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7	Simultaneous estimation of the soil hydraulic conductivity and the van
8	Genuchten water retention parameters from an upward infiltration
9	experiment
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#### 26 ABSTRACT

Accurate characterization of the saturated hydraulic conductivity,  $K_s$ , and the water 27 retention curve,  $\theta(h)$ , are crucial to correctly model the water flow into the soil. This 28 paper presents a new laboratory method to simultaneously estimate  $K_s$  and  $\alpha$  and n29 parameters of the van Genuchten (1980)  $\theta(h)$  from the inverse analysis of an upward 30 infiltration curve measured in a 5-cm high soil column. The method was evaluated on 31 synthetic 1D infiltration curves generated for a theoretical loamy sand, loam and clay 32 soil. In a first step, the  $K_s$ - $\alpha$ , n- $K_s$  and  $\alpha$ -n error maps were evaluated, using in each case 33 the remaining theoretical hydraulic parameter. The influence of the soil initial condition 34 35 on the inverse analysis was also studied. Next, an optimization method was presented 36 and tested on eight theoretical soils (from loamy sand to clay). The method was subsequently applied to experimental infiltration curves measured on five sieved soils 37 38 (from sand to clay) packed in 5-cm high and diameter cylinders. The  $K_s$ ,  $\alpha$  and n values estimated from the inverse analysis of the experimental curves were compared to those 39 measured by Darcy and the pressure cell method (PC). The initial soil tension,  $h_i$ , which 40 had an important influence on the optimization, was fixed to  $-6.0 \ 10^5$  cm. A unique 41 42 minimum was observed in all  $K_s$ - $\alpha$ , n- $K_s$  and  $\alpha$ -n error maps generated for the synthetic 43 loamy sand, loam and clay soils. The optimization method resulted robust and allowed accurate estimates of the actual hydraulic parameters. A close to one relationship ( $R^2 =$ 44 0.99) was observed between the theoretical  $K_s$ ,  $\alpha$  and n and the corresponding values 45 obtained with the inverse analysis. Regarding to the experimental soils, significant 46 relationships close to one were obtained between  $K_s$  and n ( $\mathbb{R}^2 > 0.98$ ) estimated from 47 inverse analysis and those measured with Darcy and PC. A non-significant relationship 48 with slope away from one was found for  $\alpha$ . 49

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# 52

**1. INTRODUCTION** 

Characterization of the hydraulic conductivity, K, and the water retention curve,  $\theta(h)$ , 54 is crucial to determine the water flow in the vadose zone. K is a measure of the soil 55 ability to transmit water when soil is submitted to a hydraulic head gradient. This 56 parameter depends on the soil water content, the pressure head and the flux across the 57 58 boundary of a soil compartment (Dane and Hopmans 2002). The soil water retention curve describes the relationship between the volumetric water content,  $\theta [L^3 L^{-3}]$ , and 59 the matric potential, h [L].  $\theta(h)$  depends upon the particle-size distribution, which 60 determines the soil texture, and the arrangement of the solid particles, which refers to 61 the soil structure (Dane and Hopmans, 2002). One of the most common functions used 62 to describe  $\theta(h)$  is the unimodal van Genuchten (1980) model, which is defined by the 63 64 saturated  $(\theta_s)$  and residual  $(\theta_r)$  volumetric water content and the empirical  $\alpha$  and n factors. An additional m parameter, commonly defined as  $m = 1 - \left(\frac{1}{n}\right)$ , is also 65 employed.  $\theta_r$  is defined as the water content for which the gradient  $d\theta/dh$  becomes zero 66 (excluding the region near  $\theta_s$  which also has a zero gradient), n [-] is the slope of  $\theta(h)$ 67 and is related to pore-size distribution, and  $\alpha$  [L<sup>-1</sup>] is a scale factor that defines the shape 68 69 of  $\theta(h)$  near  $\theta_s$ .

*Keywords*: Soil Hydraulic Properties; Sorptivity; Inverse Analysis; Richard's Model.

The saturated hydraulic conductivity,  $K_s$ , can be measured with either the constant head or the falling-head method (Klute and Dirksen, 1986). The reference laboratory method used to determine  $\theta(h)$  is the pressure extractor (Klute, 1986). Although this technique has been improved by incorporating alternative methods to determine  $\theta$ (Jones et al., 2005; Moret-Fernández et al., 2012), the long time needed to conclude a measurement together with its limitations on fine textured soils (Solone et al., 2012) can
restrict its use.

77 Other family of methods to estimate K and  $\theta(h)$  are based on the inverse numerical 78 analysis of Richard's transient water flows. The main advantage of these techniques is 79 the simultaneous estimation of  $\theta(h)$  and K(h). To date, four different methods based on 80 the inverse analysis of a transient water flow are available: evaporation and horizontal, downward- and upward-infiltration processes. The evaporation method is based on the 81 Wind (1968) formulation, where soil tension is measured within a vertical soil column 82 83 as water evaporates from its surface using tensiometers installed at multiple depths, and water content and flux are determined by weighing the column. In more recent studies, 84 85 Wind's method has been modified and simplified (e.g., Schindler, 1980; Simunek et al., 1996; Schindler and Müller, 2006; Schindler et al., 2010; Masaoka and Kosugi, 2018). 86 The horizontal infiltration method is based on the Shao and Horton (1998) procedure, 87 88 where the saturated hydraulic conductivity is measured by Darcy, and  $\alpha$  and n van Genuchten (1980) parameters are estimated with an integral method that solves the 89 problem of water absorption into a horizontal soil column. To this end, a soil column 90 inserted in a 20 cm-length transparent cylinder should be used. The downward 91 92 infiltration method analyzes cumulative infiltration rates measured with a disc infiltrometer at several consecutive tensions (Simunek and van Genuchten, 1997). The 93 combination of multiple tension cumulative infiltration data with measured initial and 94 final water contents yields unique solutions of the inverse problem for the unknown 95 96 parameters. This method has been successfully used in several studies, such as Ramos et al. (2006), Caldwell et al. (2013) or Rashid et al. (2015), among others. 97

98 Up to date, different laboratory upward infiltration methods have been developed. 99 Hudson et al. (1996) estimated  $\theta(h)$  and K(h) from the inverse analysis of an upward

flow using a constant flux of water at the bottom of the soil sample. Young et al. (2002) 100 combined the water cumulative flux and the soil pressure head measured by two 101 tensiometers installed along a 15-cm-long soil column. Although this technique gave 102 103 satisfactory results, the long soil columns used in the experiment together the use of tensiometers may prevent its use in undisturbed soil samples. Moret-Fernández et al. 104 105 (2016b) developed a method where  $K_s$  was calculated according to the Darcy's law and the  $\theta(h)$  parameters were estimated from the inverse analysis of a multiple tension water 106 absorption curve. Although the method proved effective, the high negative pressure 107 108 head needed at the beginning of the experiment restricted its use to sieved soils. Peña-Sancho et al. (2017) estimated the soil hydraulic properties from a capillary wetting 109 process at saturation followed by an overpressure step and an evaporation process. In 110 this case,  $K_s$  was calculated by Darcy and the hysteresis phenomenon was introduced 111 using an empirical model. Finally, Moret-Fernández and Latorre (2017) estimated the 112  $\theta(h)$  parameters from  $K_s$  measured by Darcy and the sorptivity, S, and  $\beta$  parameter 113 (Haverkamp et al., 1994). In this case S and  $\beta$  were estimated from the inverse analysis 114 115 of an upward infiltration curve. Although this technique was satisfactorily validated on 5-cm high theoretical and experimental soils, the employed formulation restricted its 116 117 use to soils ranged from sand to silt textural classes (Lassabatere et al., 2009).

118 Although all above cited references show that the upward infiltration is an effective 119 process to estimate  $\theta(h)$  and K(h), further efforts are needed to develop an alternative 120 method that allows simultaneous estimate of all hydraulic properties, in any kind of soil 121 and using short soil columns. This work presents a new method to determine  $K_s$ ,  $\alpha$  and 122 *n* from the inverse analysis of an upward infiltration curve measured on a 5-cm high soil 123 column. The method was firstly evaluated with a global analysis applied on upward 124 infiltration curves generated by HYDRUS-1D for a loamy sand, loam and clay soil. The influence of the initial soil pressure head on the inverse analysis was also studied. Next,
an optimization method was proposed and tested on eight theoretical soils. The method
was finally applied on experimental infiltration curves measured on different sieved
soils of known hydraulic properties.

129

#### 130 2. MATERIAL AND METHODS

## 131 **2.1. Theory**

132 The one-dimensional water flow equation in a variably saturated rigid porous medium133 is defined by the Richards model

134 
$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left( K \frac{\partial h}{\partial z} + K \right)$$
(1)

135 where  $\theta$  is the volumetric soil water content [L<sup>3</sup> L<sup>-3</sup>], *t* is time [T], *z* is a vertical 136 coordinate [L], positive upward, *h* is the soil-water pressure head [L] and *K* is the 137 hydraulic conductivity [L T<sup>-1</sup>].

138 The soil hydraulic functions can be described by the van Genuchten-Mualem functions139 (van Genuchten, 1980)

140 
$$S_e(h) = \frac{\theta(h) - \theta_r}{\theta_s - \theta_r} = \left[1 + (\alpha h)^n\right]^m$$
(2)

141 
$$K(S_{e}) = K_{s}S_{e}^{l} \left[1 - \left(1 - S_{e}^{\frac{1}{m}}\right)^{m}\right]^{2}$$
(3)

where  $S_e$  is the effective saturation [-],  $\theta_s$  and  $\theta_r$  are the saturated and residual water content, respectively,  $\alpha$  [L-1] and n [-] are shape parameters, m=1-1/n, l is a poreconnectivity parameter and  $K_s$  is the saturated hydraulic conductivity. Similar to defined by Simunek et al. (1996, 1998), Simunek and van Genuchten et al. (1997) and Young et al. (2002), among others, *l* was fixed to 0.5. Because  $\theta_r$  and  $\theta_s$  can be easily measured at the beginning and the end of the experiment, respectively, the hydraulic characteristics defined by Eq. (2) and (3) were reduced to three unknown parameters:  $\alpha$ , *n* and *K*<sub>s</sub>. In our case, these equations represent the wetting branch of the unsaturated hydraulic properties.

The soil sorptivity, *S*,  $[L T^{-0.5}]$  is defined as the capacity of a porous medium to absorb liquid by capillarity (Philip, 1957). *S*, expressed as function of the van Genuchten (1980) parameters, results (Moret-Fernández, et al., 2017a)

$$S^{2} = \frac{(1-m)K_{s}}{\alpha m(\theta_{s}-\theta_{r})} \int_{\theta_{i}}^{\theta_{s}} \left[\theta_{s}+\theta-2\theta_{i}\right] S_{e}^{\frac{\gamma_{2}-\gamma_{m}}{m}} \left[\left(1-S_{e}^{\frac{\gamma_{m}}{m}}\right)^{-m}+\left(1-S_{e}^{\frac{\gamma_{m}}{m}}\right)^{m}-2\right] d\theta$$

$$(4)$$

where  $\theta_i$  is the initial water content. The soil sorptivity expressed as function of an upward infiltration curve,  $S^*$ , can be expressed as (Moret-Fernández, et al., 2017a)

$$157 I = S^* \sqrt{t} - Ct (5)$$

where I [L] is the cumulative upward infiltration and C is a constant that is related to the soil hydraulic conductivity (Minasny and McBratney, 2000). This equation is only valid for short-medium infiltration times.

161

# 162 **2.2. Numerical simulations**

163 The synthetic upward infiltration data was generated using the HYDRUS-1D 164 software (Simunek et al., 1996). The method was tested on eight theoretical soils 165 (Carsel and Parrish, 1988) ranged from loamy sand to clay soil textural classes (Table 166 1).

A 5 cm-high soil column was discretized with a 1-D mesh of 1000 cells. Previous 167 168 conducted numerical analysis demonstrated that, under this discretization, the solution was grid independent. The initial time step in the simulation, which value depended on 169 the total infiltration time, varied from  $10^{-5}$  s to 0.025 s for sand to clay, respectively. 170 The tension at the base of the soil column was 0 cm. The evaporation rate was 171 considered null and atmospheric conditions with a maximal tension of 0 cm was 172 173 imposed at the top boundary. Time cero corresponded to the beginning of the upward 174 infiltration process, and the simulation finished when the wetting front arrived to the soil surface. 175

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# 177 **2.3. Inverse analysis**

178 The  $\alpha$ , *n* and  $K_s$  parameters were calculated by minimizing an objective function, 179  $\Phi(\alpha, n, K_s)$ , that represents the difference between HYDRUS-1D simulated curves and 180 synthetic or experimental infiltration data

181 
$$\Phi = \sqrt{\frac{\sum_{i=1}^{N} (I_e(t_i) - I_s(t_i))^2}{N}}$$
(6)

where N is the number of measured *I* values,  $I_e(t_i)$  and  $I_s(t_i)$  are specific measurements at time  $t_i$ . The values of the objective function were initially summarized as contours lines in the  $K_s$ -n,  $\alpha$ -n, and  $K_s$ - $\alpha$  error maps, given in each plane the remaining theoretical hydraulic parameter.  $K_s$ ,  $\alpha$  and n values ranged from 10<sup>-5</sup> to 10<sup>-2</sup> cm s<sup>-1</sup>, 0.01 to 0.1 cm<sup>-1</sup>, and 1.01 to 3.0, respectively, and  $K_s$  and  $\alpha$  were logarithmically sampled. The parameter combination for each response surface were calculated on a rectangular grid. Each parameter was discretized into 100 points, resulting in 10000 grid points for each response surface. These error maps were generated for a theoretical loamy sand, loamand clay soil.

The influence of the initial pressure head  $(h_i)$  on the global optimization was studied on a synthetic loam soil. Two different initial soil tensions were compared: -1.0  $10^3$ , -6.0  $10^5$  cm. These  $h_i$  correspond to a soil sample in equilibrium with an atmosphere at 20 °C and relatively humidity of ~100 and 60%, respectively (RILEM, 1980).

196 Experimental data is subject to several sources of uncertainty (i.e. water level drop in the water reservoir, initial and final water content, etc.). Only the experimental error 197 198 corresponding to the water level measurement in the water reservoir was considered. A preliminary experiment performed with a  $\pm 72$  cm pressure transducer installed in a 1.9 199 cm-diameter water reservoir and connected to a 5 cm-diameter soil cylinder resulted in 200 201 a soil water infiltration measurement uncertainty of  $\pm 0.02$  mm. The change of the 202 objective function (Eq. 5) associated to the uncertainty source was first calculated and 203 superimposed on the response surfaces in the form of a contour line (0.02 mm).

The soil sorptivity defined in the cumulative upward infiltration curve (Eq. 5),  $S^*$ , was calculated by applying an objective function that calculates the squared difference between numerically generated and predicted cumulative infiltration curves, where we set it to be minimized based the target parameters (*S*,*C*).

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## 209 **2.4. Optimization method**

Previous studies on upward infiltration processes (Moret-Fernández et al., 2016,
Peña-Sancho et al., 2017) have shown ill-conditioned error maps with long ellipsoid

212 contours or elongated valleys. Given that a brute-force search is time-consuming (Horst 213 and Romeijn, 2002), local optimization methods should be employed. First-order 214 optimization methods, like gradient descent, oscillate quickly across the valley but 215 move slowly along the valley floor. This results in extremely low convergence. Newton 216 methods overcome this problem relying on the two first derivatives of the function: the gradient and the Hessian (Avriel, 2003). In the case of the Richards equation, the 217 gradient function is not given and it is computed numerically. Any noise in this 218 219 calculation, such as that introduced by numerical simulation, amplifies when the Hessian is inverted and introduces noise and instabilities. 220

Random search (RS) is a family of stochastic optimization methods that do not require the gradient of the function to be optimized (Brooks, 1958). The basic RS algorithm can be described as follows:

1. Initialize x with a random position in parameter-space.

225 2. Until a termination criterion is met, repeat the following:

1. Sample a new position y, moving x in a random direction a given fixed step

227 2. If f(y) < f(x) then move to the new position by setting x = y

Adaptive Step Size Random Search (ASSRS) (Schumer and Steiglitz, 1968) attempts to heuristically adapt the step size to improve the performance of the search. Though ASSRS is quite effective in reducing the objective function during the initial search phases, the average linear convergence rate is rather slow for more precise solutions. In order to obtain accurate estimations, deterministic optimization techniques are needed (Haiping, 1996).

In this work, ASSRS was combined with a gradient search method. In each iteration, 234 a random direction is first proposed and explored. Subsequently a deterministic 235 direction is computed based on the linear regression of the last five successfully points 236 and is also explored. In both cases, an initial step size of  $10^{-3}$  is considered which is 237 incremented exponentially while the error is reduced. The explored variables were 238 transformed to the (0,1) interval using the following extreme values:  $K = [10^{-6}, 10^{-2}]$  cm 239 s<sup>-1</sup>,  $\alpha = [10^{-3}, 0.5]$  cm<sup>-1</sup>, n = [1.0, 3.5] and considering logarithmic transformations in the 240 241 case of K and  $\alpha$ . This transformation simplifies calculations, guarantees the same properties in all explored directions and allows to accurately explore physical variables 242 covering several orders of magnitude. 243

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#### 245 **2.5. Experimental validation**

246 The experimental upward infiltration curves were measured with a sorptivimeter device (Moret-Fernández et al., 2017a). This consists of a saturated perforated base 5 247 cm-internal diameter (i.d.) that accommodates a stainless steel cylinder (5 cm-i.d. x 5 248 249 cm-high) that contains the soil sample. The bottom of the perforated base is connected to a Mariotte water supply reservoir (30 cm high, 1.9 cm-i.d). A ±7.2 kPa differential 250 pressure transducer (Microswitch; Honeywell International Inc.) connected to a 251 datalogger (CR1000; Campbell Scientist, Inc., Logan, UT, USA) was installed at the 252 253 bottom of the water supply reservoir. The time interval of the water level measurements 254 was 1 s. To minimize the water losses by evaporation, the surface of the soil column was covered with a lid. More details of the sorptivimeter can be found in Moret-255 256 Fernández et al. (2017a).

257 The upward infiltration method was applied on five 2-mm sieved soils with textural classes ranging from sand to clay (Table 2). The sieved material was initially stored at  $\approx$ 258 259 20 °C and  $\approx$  30% of relative humidity during several months. Since the soil is in equilibrium with the air in the chamber, the soil tension corresponding to this 260 atmospheric condition is  $-1.6 \ 10^6$  cm (RILEM, 1980). The soils were next 261 homogenously packet in 5-cm high and diameter cylinders and weighted. To this end, 262 263 the sieved soil was poured in by hand and gently tapped in small incremental steps to achieve a uniform bulk density. This initial weight defined the residual gravimetric 264 water content. Next, the cylinders were stored during several months at a temperature of 265  $\approx 20$  °C and relative humidity of  $\approx 60$  %, which corresponds to a soil pressure head of -266  $6.0 \, 10^5$  cm (RILEM, 1980). The upward infiltration started when the cylinder 267 containing the soil was placed on the sorptivimenter, and finished when the wetting 268 front arrived at the soil surface. At this time, the soil sample was saturated by raising the 269 air inlet tube of the Mariotte reservoir to the soil surface. Once the soil sample was 270 saturated, the core was disassembled, weighted, dried at 105 °C during 24 h, and 271 272 weighted again. Soils with high gypsum content (Table 1) were dried at 50 °C during 48 h (Moret-Fernández et al. 2016b). The soil bulk density ( $\rho_b$ ) was calculated as the 273 product between the core volume and the dry-weight of the soil.  $\theta_s$  and  $\theta_r$  were 274 275 calculated as the product between  $\rho_b$  and the corresponding gravimetric data. Once  $\theta_s$ and  $\theta_r$  calculated,  $K_s$  and  $\alpha$  and n were finally estimated by applying the optimization 276 method to the corresponding upward infiltration curves. 277

The  $K_s$  and  $\alpha$  and n parameters estimated from the inverse analysis were compared with those calculated by Darcy and the pressure cell, PC, method (Moret-Fernández et al. 2012), respectively. The volumetric water content in the PC was measured by TDR 281 at air-dried soil conditions, which corresponds to a pressure head (h) of approximately – 1.6 MPa, at soil water saturation and at pressure heads of -0.5, -1.5, -3, -10 and -50282 kPa. In this case,  $\theta_r$  and  $\theta_{sat}$  corresponded to the air-dried and saturated water content 283 measured by TDR, respectively. The measured pairs of  $\theta$  and h values were numerically 284 fitted to the van Genuchten (1980) model (Eq. 2). To this end,  $\theta_{sat}$  and  $\theta_r$  were 285 considered as known values, and  $\alpha$  and *n* were estimated by minimizing an objective 286 287 function that represents the difference between model and experimental data (Moret-Fernández et al., 2017b). The saturated hydraulic conductivity was estimated by the 288 Darcy's law. Because the inverse analysis of upward infiltration curves and PC methods 289 define the opposite branches of the water retention curve,  $\alpha$  values obtained with PC 290 were converted to the wetting branch of the water retention curve using the Gebrenegus 291 292 and Ghezzehei (2011) hysteresis index.

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#### **3. RESULTS AND DISCUSSION**

The analysis of the results obtained on the synthetic loam soil shows that  $h_i$  had an 295 296 important influence on the error maps (Fig. 1). When the initial tension is located in the transition zone of the water retention curve (i.e. -1.0 10<sup>3</sup> cm) (Fig. 1), small variations 297 298 of *n* and  $\alpha$  produce large changes in the initial soil water content. This translates into error maps with a focused minimum. Although the contour lines of the error maps tend 299 300 to length when initial tension is shifted to the flat zone of the water retention curve (i.e. 6.0  $10^{-5}$ ), the minimum is still preserved (Fig. 1). These results indicate that very 301 extremely negative  $h_i$  should not be employed. Overall, initial soil tension of  $-10^3$  cm 302 303 could be experimentally obtained with a pressure extractor. However, we discard this 304 technique because the pressure plates method is not consistent in fine soils (Solone et al., 2012), and it has little effectiveness in long cores (i.e. 5 cm high), where the very 305

306 long draining time needed to stabilize the water content into the soil core can restrict its 307 use. On the other hand, the soil water draining process within the pressure plates, which can alter the soil structure by collapsing the more unstable soil macrostructure (Moret-308 309 Fernández et al. 2016a), can modify the actual soil hydraulic properties. In any case, the use of a pressure extractor would be only recommendable in very stable and permeable 310 soils. Alternatively, suitable  $h_i$  can be achieved by placing the soil samples in 311 equilibrium in an atmosphere with high relatively humidity. For instance, a pressure 312 head of -6.0  $10^5$  cm can be obtained when a soil sample is stored at 20 °C and 60% 313 relative humidity (RILEM, 1980). Given that these atmospheric conditions are not 314 315 difficult to accomplish, the initial tension considered from now on, both in the theoretical and experimental analysis, will be fixed to  $-6.0 \ 10^5 \text{ cm}$ . 316

Upward infiltration curves were longer in finer soils (Fig. 2). The  $\alpha$ -n, K<sub>s</sub>-n and K<sub>s</sub>-317 318  $\alpha$  response surfaces calculated for the loamy sand, loam and clay soils showed, in all cases, an unique minimum (Fig. 2). These results indicate that  $K_s$ ,  $\alpha$  and n can be 319 estimated from the inverse analysis of a single upward infiltration curve. However, the 320 321 shapes of the error map varied depending on the soil type. For instance, the vertical and 322 elongated  $\alpha$ -n and  $K_s$ -n error maps observed in loamy sand makes that small changes in  $\alpha$  or  $K_s$  promoted important variations of n. This can be related to the commonly abrupt 323  $\theta(h)$  shapes observed in coarse soils, where small changes of the water retention slope 324 make important variations in n. An opposite behavior was observed in clay, where the 325 more horizontal  $\alpha$ -n and  $K_s$ -n error maps made that minor changes in n promoted large 326 327 variations of  $\alpha$  and K. This dependence can be related to the flatter  $\theta(h)$  shapes observed in fine soils, where large changes of  $\alpha$  may induce small variations in the  $\theta(h)$  slope. An 328 intermediate behavior was observed in the loam soil (Fig. 2). These results, however, 329 contrast with those obtained by Moret-Fernández et al. (2016a) and Peña-Sancho et al. 330

(2017), where error maps calculated from the inverse analysis of an upward infiltration 331 332 curve did not show an absolute minimum. These differences are explained because the soil initial condition used in those works was fixed in volumetric water content instead 333 on pressure head. Under these circumstances,  $\theta_i$  was set close to the measured  $\theta_r$ , and  $h_i$ 334 resulted free and dependent of  $\alpha$  and n. These results indicate the initial soil tension is a 335 key physical parameter in the capillarity processes. Moreover, the differences regarding 336 337 to the above cited works could be also explained because of the steady-state phase at the end of the upward infiltration was not included in the inverse analysis. This assumption 338 suggests that the measurement of the steady-state section is crucial to optimize the soil 339 340 hydraulic properties.

341 Given the ill-conditioning of the error maps, the hydraulic parameters were estimated using an stochastic optimization method. The procedure was based on the ASSRS 342 343 method, introducing preferential directions in the random search to increase 344 convergence rate at the final stage of the optimization. The last ten successful points explored by the ASSRS method were linearized to approximate the direction that leads 345 346 to the minimum. The satisfactory convergences of the optimization method in a loam soil, starting from four different initial values, indicate the proposed method allows 347 accurate estimates of  $\alpha$ , *n* and *K*<sub>s</sub>, independently of the initial value (Fig. 3). A robust 348 relationship (Fig. 4a) ( $\mathbb{R}^2 > 0.99$ ) was observed between the theoretical  $K_s$ ,  $\alpha$  and n and 349 the corresponding optimized values (Table 1). In all cases,  $\Phi$  (Eq. 6) was lower than 5.0 350  $10^{-4}$  cm. The week dispersion found in  $K_s$  and  $\alpha$  on clay can be related to the quasi-351 horizontal  $\alpha$ -n and  $K_s$ -n error maps observed in this soil (Fig. 2), where small variations 352 in *n* can make large changes in  $\alpha$  and *K*. An also robust relationship ( $\mathbb{R}^2 > 0.99$ ) was 353 found between the theoretical hydraulic properties and the intermediate values for a 354 0.02 mm error (Fig.4b), which corresponds with the experimental threshold error 355

defined in Section 2.3. These results indicate that the proposed optimization can be satisfactorily applied to any kind of soil. The optimization, however, could be accelerated if initial hydraulic parameters ( $K_s$ ',  $\alpha$ ' and n') close to the actual values were selected. For instance, these initial values could be obtained from the  $K_s(S)$ ,  $\alpha(S)$  and n(S) regressions (Fig. 5), where S is integrated between  $\theta_s$  and  $\theta_i$  (Eq. 4). This relationship will be subsequently used to estimate  $K_s$ ',  $\alpha$ ' and n' (Table 1) from  $S^*$  (Eq. 5).

The  $S^*$  values estimated from the experimental infiltration curves (Eq. 5), together 363 364 with the corresponding  $K_s$ ,  $\alpha$  and n are summarized in Table 2. Overall, good fittings 365 were observed between the measured upward infiltration curves and the optimized ones 366 (Table 2). For instance, Figure 6 compares the experimental vs. the best optimized 367 curve, as well as the iterations followed by the optimization method applied to the 368 experimental clay soil. A robust and significant relationship, with slope close to one and an average dispersion of 0.4% (Fig. 7), was observed between *n* measured with PC and 369 the corresponding values estimated from the inverse analysis of the experimental 370 371 infiltration curves (Fig. 7). This strong relationship could be associated to the fact that n372 is more related to the soil textural characteristics (Jirku et al., 2013), and hence, less affected by the influence of the wetting-drainage process on the soil structure (Moret-373 374 Fernández et al., 2016a). Similar results were obtained by Moret-Fernádnez et al. (2016b) and Moret-Fernández and Latorre (2017) with comparable upward infiltration 375 methods. An also significant relationship, with slope close to one, was observed 376 377 between the optimized  $K_s$  and the corresponding value obtained by Darcy. In this case,  $log(K_s)$  measured by Darcy was 2.5% higher than that estimated by the inverse analysis. 378 A no-statistically significant relationship, with a slope away from the 1:1 line, was 379 observed between  $\alpha$  estimated with PC and that obtained with the infiltration method. 380

Similar results were obtained by Moret-Fernández and Latorre (2017) with a 381 comparable upward infiltration method. This behavior could be explained by the 382 different wetting processes used in both methods (Moret-Fernández and Latorre, 2017), 383 384 which may modify the contact angle of water with the soil particles, the amount of air entrapped in the pores, or the interconnection in the pore network (Bachmann and van 385 der Ploeg, 2002; Magsoud et al., 2004). Other explanation could be found in the 386 empirical Gebrenegus and Ghezzehei (2011) hysteresis model, that could give an 387 388 inaccurate description of  $\alpha$  for a wetting process. An indirect confirmation for this hypothesis is given by the good correlation found in  $K_s$  and n, which are less affected by 389 the hysteresis. A robust and significant relationship with slope close to one (Fig. 8) was 390 observed between S calculated by applying the optimized  $\alpha$ , n and  $K_s$  values to Eq.(4) 391 and the corresponding  $S^*$  (Eq. 5) estimated from the upward infiltration curve. This 392 393 satisfactory relationship corroborates the robustness of the inverse analysis.

394

## 395 CONCLUSIONS

396 This work demonstrates that  $K_s$ ,  $\alpha$  and n can be estimated from the inverse analysis of a single upward infiltration curve measured on a 5-cm high cylinder, when the initial 397 soil tension is fixed to  $-6.0 \ 10^5$  cm. A robust and efficient optimization method was 398 proposed and satisfactorily validated on theoretical and experimental sieved soils 399 400 contained in 5-cm high cylinders. Unlike previous methods, this new technique is 401 simple, inexpensive, fast to implement, allows simultaneous estimates of all hydraulic 402 parameters, can be applied to any kind of sieved soils and on the 5-cm high cores 403 commonly employed for soil bulk density determination. However, new efforts should 404 be done to test the method on heterogeneous and undisturbed soil samples, and to study

405 the influence of the core length on the hydraulic properties estimation.

406

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# 414 **References**

- Avriel, M. Nonlinear Programming: Analysis and Methods. Englewood Cliffs (N.J.).
  Prentice-Hall, 2003.
- Bachmann, J., van der Ploeg, R.R., 2002. A review on recent developments in soil water
  retention theory: interfacial tension and temperature effects. Journal of Plant
  Nutrition and Soil Science 165, 468–478.
- Brooks, S.H., 1958. A Discussion of Random Methods for Seeking Maxima. Operations
  Research 6, 244-251.
- Caldwell, T.G., Wohling, T., Young, M.H., Boyle, D.P., McDonald, E.V. 2013.
  Characterizing disturbed desert soils usingmultiobjective parameter
  optimization. Vadose Zone Journal 12 (1).

- 425 Carsel, R.F., Parrish, R.S., 1988. Developing joint probability distributions of soil water
  426 retention characteristics. Water Resources Research. 24, 755–769.
- 427 Dane J.H., Hopmans J.W. 2002. Water retention and storage. In Methods of Soil
  428 Analysis. Part. 4, Dane JH and Topp GC (editors). SSSA Book Series No. 5.
  429 Soil Science Society of America, Madison, WI.
- Gebrenegus, T., Ghezzehei, T.A., 2011. An index for degree of hysteresis in water
  retention. Soil Science Society of America Journal 75, 2122–2127
- Haverkamp, R., Ross, P.J., Smettem, K.R.J., Parlange, J.Y. 1994. Three dimensional
  analysis of infiltration from the disc infiltrometer. Part 2. Physically based
  infiltration equation. Water Resources Research 30, 2931-2935.
- Haiping, Z., Yamada K. 1996. Estimation for urban runoff quality modeling. Water
  Science and Technology. 34, 49-54.
- 437 Horst, R., Romeijn, H.E. (Eds.), 2002. Handbook of Global Optimization, vol. 2.
  438 Springer Science & Business Media.
- Hudson, D.B., Wierenga, P.J., Hills, R.G., 1996. Unsaturated hydraulic properties from
  upward flow into soil cores. Soil Science Society of America Journal 60, 388–
  396.
- Jirku, V., Kodesová, R., Nikodem, A., Mühlhanselová, M., Zigová, A., 2013. Temporal
  variability of structure and hydraulic properties of topsoil of three soil types.
  Geoderma 204, 43–58.

445	Jones, S.B., Mace, R.W., Or, D., 2005. A time domain reflectometry coaxial cell for
446	manipulation and monitoring of water content and electrical conductivity in
447	variable saturated porous media. Vadose Zone Journal 4, 977–982.

Klute, A. 1986. Water retention curve: laboratory methods. In: Klute, A. (Ed.), Methods
of Soil Analysis. Part 1. SSSA Book Series No. 9. Soil Science Society of
America, Madison WI.

- Klute, A. and Dirksen, C. 1986. Hydraulic conductivity and diffusivity: Laboratory
  methods. In: Klute, A. Ed., Methods of Soil Analysis Part 1 Physical and
  Mineralogical Methods, American Society of Agronomy, Madison, 687-734.
- Lassabatere, L., Angulo-Jaramillo, R., Soria-Ugalde, J.M., Simunek, J., Haverkamp, R.,
  2009. Numerical evaluation of a set of analytical infiltration equations. Water
  Resources Research 45. http://dx.doi.org/10.1029/2009WR007941.
- Latorre, B., Peña, C., Lassabatere L., Angulo-Jaramillo R., Moret-Fernández, D. 2015.
  Estimate of soil hydraulic properties from disc infiltrometer three-dimensional
  infiltration curve. Numerical analysis and field application. Journal of Hydrology
  57, 1-12.
- Maqsoud, A., Bussiere, B., Mbonimpa, M., Aubertin, M., 2004. Hysteresis effects on
  the water retention curve: a comparison between laboratory results and predictive
  models. In: Proc. 57th Can. Geotech. Conf. and the 5th joint CGS-IAH Conf.,
  Quebec City. 24–27 October. The Canadian Geotechnical Soc., Richmond, BC,
  pp. 8–15.

- Masaoka, N., Kosugi, K. 2018. Improved evaporation method for the measurement of
  the hydraulic conductivity of unsaturated soil in the wet range. Journal of
  Hydrology 563, 242–250.
- Minasny, B., McBratney, A.B. 2000. Estimation of sorptivity from disc-permeameter
  measurements. Geoderma 95, 305-324.
- 471 Moret-Fernández, D., Latorre, B. 2017. Estimate of the soil water retention curve from
  472 the sorptivity and β parameter calculated from an upward infiltration experiment.
  473 Journal of Hydrology 544, 352–362.
- 474 Moret-Fernández, D., Peña-Sancho, C., López, M.V. 2016a. Influence of the wetting
  475 process on estimation of the water retention curve of tilled soils. Soil Research
  476 doi.org/10.1071/SR15274.
- 477 Moret-Fernández, D., Latorre, B., Angulo-Martínez, M. 2017a. Comparison of different
  478 methods to estimate the soil sorptivity from an upward infiltration curve. Catena
  479 155, 86–92.
- Moret-Fernández, D., Latorre, B., Peña-Sancho, C., Ghezzehei, T.A., 2016b. A
  modified multiple tension upward infiltration method to estimate the soil
  hydraulic properties. Hydrological Processes.
  http://dx.doi.org/10.1002/hyp.10827.
- Moret-Fernández, D., Peña-Sancho, C., Latorre, B., Pueyo, Y., López, M.V. 2017b.
  Estimating the van Genuchten retention curve parameters of undisturbed soil from
  a single upward infiltration measurement. Soil Research
  doi.org/10.1071/SR16333

- Moret-Fernández, D., Vicente, J., Latorre, B., Herrero, J., Castañeda, C., López, M.V.,
  2012. TDR pressure cell for monitoring water content retention curves on
  undisturbed soil samples. Hydrological Processes 26, 246–254.
- 491 Peña-Sancho, C., Ghezzehei, T.A., Latorrea, B., Moret-Fernández, D. 2017.Water
  492 absorption-evaporation method to estimate the soil hydraulic properties.
  493 Hydrological Science Journal 62, 1683-1693.
- Philip J.R. 1957. The theory of infiltration: 4. Sorptivity and algebraic infiltration
  equations. Soil Sci. 84, 257-264.
- Shao, M., Hudson, R. 1998. Integral method for estimating soil hydraulic properties.
  Soil Science Society of America Journal 62, 585-592.
- Ramos, T., Gonçalves, M., Martins, J., van Genuchten, M.T., Pires, F., 2006. Estimation
  of soil hydraulic properties from numerical inversion of tension disk infiltrometer
  data. Vadose Zone Journal 5, 684–696.
- Rashid, N., Askari, M., Tanaka, T., Simunek, J., van Genuchten, M., Th. 2015. Inverse
  estimation of soil hydraulic properties under oil palm trees. Geoderma 241–242,
  306-312
- RILEM (1980). Essais recommandés pour mesurer l'altération des pierres et évaluer
  l'efficacité des méthodes de traitement. Matériaux et Constructions, Bull. RILEM
  13 (75), 175-253.
- 507 Schumer, M.A., Steiglitz, K. 1968. Adaptive step size random search. IEEE
  508 Transactions on Automatic Control. 13, 270-276.

- Schindler, U. 1980. Ein Schnellverfahren zur Messung der Wasserleitfähigkeit im
  teilgesättigten Boden an Stechzylinderproben. Arch. Acker- Pflanzen- bau
  Bodenkd. 24, 1–7.
- Schindler, U., Müller, L., 2006. Simplifying the evaporation method for quantifying soil
  hydraulic properties. Journal of Plant Nutrition and Soil Science 169, 623–629.
- Schindler, U., Durner, W., von Unold, G., Müller, L., 2010. Evaporation method for
  measuring unsaturated hydraulic properties of soils: extending the measurement
  range. Soil Science Society of America Journal 74, 1071–1083.
- 517 Simunek, J., van Genuchten, M.T., 1997. Estimating unsaturated soil hydraulic
  518 properties from multiple tension disc infiltrometer data. Soil Science 162, 383–
  519 398.
- Simunek, J., van Genuchten, M.T., 1996. Estimating unsaturated soil hydraulic
  properties from tension disc infiltrometer data by numerical inversion. Water
  Resources Research. 32, 2683–2696.
- Simunek, J., Wendroth, O., van Genuchten, M.T., 1998. Parameter estimation analysis
  of the evaporation method for determining soil hydraulic properties. Soil Science
  Society of America Journal 62, 894–895.
- Solone, R., Bittelli, M., Tomei, F., Morari, F., 2012. Errors in water retention curves
  determined with pressure plates: effects on the soil water balance. Journal of
  Hydrology 470, 65–75.

529	van Genuchten, M.T., 1980. A closed form equation for predicting the hydraulic
530	conductivity of unsaturated soils. Soil Science Society of America Journal 44,
531	892–898.

- Young, M.H., Karagunduz, A., Siumunek, J., Pennell, K.D., 2002. A modified upward
  infiltration method for characterizing soil hydraulic properties. Soil Science
  Society of America Journal 66, 57–64.
- Wind, G.P., 1968. Capillary conductivity data estimated by a simple method. In:
  Rijtema, P.E., Wassink, H. (Eds.), Water in the unsaturated zone. Vol. 1. Proc.
  Wageningen Symp. June 1966. Int. Assoc. Scientific Hydrol. Gentbrugge,
  Belgium, pp. 181–191.

## **Figures captions**

539

Figure 1. Water retention curve and response surfaces for the  $\alpha$ -*n*,  $K_s$ -*n* and  $K_s$ - $\alpha$  planes calculated on a theoretical loam soil for two different initial soil tensions ( $h_i$ ) (Table 1). Contour lines indicate errors of 0.05, 0.1, 0.2, 0.5, 1, 2 and 5 mm, respectively, red line is the contour line for an error of 0.02 mm and blue circle denotes the theoretical value.

Figure 2. Simulated cumulative infiltration curves and response surfaces for the  $\alpha$ -*n*, *K<sub>s</sub>*-*n* and *K<sub>s</sub>*- $\alpha$  planes calculated for theoretical loamy sand, loam and clay soils (Table 1). Contour lines indicate errors of 0.05, 0.1, 0.2, 0.5, 1, 2 and 5 mm, respectively, red line is the contour line for an error of 0.02 mm and blue circle denotes the theoretical value.

- **Figure 3.** Convergence of the optimization to the  $K_s$ ,  $\alpha$  and n values of a theoretical loam soil from four different initial values.
- **Figure 4.** Relationship between the theoretical  $K_s$ ,  $\alpha$  and n of Table 1 and the corresponding values obtained with the optimization for (a) the best result and (b) the intermediate iteration reaching 0.02 mm error.

**Figure 5.** Experimental relationship between *S* (Eq. 4) and  $K_s$ ,  $\alpha$  and *n* of the theoretical soils of Table 1.

**Figure 6.** (a) Experimental (circles) and optimized (red line) upward infiltration curve and (b) convergence of  $K_s$ ,  $\alpha$  and n during the optimization of the experimental sieved clay soil.

561	<b>Figure 7.</b> Relationship between $K_s$ , $\alpha$ and $n$ estimated on the experimental soils with
562	the Darcy's and PC methods and the corresponding hydraulic values estimated
563	from the inverse analysis (opt) of the upward infiltration curves.

**Figure 8.** Relationship between the sorptivity (*S*) of the experimental soils estimated from Eq.(4) and the optimized  $\alpha$ , *n* and *K<sub>s</sub>* values and the corresponding sorptivity estimated with Eq.(5) ( $S^*$ ).

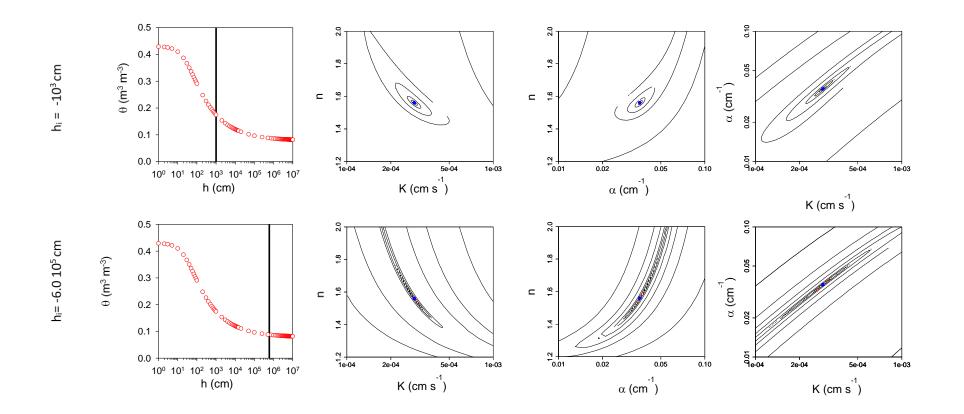
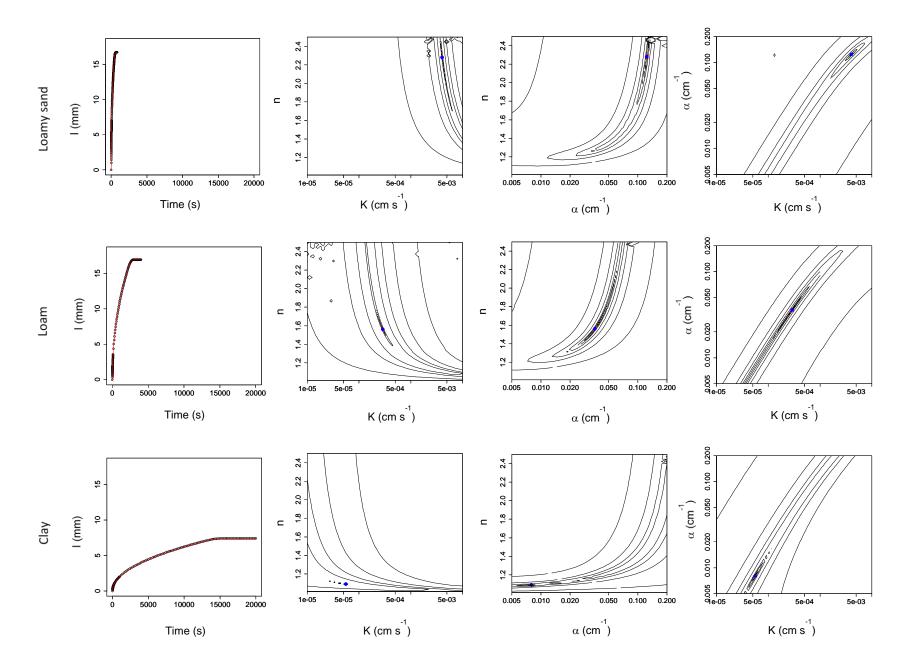


Figure 1.





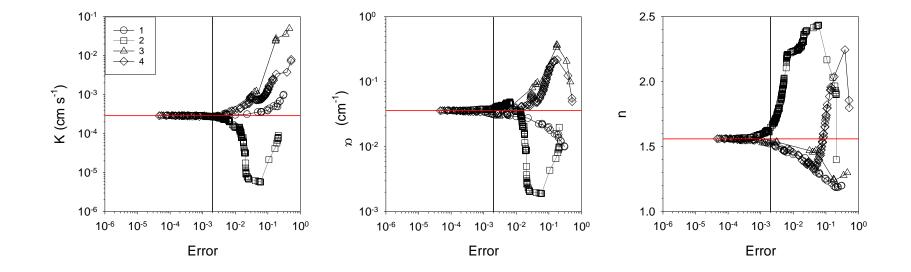


Figure 3.

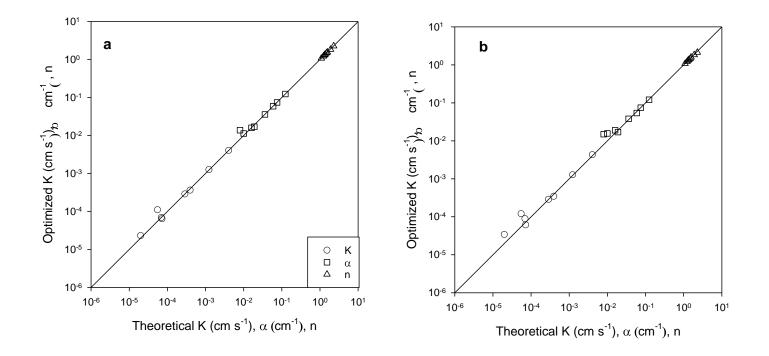


Figure 4

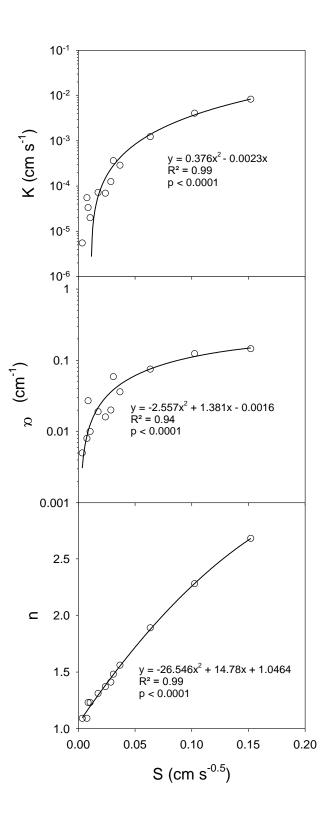
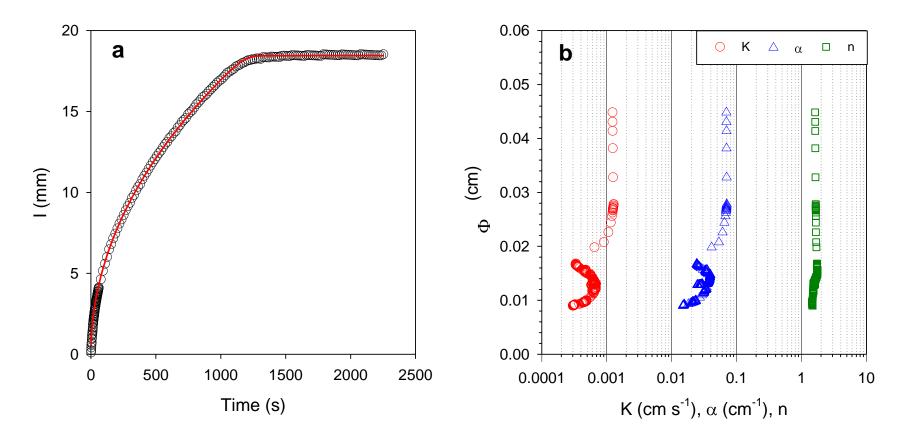


Figure. 5





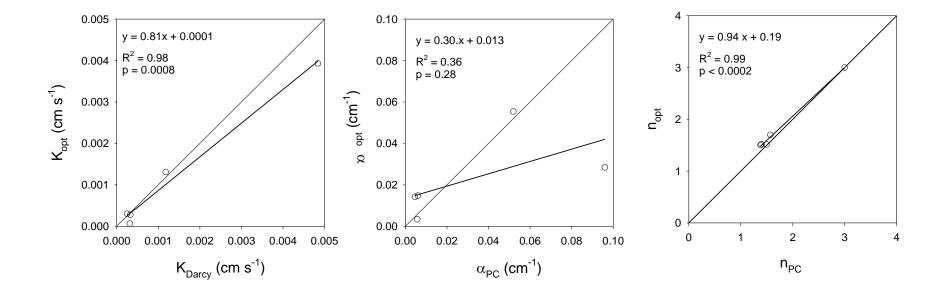


Figure 7.

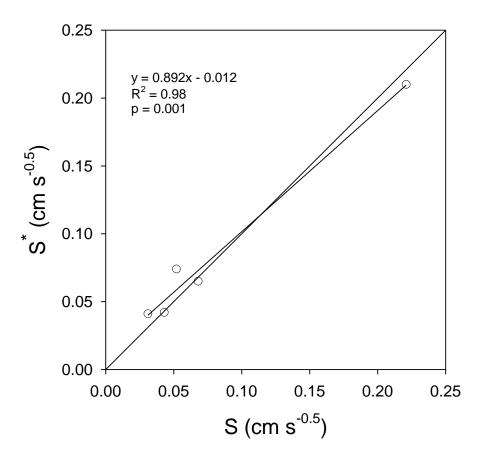


Figure 8.

**Table 1**. Theoretical values of initial ( $\theta_i$ ), saturated ( $\theta_s$ ) and residual ( $\theta_r$ ) water content,  $\alpha$  and n parameters of the van Genuchten (1980) water retention curve, saturated hydraulic conductivity ( $K_s$ ), sorptivity calculated with Eq. (4) (*S*) and estimated from Eq. (5) ( $S^*$ ), and  $K_s$ ,  $\alpha$  and n parameters ( $K_s$ ',  $\alpha$ ' and n') estimated from  $K_s(S)$ ,  $\alpha(S)$  and n(S) relationships (Fig. 3).

	$ heta_i$	$\theta_r$ - cm <sup>3</sup> cm <sup>-3</sup>	$\theta_s$	$\alpha$ cm <sup>-1</sup>	п	$K_s$ cm s <sup>-1</sup>	<i>S</i> cm :	s <sup>-0.5</sup>	$\alpha'$ cm <sup>-1</sup>	n'	$K_s$ ' cm s <sup>-1</sup>
Loamy sand	0.057	0.057	0.41	0.124	2.28	4.05 10 <sup>-3</sup>	0.1025	0.1021	0.106	2.28	3.58 10 <sup>-03</sup>
Sandy loam	0.065	0.065	0.41	0.124	1.89	$4.03\ 10^{-3}$	0.1023	0.1021	0.100	1.87	$1.42 \ 10^{-03}$
Loam	0.005	0.078	0.43	0.075	1.56	$2.88 \ 10^{-4}$	0.0367	0.0366	0.047	1.55	8.05 10 <sup>-05</sup>
Silt	0.048	0.034	0.46	0.016	1.37	6.93 10 <sup>-5</sup>	0.0238	0.0235	0.031	1.38	$1.67 \ 10^{-04}$
Sandy clay loam	0.102	0.100	0.39	0.059	1.48	3.64 10 <sup>-4</sup>	0.0309	0.0307	0.036	1.48	2.79 10 <sup>-04</sup>
Clay loam	0.112	0.095	0.41	0.019	1.31	7.22 10 <sup>-5</sup>	0.0174	0.0176	0.022	1.29	$7.40 \ 10^{-05}$
Silty clay loam	0.135	0.089	0.43	0.010	1.23	1.99 10 <sup>-5</sup>	0.0104	0.0105	0.013	1.19	$1.68  10^{-05}$
Clay	0.213	0.068	0.38	0.008	1.09	5.55 10 <sup>-5</sup>	0.0076	0.0078	0.009	1.17	3.55 10 <sup>-06</sup>

**Table 2**. Soil particle size, gypsum and organic carbon content, OC, bulk density,  $\rho_b$ , residual,  $\theta_r$ , and saturated,  $\theta_s$ , volumetric water content, saturated hydraulic conductivity,  $K_s$ ',  $\alpha$ ' and n' calculated form the estimated sorptivity ( $S^*$ ), and error,  $\Phi$  (Eq. 6), obtained by the inverse analysis of the experimental soils

Treatment *	Sand	Silt	clay	Gypsum	OC	$ ho_b$	$\theta_r$	$\theta_s$	<i>S</i> *	$K_s$ '	α'	n'	Φ
			- g kg <sup>-1</sup>			g cm <sup>-3</sup>	— m <sup>2</sup>	$m^{-3}$ —	$\mathrm{cm}~\mathrm{s}^{-0.5}$	$\mathrm{cm}~\mathrm{s}^{-1}$	$cm^{-1}$		mm
Sand	1000	-	-	-	-	1.64	0.02	0.35	0.210	1.65 10 <sup>-2</sup>	0.175	2.97	0.08
Loam	280	470	250	-	11.7	1.25	0.03	0.47	0.074	2.05 10 <sup>-3</sup>	0.086	1.99	0.11
Clay loam	205	497	298	-	19.9	1.33	0.03	0.44	0.065	1.58 10 <sup>-3</sup>	0.077	1.89	0.15
Silt-Gypeseous	316	591	129	703	1.50	1.02	0.01	0.37	0.042	6.61 10 <sup>-4</sup>	0.052	1.62	0.08
Clay	151	344	465	-	12.4	1.30	0.03	0.40	0.041	6.29 10 <sup>-4</sup>	0.051	1.60	0.09

\* S estimated from the inverse analysis of the upward infiltration curve using Eq. (5)