. Geoderma 166, 34–42.

Asgarzadeh, H., Mosaddeghi, M.R., Nikbakht, A.M., 2014. SAWCal: A user-friendly program for calculating soil available water quantities and physical quality indices. Comput. Electron. Agric. 109, 86–93.

Busscher, W.J., 1990. Adjustment of flat-tipped penetrometer resistance data to a common water content. Trans. ASAE 33, 519–524.

Groenevelt, P.H., Grant, C.D., Murray, R.S., 2004. On water availability in saline soils. Aust. J. Soil Res. 42, 833–840.

Groenevelt, P.H., Grant, C.D., Semetsa, S., 2001. A new procedure to determine soil water availability. Aust. J. Soil Res. 39, 577–598.

Guedes Filho, O., Blanco-Canqui, H., Silva, A.P., 2013. Least limiting water range of the soil seedbed for long-term tillage and cropping systems in the central Great Plains, USA. Geoderma 207–208, 99–110.

Leão, T.P., da Silva, A.P., 2004. A simplified Excel® algorithm for estimating the least limiting water range of soils. Sci. Agricola 61, 649–654.

Leão, T.P., da Silva, A.P., Perfect, E., Tormena, C.A., 2005. An algorithm for calculating the least limiting water range of soils. Agrono. J. 97, 1210–1215.

Letey, J., 1985. Relationship between soil physical properties and crop production. Adv. Soil Sci. 1, 277–294.

Minasny, B., McBratney, A.B., 2003. Integral energy as a measure of soil–water availability. Plant Soil 249, 253–262.

Mualem, Y., 1976. A new model for predicting the hydraulic conductivity of unsaturated porous media. Water Resour. Res. 12, 513–522.

Omuto, C.T., Gumbe, L.O., 2009. Estimating water infiltration and retention characteristics using a computer program in R. Comput. Geosci. 35, 579–585.

R Core Team, 2015. *R:* A language and environment for statistical computing. R Foundation for Statistical Computing, Vienna, Austria. Available from: <http://www.R-project.org/. Verified on May 03, 2015>.

Richards, L.A. (Ed.), 1953. Diagnosis and Improvement of Saline and Alkali Soils. USDA Agricultural Handbook No. 60. United States Saline Laboratory Staff, Riverside CA.

Ross, P.J., Willians, J., Bristow, K.L., 1991. Equations for extending water retention curves to dryness. Soil Sci. Soc. Am. J. 55, 923–927.

Silva, A.P., Kay, B.D., Perfect, E., 1994. Characterization of the least limiting water range of soils. Soil Sci. Soc. Am. J. 58, 1775–1781.

Spiegel, M.R., 1990. Mathematical Handbook of Formulas and Tables. Schaum's Outline Series, 25th Printing. McGraw-Hill Publishing Company.

van Genuchten, M.T., 1980. A closed-form equation for predicting the hydraulic conductivity of unsaturated soils. Soil Sci. Soc. Am. J. 44, 892–898.

Veihmeyer, F.J., Hendrickson, A.H., 1927. The relation of soil moisture to cultivation and plant growth. In: Proceedings of 1st International Congress of Soil Science, vol. 3, pp. 498–513.

Veihmeyer, F.J., Hendrickson, A.H., 1931. The moisture equivalent as a measure of the field capacity of soils. Soil Sci. 32, 181–193.