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Abstract

The objective function of the inverse problem in Soil Vegetation Atmosphere Transfer (SVAT) models can be expressed as the aggregation of two criteria, accounting for the uncertainties of surface soil moisture (θ) and evapotranspiration (ET), retrieved from remote sensing (RS). In this context, we formulate a Weighted Objective Function (WOF) with respect to model effective soil hydraulic parameters, comprising of two components for θ and ET, respectively, and a dimensionless coefficient w . Given that the sensitivity of θ is increased by omitting the periods when soil moisture decoupling occurs, we also introduce within the WOF a threshold, θ_d , which outlines the decoupling of the surface and root-zone moisture. The optimal values of w and θ_d are determined by using a novel framework, Weighted Objective Function Selector Algorithm (WOFSA). This performs numerical experiments, assuming known reference conditions. In particular, it solves the inverse problem for different sets of θ and ET, considering the uncertainties of retrieving them from RS, and then runs the hydrological model to obtain the simulated water fluxes and their residuals, ΔWF , against the reference responses. It estimates the two unknown variables, w and θ_d , by maximizing the linear correlation between the WOF and maximum ΔWF . The framework is tested using a modified Soil-Water-Atmosphere-Plant (SWAP) model, under 22 contrasting hydroclimatic scenarios. It is shown that for each texture class, w can be expressed as function of the average θ and ET-fraction, while that for all scenarios θ_d can be modeled as function of the average θ , average ET and standard deviation of ET. Based on the outcomes of this study, we also provide recommendations on the most suitable time period for soil moisture measurements for capturing its dynamics and thresholds. Finally, we propose the implementation of WOFSA within multiobjective calibration, as a generalized tool for recognizing robust solutions from the Pareto front.

KEYWORDS:

Inverse modeling; Soil Hydraulic parameters; SVAT; Water fluxes; Decoupling; Multi-objective calibration; Uncertainty; Soil moisture; Evapotranspiration; Remote sensing.

ACRONYMS:

DR: deep roots, **HYDRAU_{ref}**: reference sets of hydraulic parameters; **HYDRAU_{sim}**: simulated sets of hydraulic parameters; **LAI:** leaf area index; **MEDP:** Minimizing the Euclidean Distance of the Pareto set; **OF _{θ}** : objective function based on soil moisture; **OF_{et}**: objective function based on evapotranspiration; **RS:** remote sensing; **SR:** shallow roots; **SVAT:** Soil Vegetation Atmosphere Transfer water flow model; **SWAP:** Soil-Water-Atmosphere-Plants model; **SWAP_{inv}**: modified Soil-Water-Atmosphere-Plant model suitable for inverse modeling; **WOF:** weighted objective function; **WOFSA:** Weighted Objective Function Selector Algorithm, **WF:** water fluxes.

23 1. Introduction

24 In the hydrological community there is a growing interest to make suitable usage of data retrieved from
25 remote sensing (RS), to be employed within physically-based models. Two of the most typical variables,
26 which are of key importance in hydrological modeling, are surface soil moisture, θ [Sun et al., 2007; Wang et
27 al., 2008; Zhan et al., 2008; Naeimi et al., 2009; Entekhabi et al., 2010], and actual evapotranspiration, ET
28 [e.g., Wang et al., 2008; Wu et al., 2008; Hong et al., 2009; Ramos et al., 2009; Teixeira et al., 2009a]. In
29 particular, RS data of this type have been used to invert the soil hydraulic parameters of Soil Vegetation
30 Atmosphere Transfer (SVAT) models [e.g. Mohanty and Zhu, 2007; Ines and Mohanty, 2008a; Ines and
31 Mohanty, 2009; Gutmann and Small, 2010]. Recently, Pollacco and Mohanty [2012] performed numerical
32 experiments under 18 contrasting hydroclimatic scenarios to estimate the uncertainties of computing the
33 water fluxes (WF) through a modified SVAT model, by inverting its soil hydraulic parameters from θ and ET.
34 They found that the predictive capacity of the model against its simulated fluxes strongly depends on the
35 hydroclimatic conditions; specifically, the uncertainty increases under dry climates, coarse textures and
36 deep rooted vegetation.

37 In this paper we provide a novel methodological framework, termed Weighted Objective Function
38 Selector Algorithm (WOFSA), to improve predictions by SVAT models, by ensuring the most appropriate
39 combination of these two types of information (θ & ET), for a wide range of hydroclimatic conditions and soil
40 texture patterns. In the simulations we use a modified SWAP 3.2 model, for which we are interested in
41 inverting the effective soil hydraulic parameters, while the vegetation parameters are assumed known. The
42 modified SWAP 3.2, introduced by Pollacco and Mohanty [2012] and next termed SWAP_{inv}, is briefly
43 described in section 2.1.

44 In the proposed framework, the inverse problem is expressed in multiobjective terms, by formulating a
45 Weighted Objective Function (WOF) of two criteria, OF_{θ} and OF_{et} , which account for the deviation of the
46 simulated to the “reference” surface soil moisture θ and evapotranspiration ET, i.e.:

$$47 \quad WOF = w OF_{\theta} + (1 - w) OF_{et} \quad (1)$$

48 where w is a dimensionless weighting coefficient. Multiobjective approaches have been widely documented

49 in all aspects of hydrological modeling, starting from the late '90s [e.g., *Mroczkowski et al.*, 1997; *Gupta et al.*,
50 1998; *Yapo et al.*, 1998; *Bastidas et al.*, 1999; *Gupta et al.*, 1999]. The rationale is that as more information is
51 embedded within calibration, it is expected that the identifiability of parameters is improved, thus also
52 ensuring an improved predictive capacity. These advantages have been demonstrated in several applications
53 involving SVAT and land surface models [e.g., *Bastidas et al.*, 1999; *Franks et al.*, 1999; *Gupta et al.*, 1999;
54 *Demarty et al.*, 2004; 2005; *Coudert et al.*, 2006; *Mo et al.*, 2006]. In this respect, conditioning the hydraulic
55 parameters of SVAT models against both θ and ET data is generally accepted, although not all researchers
56 found advantageous of calibrating SVAT models simultaneously with θ and ET data [*Ines and Droogers*, 2002;
57 *Jhorar et al.*, 2002; *Jhorar et al.*, 2004; *Ines and Mohanty*, 2008b].

58 In order to increase the information embedded in calibration, the WOF is further parameterized by
59 introducing a threshold soil moisture θ_d , which indicates the period when soil moisture θ can be calibrated,
60 in order to avoid decoupling between surface and subsurface θ . The concept of θ_d is one of the novelties of
61 our framework, as explained in section 2.4.2. It is well-known that by tuning the weighting coefficient w and
62 next solve the inverse (calibration) problem for a given value of θ_d , we can obtain different sets of optimized
63 hydraulic parameters. The later are called non-dominated or Pareto-optimal and lie in the boundary of the
64 feasible objective space (Fig. 1). By assigning a specific value to w and θ_d we assert that the solution obtained
65 by minimizing WOF ensures an acceptable compromise between OF_θ and OF_{et} . In this respect, the “optimal”
66 combination of θ and ET data is mathematically represented as the determination of the weighting
67 coefficient w and the decoupled soil moisture θ_d . The **W**eighted **O**bjective **F**unction **S**elector **A**lgorithm
68 (WOFSA) is a novel numerical procedure, which allows for identifying the optimal values of both the control
69 variables of the multiobjective function (i.e., w and θ_d) and the model hydraulic parameters. The suitability of
70 w and θ_d is evaluated on the basis of the information provided by the simulated water fluxes (model
71 outputs), in terms of uncertainty, in an attempt to constrain the feasible parameter space. In contrast to the
72 classic calibration paradigm, which merely aims to achieve the smallest departure between the observed and
73 simulated model responses, the WOFSA also takes into account the uncertainties due to errors in input data.
74 For convenience, in the investigations we use synthetic data provided by numerical experiments with known
75 parameter sets, in order to eliminate the impacts of other sources of uncertainty, e.g., structural (model)

76 errors. In this context, WOFSA assumes that the uncertainties of the water fluxes are only caused by
77 prescribed uncertainties of the observed θ and ET.

78 Specifically, we consider that the top 5cm soil moisture retrieved from remote sensing has an average
79 accuracy of root mean square error (RMSE) of $0.04 \text{ m}^3 \text{ m}^{-3}$, in terms of volumetric soil moisture [e.g., *Kerr et*
80 *al.*, 2001; *Simmonds et al.*, 2004; *Davenport et al.*, 2005; *Choi et al.*, 2008; *Das et al.*, 2008; *Sahoo et al.*, 2008;
81 *Verstraeten et al.*, 2008; *Vischel et al.*, 2008]. This has been validated with field campaigns, typically under
82 low vegetated area for which the biomass is up to $4\text{-}8 \text{ Kg m}^{-2}$ (for example, under mature corn and soybean),
83 by using passive microwave remote sensing [e.g., *Jackson and Schmugge*, 1991; *Bindlish et al.*, 2006; *Li et al.*,
84 2006; *Njoku and Chan*, 2006]. On the other hand, the procedures for retrieving the actual evapotranspiration
85 from remote sensing exhibit an average relative error of 20%, as also validated from field campaigns. This
86 value is suggested by Kalma et al. [2008], from a compilation of 30 publications [e.g., *Zhang et al.*, 2006; *Gao*
87 *and Long*, 2008; *Opoku-Duah et al.*, 2008; *Bashir et al.*, 2009; *Ramos et al.*, 2009; *Teixeira et al.*, 2009b]. We
88 note that the uncertainties of retrieving θ are different when compared to the uncertainties of ET, and
89 therefore have different implication on the uncertainties of the modeled/inverted water fluxes. Moreover,
90 the behavior of the uncertainties of θ and ET retrieved from RS with increasing θ and ET is still poorly
91 understood [e.g., *Fernández-Gálvez*, 2008]. For this reason, we also assume that the uncertainties of θ and ET
92 linearly increase with increasing θ and ET, thus suggesting that the WOF and the corresponding residuals
93 are correlated. Under this premise, the optimal w and θ_d are those which achieve the maximum linear
94 correlation between the WOF and the residuals of the simulated water fluxes. This is a key point of the
95 methodology, which is analytically presented in section 3.

96 Our methodology is validated by employing numerical experiments with SWAP_{inv}. Following the recent
97 research study by Pollacco and Mohanty [2012], we used as reference states/fluxes the surface and root-
98 zone soil moisture, groundwater recharge, actual evapotranspiration, actual evaporation and actual
99 transpiration. In order to investigate the variability of the optimized w and θ_d , we formulated 22 contrasting
100 hydroclimatic scenarios, which are composed as combination of five climates across the USA, three soil
101 textures and two rooting depths. The need for investigating different rooting depths is justified by Ines and
102 Mohanty [2008b], who found that the predictions of the hydraulic parameters of SVAT models are much

103 more sensitive to rooting depths than other vegetation parameters. In the numerical experiments, we
104 assumed that the soil hydraulic parameters are unknown and that the vegetation parameters are not subject
105 to calibration, since these can be readily retrieved from MODIS (MODerate resolution Imaging
106 Spectroradiometer) [e.g., Huete et al., 2002; Simic et al., 2004; Nagler et al., 2005; Vegas Galdos et al., 2012].
107 In all simulations, we assumed that the soils are homogeneous, based on the work by Jhorar et al. [2004],
108 who found that, in most cases, a reliable water balance can be obtained by replacing the heterogeneous soil
109 profile by an equivalent single one. Finally, we selected a deep water table, since Pollacco and Mohanty
110 [2012] showed that inverting the soil hydraulic parameters with ET in presence of shallow water table
111 causes extra uncertainties.

112 The goals of this study include:

- 113 • Development of the *Weighted Objective Function Selector Algorithm* (WOFSA), for determining the
114 best-compromise weights of a WOF;
- 115 • Application of WOFSA within $SWAP_{inv}$, in order to investigate the variability of the optimal coefficient
116 w and threshold θ_d under contrasting hydroclimatic conditions, on the basis of synthetic data obtained
117 through numerical experiments, i.e. by inverting the soil hydraulic parameters;
- 118 • Determination of the most suitable calibration period (in terms of soil moisture thresholds), to take
119 full advantage of the information provided simultaneously by θ and ET retrieved from remote sensing;
- 120 • Development of empirical relationships correlating w and θ_d against typical statistical metrics of θ and
121 ET ;
- 122 • Comparison with the minimum Euclidian distance approach, which is usually employed in
123 multiobjective calibration problems;
- 124 • Discussion of future research perspectives, for implementing WOFSA within a multi-objective
125 calibration framework, and on the basis of actual (i.e., field) data.

126

2. Modeling framework and set-up of numerical experiments

2.1 Soil-Water-Atmosphere-Plant hydrological model

We introduce a modified version of the so-called **S**oil-**W**ater-**A**tmosphere-**P**lant (SWAP 3.2), which is a physically-based **S**oil **V**egetation **A**tmosphere **T**ransfer (SVAT) water flow model for representing the unsaturated zone soil water fluxes of vegetated land [e.g., *Van Dam et al.*, 1997; *Kroes et al.*, 2000; *Van Dam et al.*, 2008]. SWAP has been extensively used to calibrate the hydraulic parameters by matching θ and/or ET retrieved from remote sensing [e.g., *Ines and Mohanty*, 2008a; b; c; 2009; *Shin et al.*, 2012]. The governing equation solves the mixed form of the Richards' equation, combined with a sink term for root water extraction, to simulate the variably saturated soil moisture movement in the soil profile:

$$\frac{\partial \theta}{\partial t} = \frac{\partial \left(K(\theta) \left(\frac{\partial h}{\partial z} + 1 \right) \right)}{\partial z} - S(h) \quad (2)$$

where θ is the volumetric water content ($L^3 L^{-3}$) or the fraction of water-filled pore space; h is the capillary pressure head (m); t is time (T); z is the vertical coordinate (L) defined as positive upwards; $K(\theta)$ is the unsaturated hydraulic conductivity ($L T^{-1}$); and $S(h)$ is the soil water extraction rate by plant roots ($L^3 L^{-3}$).

2.1.1 Soil water retention and unsaturated hydraulic conductivity

The model accuracy depends on two functions, the soil-moisture characteristic curve $h(\theta)$ and the unsaturated hydraulic conductivity $K(\theta)$. The analytical function of $h(\theta)$ is provided by the van Genuchten model [1980]:

$$\theta_e = \frac{\theta - \theta_r}{\theta_s - \theta_r} = \frac{1}{\left[1 + \left(\frac{h}{h_{ae}} \right)^n \right]^m} \quad (3)$$

where θ_e is the normalized volumetric water content ($L^3 L^{-3}$); θ_r and θ_s are the residual and saturated water contents ($L^3 L^{-3}$), respectively, with $0 \leq \theta_r < \theta < \theta_s$; h is the capillary pressure head (m), h_{ae} ($1/\alpha$) is associated

147 to the air-entry matrix potential (m^{-1}), n (> 1) is a shape parameter related to the pore-size distribution
148 (dimensionless), and m is another shape parameter. The two parameters m and n are interrelated via the
149 expression $m = 1 - 1/n$, following the assumption by Mualem [1976].

150 The unsaturated hydraulic conductivity function $K(\theta)$ is given by Mualem [1976] and van Genuchten
151 [1980]:

$$152 \quad K(\theta) = K_s \theta_e^L \left[1 - \left(1 - \theta_e \frac{1}{m} \right)^m \right]^2 \quad (4)$$

153 where L is a dimensionless shape factor and K_s is the saturated hydraulic conductivity ($m \text{ d}^{-1}$). The shape
154 factor, L is not a sensitive parameter and it is normally kept fixed to 0.5. Similarly, θ_r does not affect the
155 goodness-of-fit of the characteristic curve and it is typically eliminated [e.g. Russo, 1988; Luckner et al., 1989;
156 Tietje and Tapkenhinrichs, 1993; Boufadel et al., 1998; Schaap and Leij, 1998; Ines and Droogers, 2002].
157 Hence, in this study, θ_s , h_{ae} , n and K_s are the sole hydraulic parameters to be inverted. The expected range of
158 the above parameters are provided in Table 1; this range was computed by taking the 90% confidence
159 interval of the combined datasets of GRIZZLY [Haverkamp et al., 2005] and UNSODA [Leij et al., 1996]. In
160 particular, the minimum range of θ_s is determined for each hydroclimate by calculating the maximum range
161 of the reference θ .

162 **2.1.2 Modified sink term of SWAP 3.2 (SWAP_{inv})**

163 Building parsimonious SWAP models by reducing the number of input vegetation parameters, without
164 decreasing their predictive capacity and their physical concept, is a challenging task. In this context, we
165 modified the evaporation, transpiration and rainfall interception modules of SWAP, next termed SWAP_{inv}, in
166 order to use a reduced number of input parameters, namely the Leaf Area Index (LAI), the extinction
167 coefficient of solar radiation (K_g), the rooting depth, and the saturated (θ_s) and residual (θ_r) water contents.
168 In this respect, we use the Beer-Lambert law that partitions potential evaporation, potential transpiration
169 and potential evaporation of a wet canopy by using LAI and K_g [e.g. Ritchie, 1972; Goudriaan, 1977; Belmans
170 et al., 1983]. In addition, LAI, K_g and the potential evaporation of a wet canopy are also used to compute the

171 interception, based on the works of Noilhan and Lacarrere [1995] and Varado et al. [2006]. Thus, the
172 sensitivity of LAI and K_g are increased since they control multiple processes. The modified SWAP
173 evaporation module does not require extra parameters, since it is directly estimated from the soil moisture,
174 the potential soil evaporation and the hydraulic parameters [e.g. *Eagleson, 1978; Milly, 1986; Simmons and*
175 *Meyer, 2000; Romano and Giudici, 2007; 2009*]. Consequently, the sharing of the hydraulic parameters, which
176 computes soil moisture and evaporation, increases the sensitivity of the hydraulic parameters when they are
177 inverted simultaneously from soil moisture and evapotranspiration. The general shape of the roots in SWAP
178 is entered manually, in tabular form. Nevertheless, for large-scale modeling, a detailed description of roots is
179 not required, thus we introduced an empirical power-law root density function [*Gale and Grigal, 1987*], that
180 was further modified by Pollacco et al. [2008a]. The root density function requires two parameters, the
181 maximum rooting depths and the percentage of roots in the top 30 cm. A detailed mathematical description
182 of SWAP_{inv} is provided in Appendix A.

183 **2.2 Generation of reference data for numerical experiments**

184 The numerical experiments were carried out for 22 hydroclimatic scenarios, derived by combining three soil
185 types, two rooting depths and five climates (Table 2). In order to provide realistic simulations, deep roots
186 (DR) were not assigned to subtropical climates and shallow roots (SR) were not allocated to arid climate
187 [*Schenk and Jackson, 2002*]. Moreover, in semi-arid climates, only loamy sand was modeled. More precisely:

- 188 • The hydraulic parameters for the three contrasting benchmark soils (loamy sand, silty loam, silty clay)
189 are given in Table 3. These soil textures were selected from Carsel and Parrish [1988] and Ines and
190 Mohanty [2008b], and they ensure a large variability of annual evapotranspiration and groundwater
191 recharge.
- 192 • For the two contrasting benchmark-rooting depths (i.e. shallow and deep), the rooting depths and the
193 percentage of roots for the top 30 cm are given in Table 4. These contrasting rooting depths were
194 selected to depict shrubs, and they are provided by Schenk and Jackson [2002] and Jackson et al.
195 [1996]. Forested land use was not selected, because remote sensing platforms using passive
196 microwave still cannot retrieve soil moisture under dense canopy, the biomass of which is higher than
197 8 Kg m^{-2} (e.g., vegetation denser than mature corn) [e.g., *Jackson and Schmugge, 1991; Bindlish et al.,*

198 2006; *Li et al.*, 2006; *Njoku and Chan*, 2006].

- 199 • The values of the typical vegetation parameters that remain constant for all simulations are provided in
200 Table 5 and explained in Appendix A. It is assumed that all these parameters can be retrieved from
201 MODIS remote sensing [e.g., *Huete et al.*, 2002; *Simic et al.*, 2004; *Nagler et al.*, 2005; *Vegas Galdos et al.*,
202 2012].
- 203 • To formulate the hydroclimatic scenarios, we used daily precipitation time series and meteorological
204 data for computing the potential evapotranspiration through the Penman-Monteith formula [1965],
205 which were compiled from AmeriFlux <http://public.ornl.gov/ameriflux/> (Table 6). The contrasting
206 climates correspond to typical mainland Southern United States conditions, for which snowfall is
207 scarce. The forcing data was selected by combining a dry, a normal and a wet water year (October 1 to
208 September 30).

209 A summary of the 22 reference water fluxes computed with SWAP_{inv} is presented in Fig. 2. The
210 scenarios provide satisfactory high variability of the model fluxes. Specifically, the annual groundwater
211 recharge ranges from 30 to 800 mm, the annual transpiration ranges from 120 to 370 mm, and the annual
212 evaporation ranges from 7 to 144 mm.

213 2.3 Boundary conditions and discretization

214 Within the simulations, the soil column was discretized for deep roots of a total depth of 1.80 m and for
215 shallow roots of a total depth of 0.90 m. Finer discretization (0.25 cm) near the land atmospheric boundary
216 and coarser discretization (5 cm) at deeper depths were employed. For all scenarios, the soil columns were
217 initialized uniformly at $h = -0.1$ m and SWAP_{inv} run for 90 days (spin up time) ahead of the experiment, to
218 tune the state of the initial soil moisture profile. For the bottom boundary condition of the soil columns, the
219 free drainage was selected. The upper boundary condition was determined by the daily net precipitation,
220 which was computed with the interception model, and the potential evapotranspiration, estimated by the
221 Penman-Monteith equation. The potential evapotranspiration was partitioned into potential soil
222 evaporation, potential evaporation of wet canopy and potential transpiration by using the Beer-Lambert law
223 [e.g., *Ritchie*, 1972; *Goudriaan*, 1977; *Belmans et al.*, 1983]. Finally, a maximum of 2 cm of ponding water is
224 permitted with any overflow lost as runoff.

225 2.4 Formulation of the inverse problem

226 2.4.1 The Weighted Objective Function

227 Within the inverse problem we use a WOF comprising two fitting criteria, OF_{θ} and OF_{et} , and two control
228 variables, w and θ_d . In order to account for the differences in magnitude between the individual criteria, it is
229 preferable that all the components of the WOF are either dimensionless or normalized. The WOF is derived
230 by dividing the mean absolute error by the typical observation error (uncertainty) of the corresponding
231 reference state or flux, i.e.:

$$232 \quad OF_{\theta} = \frac{\sum_{i=1}^{N_{\theta}} |\theta_{ref} - \theta_{sim}|}{N_{\theta} \Delta\theta_{rs}} \quad \text{AND} \quad OF_{et} = \frac{\sum_{i=1}^{N_{et}} |ET_{ref} - ET_{sim}|}{N_{et} \Delta ET_{rs}} \quad (5)$$

233 where θ [$L^3 L^{-3}$] is the top 5 cm surface soil moisture where decoupling does not occur, and N_{θ} and N_{et} are the
234 lengths of daily soil moisture and evapotranspiration time series, respectively. When OF_{θ} or OF_{et} is greater
235 than one indicates that the errors of simulations are greater than the uncertainties of retrieving the
236 observation from remote sensing. We highlight that for both functions, all model outputs which provide
237 values greater than 1 are considered as non-acceptable. Hence, a trial set is rejected if $OF_{\theta} > 1$ or $OF_{et} > 1$.

238 To provide a proper configuration of the multiobjective calibration problem, it is essential to ensure that
239 the two fitting criteria, OF_{θ} and OF_{et} , are approximately uncorrelated. Indeed, Pollacco and Mohanty [2012]
240 showed that for contrasting hydroclimatic conditions the related processes θ and ET are rather independent.
241 This is because the surface θ is influenced by the evaporation and decouples between the surface and root-
242 zone soil moisture, while ET is a signature of the whole root-zone θ , since ET results in the uptakes of water
243 stored at depth. In addition, the storage of θ in the root-zone profile is dependent on the past weather
244 events, whereas the near-surface θ reflects the present weather condition.

245 2.4.2 Introducing decoupling within WOF

246 One of the peculiarities when calibrating hydrological models against surface soil moisture is that soil
247 moisture is prone to decoupling. This originates from the significantly faster drying of the surface compared
248 to the root-zone, due to evaporation and shallow root water uptake, causing a sharp vertical soil water

249 gradient near the surface. When this occurs, the surface θ is no more representative of the soil moisture
250 dynamics in the rooting zone [Capehart and Carlson, 1997; Walker et al., 2002; De Lannoy et al., 2007;
251 Pollacco and Mohanty, 2012]. For instance, large-scale decoupling was evidenced in New Zealand by Wilson
252 et al. [2003] between 0-6 cm and 0-30 cm *in situ*. Decoupling is more prominent when surface θ is in the
253 drying phase and it is below the threshold θ_d ($L^3 L^{-3}$), which is computed by:

$$254 \quad \theta_{\text{ref}}(t) < \theta_d \text{ and } \theta_{\text{ref}}(t + 1) < \theta_{\text{ref}}(t) \quad (6)$$

255 On the basis of Eq. (6), we modified OF_{θ} such that to increase its sensitivity by omitting the period when
256 surface and root-zone decoupling occurs. If $\theta_d = 0$, decoupling is not taken into account within WOF.

257 **3. Outline of the Weighted Objective Function Selector Algorithm (WOFSA)**

258 **3.1 Identification of the best-compromise parameter set in multiobjective calibration:** 259 **approaches and drawbacks**

260

261 Equation (1) is a specific case of aggregated objective functions that represent an overall measure of the
262 model performance, in which the characteristics of the best-compromise solution, which also reflect the
263 relative importance of the individual criteria, are specified *a priori*. The later are expressed in terms of
264 multipliers (e.g. weighting method), target-values combined with distance metrics (e.g., goal-programming
265 and ϵ -constraint methods [e.g., Laumanns et al., 2002; Reed et al., 2003]) or priorities (e.g. lexicographic
266 ordering). Besides, the detection of the best-compromise parameter set remains an open issue in
267 hydrological calibration, which has not been thoroughly addressed in the literature [e.g., Dumedah et al.,
268 2010].

269 Most approaches employ hybrid strategies, based on combined objective and subjective criteria, to
270 support the manual identification of the “most prominent” parameter values [e.g., Efstratiadis and
271 Koutsoyiannis, 2010]. In particular, a well-accepted technique for detecting the best-compromise
272 parameters, which is usually employed in subsurface flow modes, is by minimizing the Euclidean distance of
273 the Pareto set to the origin [e.g., Refsgaard and Storm, 1996; Madsen, 2003; Twarakavi et al., 2008]. Although
274 this methodology, which is a sub-case of goal-programming, appears to be statistically reasonable, its

275 hydrological meaning is not well-understood. On the other hand, few are the procedures for recognizing
276 effective non-dominated solutions *a posteriori*, through systematic filtering of the Pareto set. Some of the
277 proposed approaches are preference ordering and compensation between model objectives [e.g., *Khu and*
278 *Madsen, 2005*] as well as cluster analysis [e.g., *Taboada and Coit, 2006; Crispim and de Sousa, 2009; Dumedah*
279 *et al., 2010*]. For instance, Dumedah et al. [2010; 2012b; 2012a] used cluster analysis to evaluate the
280 distribution of solutions on the trade-off surface, to find relationships in both objective space and parameter
281 space. The linkage between the two spaces describes the level of robustness for the parameter sets
282 (according to Deb and Gupta [2005], robust solutions are less sensitive to variable perturbations in their
283 vicinity). They also showed that the use of criteria that are based on a compromise between representative
284 pathways in the parameter space and a dominant variability in the objective space provides solutions that
285 remain non-dominated across different validation sub-sets.

286 The above, rather subjective, approaches for detecting the best compromise parameter set in
287 multiobjective calibration problems, ignore uncertainties that are due to errors in input data, which prevents
288 providing robust solutions. In this respect, we are proposing a systematic procedure, called **W**eighted
289 **O**bjective **F**unction **S**elector **A**lgorithm (WOFSA), which identifies the most appropriate **W**eighted **O**bjective
290 **F**unction (WOF), by performing inverse modeling, where the uncertainties in retrieving θ and ET data are
291 directly accounted for. Next are described the key assumptions of the methodology, as well as the detailed
292 computational procedure.

293 **3.2 Key assumptions of WOFSA**

294 The key idea of WOFSA is based on the postulation that the optimal weighting between the individual
295 objectives is the one ensuring the maximum linear correlation between the residuals ΔWF of the computed
296 model responses of interest (water fluxes) and the WOF. The rationality is that if the inverse modeling is
297 well-posed, then an increase in the OF should cause the error of each specific simulated flux to also increase
298 and vice versa [Pollacco et al., 2008a]. If the later is insensitive against to variations of θ and ET , the problem
299 is ill-posed as the modeled flux cannot be calibrated solely from the observed θ and ET ; thus, additional
300 observations should be included into the WOF.

301 This assumption is further illustrated in Fig. 3, where we plot three hypothetical relationships

302 between a normalized WOF* and a dimensionless residual metric (e.g. relative bias) ΔQ^* , which is a measure
303 of uncertainty of the corresponding water flux (in the specific case, the groundwater recharge). It is assumed
304 that the optimal relationship is the 1:1 line (intermediate curve of Fig. 3, e.g. 2), which indicates that a
305 specific change of the WOF* value results to an equal change of the model uncertainty ΔQ^* . Therefore, this
306 expression is the most suitable to be used in calibration. Any other relationship, derived by different
307 combinations of weights, is sub-optimal. For instance, the right curve of Fig. 3 (e.g. 1) demonstrates a
308 weighted function that initially has limited sensitivity against the model uncertainty (a significant change of
309 the WOF* results to a much less significant change of ΔQ^*), followed by sharply varying model uncertainty
310 for small changes of the WOF*. On the other hand, the left curve of Fig. 3 (e.g. 3) represents an opposite
311 performance, which is also far from desirable. This feature forms the basis for our linearity assumption
312 between WOF* and ΔQ^* in WOFSA.

313 **3.3 Description of computational procedures**

314 The algorithm is applied to a SWAP_{inv} model, using the objective functions of section 2.4. The model runs on
315 daily basis. The water fluxes of interest are groundwater recharge Q (mm d⁻¹), evaporation E (mm d⁻¹),
316 transpiration T (mm d⁻¹), evapotranspiration ET (mm d⁻¹), while the modeled state variables are the root-
317 zone soil moisture θ_{rz} (m³ m⁻³) and the surface soil moisture θ (m³ m⁻³). The method is performed in three
318 successive steps, as also shown in the flowchart of Fig. 4

319 **3.3.1 STEP 1: Generation of reference runs**

320 WOFSA performs numerical experiments to determine the optimal control variables w and θ_d of the WOF,
321 which requires that the soil moisture θ , evapotranspiration ET, and water fluxes (as well as state variables)
322 WF, are known *a priori*. The later will be next called “reference” data, symbolized θ_{ref} , ET_{ref} and WF_{ref} ,
323 respectively. In particular, WF_{ref} are computed by inputting known sets of hydraulic parameters
324 (HYDRAU_{ref}), vegetation parameters (VEGETATION_{ref}) and daily forcing (precipitation, potential
325 evapotranspiration) data into SWAP_{inv} (Fig. 4, Loop 1). We remark that the vegetation parameters are
326 treated as known properties of the model (cf. section 2.2), while the soil hydraulic parameters are to be
327 inverted through optimization.

328 **3.3.2 STEP 2: Monte Carlo simulation and calculation of uncertainties**

329 In order to assess the uncertainties in retrieving θ_{ref} and ET_{ref} from remote sensing, we use different sets of
330 θ_{sim} and ET_{sim} , provided through Monte Carlo simulation (Fig. 4, Loop 2). Each trial set is formulated on the
331 basis of different values of soil hydraulic parameters ($HYDRAU_{sim}$), which are generated by $SWAP_{inv}$ to
332 provide the corresponding simulated time series WF_{sim} , θ_{sim} and ET_{sim} . The “unknown” constrained
333 $HYDRAU_{sim}$ are estimated by minimizing the WOF. To initialize the search procedure, the typical values
334 $w = 0.5$ and $\theta_d = 0$ are assigned to WOF, which are updated after the completion of Step 3. The simulations
335 are carried out by employing the **S**huffled **C**omplex **E**volution **U**niversity of **A**rizona (SCE-UA) algorithm,
336 developed by Duan *et al.* [1992; 1994]. The customized global optimization can be seen as a restrained
337 Monte Carlo simulation that seeks for different combinations of “compromise” parameter sets ($HYDRAU_{sim}$),
338 in the vicinity of the global minimum [van Griensven and Meixner, 2006; Pollacco *et al.*, 2008a, b].

339 For each trial set (i.e. hydraulic parameters and resulting fluxes), the model uncertainties, in terms of
340 residuals ΔWF , are computed by:

$$341 \quad \Delta WF = \frac{\sum_1^{t=N_{wf}} |WF_{ref}(t) - WF_{sim}(t)|}{\sum_1^{t=N_{wf}} WF_{ref}(t)} \quad (7)$$

342 where N_{wf} is the time length of simulations (days).

343 During the Monte Carlo procedure, all the different trials of $HYDRAU_{sim}$ and the corresponding WF_{sim}
344 and ΔWF are stored in the STORAGE archive (Fig 4). At the end of Step 2, the trial sets are sorted in
345 increasing order of WOF values. Fig. 5a depicts the relationship between WOF and the residuals of the
346 groundwater recharge ΔQ , for one of the experiments that are examined next (i.e. loamy sand, temperate
347 climate and short rooting depth).

348 **3.3.3 STEP 3: Estimation of w and θ_d**

349 As explained in section 3.2, in order to determine the best-compromise values of w and θ_d , it is
350 essential to ensure the greatest linearity between the so-called normalized WOF and the normalized

351 maximum uncertainties ΔWF_{\max}^* . This linearity is obtained by minimizing an “auxiliary” objective function
 352 OF_{lin} through the SCE-UA method, using the ensemble sets that are generated in Step 2. The computational
 353 procedure is the following:

354 From each generated WOF_i , the maximum corresponding error of WF_{sim} (ΔWF_{\max}) is selected and
 355 plotted. As shown in Fig. 5b (where ΔWF_{\max} is ΔQ_{\max}), the key assumption is that the relationship between
 356 WOF and ΔWF_{\max} monotonically increases is reasonable. The computation of ΔWF_{\max} is mathematically
 357 expressed as:

$$358 \quad \Delta WF_{\max}(i + 1) = \max \{ \Delta WF(i + 1), \Delta WF(i) \} \text{ and } \Delta WF_{\max}(i + 1) \geq \Delta WF_{\max}(i) \quad (8)$$

359 where index i corresponds to the i -th simulation, classified by an increasing order of WOF. We remind that
 360 here we only consider the uncertainties of the reference data that are used in calibration, and we do not take
 361 into account other error sources, such as structural errors of the model. In order to implicitly account for the
 362 later, we use the upper envelope uncertainties of the water fluxes ΔWF_{\max} and not, for instance, their average
 363 values.

364 For each flux, in order to evaluate the linearity between WOF and ΔWF_{\max} , the two variables are
 365 normalized, thus taking values in the range $[0, 1]$. This is performed by selecting the corresponding
 366 “envelopes” of simulated ΔWF_{\max} such that the following condition is fulfilled:

$$367 \quad OF_{\theta} = \Delta \theta \leq \Delta \theta_{\text{rs}} \text{ and } OF_{\text{et}} = \Delta ET \leq \Delta ET_{\text{rs}} \quad (9)$$

368 where $\Delta \theta_{\text{rs}}$ and ΔET_{rs} are typical values of the uncertainties in retrieving θ and ET, respectively, from remote
 369 sensing. In the case study, we generated 7000 sets of θ_{sim} and ET_{sim} which comply with Eq. 9. Preliminary
 370 investigations indicated that generating more sets improve the optimal values of w and θ_d only marginally.
 371 On the basis of literature data already mentioned in the introduction, for the soil moisture we assigned a
 372 volumetric root-mean-square error $\Delta \theta_{\text{rs}} = 0.04 \text{ m}^3 \text{ m}^{-3}$ while for the evapotranspiration we set a relative
 373 error $\Delta ET_{\text{rs}} = 20\%$ (apparently, in a particular study, different values can be employed, taking advantage of
 374 uncertainty estimations based on local data). The simulated ΔWF_{\max} values that comply with Eq. 9 are
 375 depicted in Fig. 5c, through the non-shaded area. WOF and ΔWF_{\max} are normalized and symbolized with (*),

376 using the maximum feasible simulated value that complies with Eq. 9, which is annotated with the circle in
 377 Fig. 5c.

378 As explained in section 3.2, the optimal WOF is determined such that to ensure the maximum linearity
 379 between WOF* and ΔWF_{max}^* . The linearity is quantified by means of the auxiliary objective function OF_{lin}
 380 (Fig. 3), which is computed separately for each water flux, as follows:

$$381 \quad OF_{lin}^* = \frac{MAX |\Delta WF_{max}^*(i) - WOF_i^*(w, \theta_d)|}{\sqrt{2}/2} \quad (10a)$$

382 where the index i corresponds to the i -th simulation, classified by an increasing order of ΔWF_{max}^* and $\sqrt{2}/2$
 383 is only used for graphical reasons, i.e. in order to normalize OF_{lin} thus being equal to half the diagonal of a
 384 unit square.

385 The value of OF_{lin}^* depicts the maximum deviation from the 1:1 line composed of ΔWF_{max}^* and WOF*, as
 386 described in Fig. 3. The value $OF_{lin} = 0$ denotes a perfect linearity, while $OF_{lin} = 1$ corresponds to the greatest
 387 deviation from the desirable line 1:1. The final value of OF_{lin} is computed by averaging OF_{lin}^* , which is
 388 calculated for each individual water flux and state variables of interest (root-zone soil moisture,
 389 groundwater recharge, evapotranspiration, evaporation and transpiration) by using the following
 390 expression:

$$391 \quad \overline{OF_{lin}^*} = \sqrt{\frac{\sum_1^{N_{OF_{lin}}} OF_{lin}^*(j)^2}{N_{OF_{lin}}}} \quad (10b)$$

392 where index j corresponds to j -th water flux of interest, and $N_{OF_{lin}}$ is the number of water fluxes of interest.
 393 An example of the relationship between the optimal WOF* and ΔWF_{max}^* for all water fluxes is provided in Fig.
 394 5d.

395 The SCE-UA optimization algorithm is next used to minimize the auxiliary function (Eq. 10b) against w
 396 and θ_a . After getting the optimal values of w and θ_a , the initial objective function (WOF) is updated and Steps
 397 2 and 3 are repeated. The iterative procedure continues until the values of w and θ_a are stabilized, thus WOF _{i}

398 $\approx \text{WOF}_{i-1}$. Typically, four runs are enough to achieve convergence.

399 **4. Results**

400 **4.1 General outcomes**

401 An overview of the WOFSA capabilities is provided by investigating the three representative scenarios,
402 which are presented in Table 7 and plotted in Fig. 6. The figure shows the relationship between WOF^* and
403 ΔWF_{\max}^* , which is computed for ET , T , E , θ , θ_{rz} and Q . The following general outcomes are drawn:

404 (a) The strength of linearity between WOF^* and ΔWF_{\max}^* can vary greatly with hydroclimate conditions
405 (Fig. 6);

406 (b) The usage of the decoupling algorithm (Eq. (6)) increases the linearity between WOF^* and ΔWF_{\max}^* (e.g.
407 for *loamy sand*; Fig. 6a);

408 (c) Deep roots compared to shallow roots tend to increase the discrepancy in the predictions of
409 transpiration (e.g. for *sandy clay*; Fig. 6b);

410 (d) The usage of WOF instead of a single OF_{et} did not improve the linearity between WOF^* and ΔWF_{\max}^*
411 (e.g. for *silty clay* under a Mediterranean climate for which we will show that it is a special case; Fig. 6c).

412 Next, we further investigate how the optimized values of w and θ_{d} vary under different hydroclimatic
413 conditions.

414 **4.2 Correlating soil moisture decoupling with hydroclimatic variables**

415 The weighting coefficient w and the decoupling threshold θ_{d} ($\text{m}^3 \text{m}^{-3}$) were optimized by minimizing OF_{lin}
416 (Eq. 10b). As already mentioned in section 2.4.2, to account for the observed θ within WOF we only used
417 periods when soil moisture decoupling does not occur. We remind that decoupling only occurs when the soil
418 is drying and the soil moisture falls below θ_{d} . For loamy sands, an example of decoupling is given in Fig. 7a,
419 where the reference time series of soil moisture θ are plotted at different depths. Fig. 7a suggests that during
420 the drying period and when $\theta < \theta_{\text{d}} = 0.07 \text{ m}^3 \text{m}^{-3}$ (where $0.07 \text{ m}^3 \text{m}^{-3}$ is the optimal value obtained through
421 the WOFSA, for the specific combination of soil texture and climate), the surface moisture is decoupled from

422 root-zone moisture.

423 For each hydroclimatic scenario, we employed preliminary simulations to express θ_d as function of
424 average surface soil moisture $\bar{\theta}$, average evapotranspiration \overline{ET} and its standard deviation σ_{ET} (Fig. 8). The
425 scatter plots indicate a negative correlation between $\overline{ET}/\sigma_{ET}$ and $(\theta_d/\bar{\theta})^{1/3}$. The ratio $\overline{ET}/\sigma_{ET}$ is a climatic
426 indicator which increases as the climate gets wetter, since there is a positive correlation ($r^2 = 0.70$) between
427 $\overline{ET}/\sigma_{ET}$ and the evapotranspiration fraction $\overline{ET}/\overline{ET}_{pot}$ (\overline{ET}_f) (results not provided here). On the other
428 hand, the ratio $\theta_d/\bar{\theta}$ can be viewed as a normalized expression of θ_d , where $\bar{\theta}$ is representative of the soil
429 texture, which is lower for coarse texture and higher for fine texture. To understand the correlation we
430 rewrite θ_d model as:

$$431 \quad \theta_d = \bar{\theta} \left(2.28 - 0.86 \frac{\overline{ET}}{\sigma_{ET}} \right)^3 \quad (11)$$

432 From the above equation it results that when the soil moisture storage $\bar{\theta}$ in the root-zone increases,
433 \overline{ET} also increases, which is reasonable. An increase in $\bar{\theta}$ also generates a decrease in soil moisture
434 decoupling, which is represented by a decrease in θ_d . However, a high value of σ_{ET} indicates more
435 pronounced periods of drying and wetting, which in turn produces an increase in soil moisture decoupling
436 θ_d , due to differences in the soil moisture storage between the surface and the root-zone. Fig. 8 shows that
437 for dry hydroclimates $\theta_d/\bar{\theta} > 1$, while for wetter hydroclimates $\theta_d/\bar{\theta} < 1$. Thus, $\overline{ET}/\sigma_{ET}$ is negatively
438 correlated with $(\theta_d/\bar{\theta})^{1/3}$. The conclusion that soil moisture decoupling is more pronounced in drier
439 climates is in line with the results of Capehart and Carlson [1997].

440 **4.3 Correlating weighting coefficient with hydroclimatic variables**

441 A major objective of this study is to relate the weighting coefficient w with easily obtainable predictors. The
442 optimal value of w is a complex tradeoff between the information gathered by OF_θ and OF_{et} . When more
443 weight is assigned to OF_θ , then the errors in $\Delta\theta_{rs}$ influences more the computation of the water fluxes (WF)
444 compared to ΔET_{rs} . On the other hand, when more weight is assigned to OF_{et} then the errors in ΔET_{rs}

445 influences more the computation of the WF compared to $\Delta\theta_{rs}$. In fact, the inverse modeling will favor the
446 weighting to OF_{θ} , since θ is a better predictor of the hydraulic parameters than ET [Pollacco *et al.*, 2008a].

447 For the three soil texture class subdivided climatically, Fig. 9a depicts the relationship of w against the
448 average evapotranspiration fraction $\overline{ET}/\overline{ET}_{pot}$, and Fig. 9b shows the correlation of w against the average
449 measured surface soil moisture $\overline{\theta}$. For every texture class, the empirical linear equations of Figs. 9a and 9b
450 are described in Table 8. No correlation of the rooting depth with w was found since the former influences
451 indirectly w through \overline{ET}_f . The hydroclimates which are enclosed in ovals are the ones for which little
452 difference arises in \overline{OF}_{lin}^* , given that OF_{et} is used instead of WOF. These hydroclimates are depicted by
453 arrows, representing threshold values of $\overline{\theta}$ and ET_f .

454 **Loamy Sand**

455 For coarser texture soils (loamy sand and sandy clay), w is negatively correlated to both \overline{ET}_f (Fig. 9a) and $\overline{\theta}$
456 (Fig. 9b). It is to be noted that $\overline{\theta}$ is small for coarse soils because, as shown in Fig. 7a, there are long periods
457 of droughts for which $\theta \approx 0$. Therefore, for dry hydroclimates, represented by low values of \overline{ET}_f , more
458 weight is assigned to OF_{θ} , and for wetter hydroclimates, represented by larger \overline{ET}_f , more weight is assigned
459 to OF_{et} .

460 These results can be explained in terms of the sensitivity of OF_{et} against ΔWF , which depends on \overline{ET}_f .
461 The later is computed from the water uptake function of Feddes *et al.* [1978], as shown in Fig. 9c. The
462 sensitivity of OF_{et} is considerably reduced when the vegetation is under arid conditions, with \overline{ET}_f as low as
463 10%. This is due to the closure of the stomata, thus more weight is assigned to OF_{θ} . For wetter hydroclimatic
464 scenarios characterized by an increase of \overline{ET}_f , the sensitivity of OF_{et} increases but at the same time OF_{θ}
465 weakens due to the enhanced surface and root-zone decoupling caused by evaporation. As \overline{ET}_f further
466 increases (hydroclimates enclosed in ovals in Fig. 9a and 9b), \overline{OF}_{lin}^* remains invariant if either OF_{et} or WOF

467 is used independently. Therefore, under these hydroclimatic conditions, it is preferable to use OF_{et} instead of
468 WOF. OF_{lin} remains invariant when $\overline{ET_f} > 68\%$ and $\theta > 0.035 \text{ L}^3 \text{ L}^{-3}$, approximately (refer to arrows in Fig.9a,
469 b), where the relationships between w vs. $\overline{ET_f}$ and w against θ change slope. These outcomes explain why
470 Ines and Droogers [2002], Ines and Mohanty [2008b] and Jhorar *et al.* [2002; 2004] did not find advantages
471 of using a WOF instead of a single OF to optimize the hydraulic parameters.

472 **Sandy clay**

473 The behavior of sandy clay soils is very similar to the loamy sands described above. Nevertheless, sandy
474 clays are less coarse than loamy sand and thus the average drainage and the evaporation rate is moderated.
475 Therefore, for the non-arid hydroclimatic scenarios ($\overline{ET_f} > 70\%$), w is clustered around 0.60.

476 **Silty clay**

477 For finer texture soils (silty clay), w is positively correlated with both $\overline{ET_f}$ (Fig. 9a) and $\bar{\theta}$ (Fig. 9b).
478 Therefore, for dry hydroclimates more weight is assigned to OF_{et} and for wetter hydroclimates more weight
479 is given to OF_{θ} . The correlation between w with $\bar{\theta}$ and w with $\overline{ET_f}$ of fine texture soils is positive, while for
480 coarse texture soils it is negative (Table 8). This difference arises because the vegetation under moist soils
481 do not experience much stress, thus ET_f remains close to unity (Fig. 9c). Under this premise, h is free to vary
482 between h_2 and h_3 (Eq. (A.8)), which reduces the sensitivity of OF_{et} . Thus, for wet hydroclimates, more
483 weight is assigned to OF_{θ} .

484 On the other hand, for drier hydroclimates, more weight is assigned to OF_{et} due to another type of
485 decoupling, which occurs for fine texture soils termed as *fine texture decoupling*. An example is provided in
486 Fig. 7b, where the reference time series θ are plotted at different depths. Fig. 7b suggests that for drier
487 climates the top soil dries up progressively and decouples with the root-zone, for which there is a substantial
488 amount of water stored at depth. Under these conditions, ET is more representative of the root-zone soil
489 moisture than the surface soil moisture, thus more weight should be assigned to OF_{et} .

5. Discussion

5.1 Selection of the most suitable calibration period

It is widely accepted that the information which is embedded in calibration data plays much more important role than the length of observations themselves. However, most of the existing hydrological calibration approaches do not provide any guidance about which sets of measurements are most informative for specific model parameters [e.g., *Vrugt et al.*, 2002]. In particular, for SVAT models, an additional quest is to determine the “optimal” period to calibrate the hydraulic parameters from reference surface θ and ET retrieved from remote sensing. The use of a multiobjective function, by means of the WOF, can adequately represent the errors that may be incurred due to the inverted parameter sets and may also help to recognize the structural errors much easier than when using a single fitting criterion. Therefore, to reduce ΔWF we need to select the period where the optimal w is theoretically around 0.6 (more weight is assigned to OF_{θ} , since θ is a better predictor of the hydraulic parameters), thus taking full advantage of the information provided simultaneously from OF_{et} and OF_{θ} .

Feddes *et al.* [1993], Ines and Mohanty [2008c], Jhorar *et al.* [2002] and Van Dam [2000] suggested that the identifiability of the parameters increases with the ranges of the data from very dry to very wet. Nevertheless, these results are partly supported by our study, which showed that better predictions are obtained when optimization is performed during periods where soil moisture decoupling does not occur. In this respect, given that soil moisture decoupling is accentuated under dry conditions (Eq. (6)), inverse estimations should be avoided during dry periods. Our investigations also indicated that under dry conditions ET_f is reduced and therefore OF_{et} , driven by the Feddes *et al.* [1978] model, becomes less significant. In section 4.3 it was also shown that for wet periods, during which ET_f remains close to unity (Fig. 9c), the sensitivity of OF_{et} is reduced. Thus, the common belief that one requires a period such that θ goes from saturated to residual water content is not supported by this study.

In practical terms, it is recommended that the hydraulic parameters should be preferably optimized after heavy rainfall events, when the soil moisture profile is homogeneous. Nevertheless, the measurements should only start after the plant is starting to experience stress and stopped when the roots are experiencing

516 excessive stress. This finding suggests that the inverse modeling should be performed during the period
517 where evaporation is not at its maximum, to avoid soil moisture decoupling.

518

519 **5.2 Comparison of the WOFSA with the minimum distance from the origin**

520 In section 3.1 we mentioned that a well-accepted technique for detecting the optimal value of w , which is a
521 complex tradeoff between the information gathered by OF_{θ} and OF_{et} , is by Minimizing the Euclidean Distance
522 of the Pareto front to the origin (MEDP). Apparently, this requires determining the shape of the Pareto front.
523 In nonlinear spaces, this is only achievable by running a suitable multiobjective evolutionary optimization
524 algorithm, which can provide representative non-dominated solutions that are uniformly distributed across
525 the objective space [Efstratiadis and Koutsyiannis, 2010]. For a given shape of the front, the computation of
526 its minimal distance from the origin is trivial. In particular, as illustrated in Fig. 1, when OF_{θ} and OF_{et} are
527 normalized this method results to $w = 0.5$, independently of the values of $\Delta\theta_{rs}$ and ΔET_{rs} , and also
528 independently of the hydroclimatic conditions.

529 The major drawback of the MEDP approach is the erroneous assumption that the magnitude of $\Delta\theta_{rs}$ is
530 similar to the one of ΔET_{rs} and that the impact of $\Delta\theta_{rs}$ and ΔET_{rs} on the WF are similar. Indeed, our extended
531 investigations within this paper concluded that w is far from constant; in opposite, it is highly dependent on
532 both the soil texture and climate (Fig. 9). Moreover, MEDP fails to take into consideration that when more
533 weight is assigned to OF_{θ} , then the errors in $\Delta\theta_{rs}$ influences more the computation of the water fluxes and
534 state variables WF, compared to ΔET_{rs} . On the other hand, when more weight is assigned to OF_{et} , the errors
535 in ΔET_r have more influence to the simulated WF, if compared to $\Delta\theta_{rs}$. Hence, the only advantage of MEDP
536 against WOFSA is the simplicity of the computational procedure, but only under the premise that the shape
537 of the Pareto front is well-approximated.

538 **5.3 Implementing WOFSA within a Pareto-optimization framework**

539 Forthcoming research needs to address how we can integrate WOFSA within global multiobjective
540 calibration procedures (e.g. MOSCEM, MOPSO, MOHBMO, [Barros et al., 2010]), by using real observations.

541 Moreover, it can provide guidance for the selection of the most robust solution, among the mathematically
542 equivalent Pareto optimal alternatives. Indeed, the best-compromise solution of the multi-objective
543 calibration problem is theoretically found in the cross-section of the optimally-weighted objective function
544 (WOF) and the Pareto-front. Yet, the task of implementing the above idea is non-trivial, since the true water
545 fluxes and state variables (WF_{ref}) are unknown. In the following we propose preliminary guidelines how to
546 use WOFSA in a multiobjective calibration setting by assuming that the inverse problem is well-posed, thus
547 exhibiting relatively steep trade-offs and that an increase in WOF would produce an increase in WF_{sim} .

548 ***STEP a: Run multi-objective optimization***

549 Perform multi-objective optimization by simultaneous minimizing OF_{et} and OF_{θ} , for which w does not need to
550 be provided. On the other hand, θ_d which depends on the climate data can be estimated from Fig. 8. During
551 the optimization, all the feasible $HYDRAU_{sim}$ and WF_{sim} which complies with Eq. 9 are kept in storage which
552 will give the sub-set of acceptable Pareto-optimal solutions (Fig. 1).

553 ***STEP b: Selection of temporary reference water fluxes***

554 A first guess of the reference parameters (WF_{ref} , $HYDRAU_{ref}$) is obtained from the cross-section of the
555 weighted objective function (WOF) and the sub-set of Pareto optimal solutions. To obtain a first guess of
556 WOF, w is approximated from Table 8 and θ_d is provided from Fig. 8. Next, ΔWF is computed for the sub-set
557 of acceptable solutions.

558 ***STEP c: Dividing the sub-set of acceptable solutions***

559 WOFSA is performed independently on different parts of the sub-set of acceptable solutions, i.e. the Pareto
560 front (Fig. 1). The area is divided on the basis on w . For instance, if the sub-set of acceptable solutions are
561 divided into four sub-areas, then the ranges of w are $[0 ; 0.25]$, $[0.25 ; 0.5]$, $[0.5 ; 0.75]$ and $[0.75 ; 1.0]$. For
562 each sub-areas, the WOFSA runs from STEP 3, (section 3.3.3), thus obtaining the corresponding $\overline{OF_{lin}^*}$.

563 **STEP d: Refining the results**

564 The WF_{ref} is updated with the new value of w based on the group which exhibits the lowest $\overline{OF_{lin}^*}$. Thus, the
565 best-compromise solution is in the cross section of the optimal WOF and the Pareto front (Fig. 1). Steps b
566 and c are repeated until convergence occurs between the new optimal w and the previously computed value.

567 We should remark that although in this study we used two fitting criteria, the WOFSA can be performed
568 with more criteria. In the current version, we suggest using a maximum of four fitting criteria, thus allowing
569 the calibration of up to three weights within the minimization of $\overline{OF_{lin}^*}$ (Eq. 10b). The introduction of more
570 criteria would result to a significantly extended Pareto front, tending to cover a large part of the entire
571 objective space. Evidently, this is far from desirable, for both theoretical (i.e. increased uncertainty) and
572 practical reasons (i.e. poor understanding of the generated trade-offs). Nevertheless, very limited are the
573 cases where more than four independent criteria have been applied in real-world applications [Efstratiadis
574 and Koutsoyiannis, 2010]. Forthcoming research will investigate whether is it practical to increase the
575 number of fitting criteria, taking into account that the WOFSA enables to constrain the feasible Pareto front,
576 as depicted in Fig. 1, thus significantly facilitating the multiobjective searching procedure.

577 **5.4 The need for validation experiments with field data**

578 The proposed WOFSA methodology, which was thoroughly tested on the basis of synthetic data for a wide
579 range of soil texture and climatic conditions, provided consistent and reasonable results. By using synthetic
580 data, we also explicitly ignored uncertainties that are related to field observation errors, thus only focusing
581 to uncertainties due to retrieval of surface soil moisture and evapotranspiration from remote sensing.
582 Evidently, in real-world conditions, inherent modeling and measurement errors and uncertainties cannot be
583 neglected.

584 Yet, for a full validation of the methodology, and in order to quantify the gain in accuracy would
585 require the collection of field data. This is by far non-trivial, due to the extent of *in situ* and remote sensing
586 data requirements as well as potential scaling problems. In fact, performing measurements of effective large
587 scale water fluxes is considered infeasible because typically θ and ET are retrieved at a scale of several
588 square kilometers. Without considering the scale issues, a way forward can be by using precise weighing

589 lysimeters for which all the water fluxes are continuously monitored (storage, drainage, and
590 evapotranspiration). The surface θ determined (for example) by neutron probe or time-domain
591 reflectometer needs to be monitored. To mimic the uncertainties in retrieving θ and ET from remote sensing,
592 noise can be introduced into the measurements of surface θ and lysimeter ET .

593 The different lysimeters experiments should contain contrasting textures and climate as described in
594 Fig. 2. Preferably, the lysimeters should be filled with representative soils and vegetation. Too dry climates
595 may be avoided since it causes strong surface and root-zone θ decoupling for which these periods can be
596 recognized through the newly introduced threshold θ_d , which is computed from Eq. (6).

597 During the validation phase, it is also important to recognize that non-daily information for observed θ
598 and ET is retrieved from thermal-band land surface temperature retrievals, which to date are limited to
599 cloud-free atmospheric conditions (e.g., Anderson et al., 2011). This implies that the collected data from
600 remote sensing is skewed toward drier conditions.

601 **6. Conclusions**

602 The inversion of the hydraulic parameters of a one-dimensional physically-based SVAT model by taking
603 advantage simultaneously of surface soil moisture (θ), and evapotranspiration (ET), requires to take into
604 consideration the uncertainties of retrieving θ and ET from remote sensing and the decoupling of the surface
605 and root-zone θ . To increase the sensitivity of θ , the optimization should not be performed during dry
606 periods, i.e. when decoupling of the surface and root-zone soil moisture occurs. These periods can be
607 recognized through the newly introduced threshold θ_d , which is computed from Eq. (6).

608 The proposed multiobjective approach, by means of a **W**eighted **O**bjective **F**unction (WOF), provides a
609 suitable compromise between fitting criteria against θ and ET , also taking into consideration the contrasting
610 uncertainties in retrieving θ and ET from remote sensing. As shown in the simulations, the uncertainties of θ
611 have different implication in the computation of the water fluxes of interest compared to the uncertainties of
612 ET . WOF comprises of two control variables, namely a weighting coefficient (w) and the decoupling
613 threshold θ_d .

614 In order to determine the best-compromise values of w and θ_d , we developed a novel inverse modeling
615 framework, called **W**eighted **O**bjective **F**unction **S**elector **A**lgorithm (WOFSA). WOFSA aims to minimize the
616 uncertainties of the computed water fluxes and state variables, following a systematic and as much as
617 objective procedure, in terms of a theoretical framework for formulating an optimal WOF, on the basis of
618 synthetic data. WOFSA performs forward simulations in order to ensure the greatest linearity between the
619 optimized WOF and the maximum uncertainties of the generated water fluxes ΔWF . The ΔWF are derived by
620 mimicking the typically recommended uncertainties of retrieving θ and ET from remote sensing.

621 To determine how the optimal w and θ_d of WOF vary under different hydroclimatic conditions, 22
622 contrasting hydroclimatic scenarios were formulated, by combining five climates, three soil textures and two
623 different rooting depths. Based on the results provided by WOFSA, we established relationships between the
624 optimized values of w and θ_d . In particular, for all scenarios we provided empirical relationships to compute
625 θ_d from the average values of θ and ET, and the standard deviation of ET. Moreover, for each texture class,
626 we correlated w with average evaporation fraction and with average surface soil moisture, for which we also
627 provided empirical linear equations. All results are interpreted in terms of hydrological evidence, which is a
628 strong justification of the proposed WOFSA methodology. For instance, we found that θ_d increases for drier
629 hydroclimates and that the rooting depths influence indirectly w through the average evapotranspiration
630 fraction. We remark that typical multiobjective calibration approaches, such as the well-known minimization
631 of the Euclidean Distance of the Pareto set, erroneously assume that the magnitude of $\Delta\theta_{rs}$ is similar to the
632 one of ΔET_{rs} and that the impacts of $\Delta\theta_{rs}$ and ΔET_{rs} on the simulated model responses are not affected by soil
633 and climate conditions.

634 In practical terms, it is recommended to employ soil moisture measurements preferably after heavy
635 rainfall, when the soil moisture column is homogenized to avoid soil moisture decoupling. Nevertheless, the
636 measurements should be performed only after the plant is starting to experience stress since it was found
637 that the fitting criteria of ET reduces the sensitivity when the Feddes plant water stress response function
638 equals to the potential evapotranspiration. The measurements should also not be taken when the plant is
639 experiencing excessive stress, since it reduces the sensitivity of the fitting criteria of ET and causes soil
640 moisture decoupling. It is also advised to perform the study during the season where evaporation is not at its

641 maximum to avoid soil moisture decoupling.

642 The proposed framework, which was thoroughly tested on the basis of synthetic data for a wide range of
643 soil texture and climatic conditions, provided consistent and reasonable results. Yet, for a full validation of
644 the methodology, and in order to quantify the gain in accuracy without considering the scale issues, a
645 number of calibration experiments with real data are necessary. Evidently, this task is not trivial, mainly
646 because it is very demanding in terms of in situ data measurements, e.g. through high-precise weighing
647 lysimeters.

648 Our next research step is the implementation of WOFSA within a multiobjective optimization context,
649 taking into account the preliminary ideas of section 5.3. This will enable to reduce the range of the Pareto set
650 in a hydrological perspective, on the basis of real (observed) data across a specific study area. The results of
651 these investigations will be reported in due course.

652

653 7. Appendix A

654 The appendix describes the sink term and the interception module of SWAP_{inv} which is substantially
655 different than the ones implemented into SWAP.

656 7.1 Potential evapotranspiration

657 The potential evapotranspiration ET_p (mm d⁻¹) is estimated by the Penman-Monteith [1965] equation
658 that was further modified by Allen et al. [1998], and is computed by:

$$659 \quad ET_p = \frac{\frac{\Delta_v}{\lambda_w} (R_n - G) + \frac{P_1 C_{air}}{\lambda_w} \frac{e_{sat} - e_a}{r_{air}}}{\Delta_v + \lambda_{air} \left(1 + \frac{r_{crop}}{r_{air}} \right)} \quad (A.1)$$

660 where Δ_v is the slope of the vapor pressure curve (ML⁻¹T⁻²θ⁻¹); λ_w is the latent heat of vaporization of water
661 (L²T⁻²); R_n is the net radiation flux density (MT⁻³) above the canopy; G is the soil heat flux density (MT⁻³);
662 p_1 accounts for unit conversion (86 400 s d⁻¹); ρ_{air} is the air density (MT⁻³); C_{air} is the heat capacity of moist
663 air (L T⁻¹θ⁻¹); e_{sat} is the saturation vapor pressure (ML⁻¹T⁻²); e_a is the actual vapor pressure (ML⁻¹T⁻²); r_{air} is
664 the aerodynamic resistance (L⁻¹T); γ_{air} is the psychrometric constant (ML⁻¹T⁻²θ⁻¹); and $r_{crop} = 70$ s m⁻¹ is the
665 crop resistance [Allen, 1986].

666 ET_p is partitioned into potential evaporation of the wet canopy E_{PW} (mm d⁻¹), potential soil evaporation
667 E_p (mm d⁻¹) and potential transpiration T_p (mm d⁻¹). The partitioning is performed using the leaf area index
668 LAI (m² m⁻²) and the fraction of the canopy, $1 - F_w$ that is not wet. It is to be noted that F_w is computed
669 differently in SWAP_{inv} (Eq. (A.15)). SWAP assumes that the net radiation inside the canopy decreases
670 exponentially and that the soil heat is negligible. The partitioning is performed by using a Beer-Lambert law
671 [e.g., Ritchie, 1972; Goudriaan, 1977; Belmans et al., 1983]:

$$672 \quad T_p = \max \{ ET_p [1 - F_w(E_{pw}, LAI)] - E_p, 0 \} \quad (A.2)$$

$$673 \quad E_p = E_{p0} F_s \quad (A.3)$$

$$F_s = \exp(-K_g \text{LAI}) \quad (\text{A.4})$$

where F_s (dimensionless) is the interception of solar radiation that will also be used in the interception model; K_g (-) is the extinction coefficient for solar radiation that is set to 0.5 [Varado et al., 2006; Wang et al., 2009]. ET_p decreases with increasing K_g and increasing LAI. E_{p0} (mm d^{-1}) is the potential evaporation of bare soil, computed for albedo equal to 0.1. For further information on the computation of ET_p , E_{PW} and E_{p0} the readers are referred to the SWAP manual (<http://www.swap.alterra.nl/>).

7.2 Sink term

To take into account tree physiology and the reduction of transpiration by soil water stress, the actual transpiration T is distributed by the sink term $S(h_i)$ over the whole root-zone and is calculated for each cell by Feddes et al. [1978]. The sink term is computed by:

$$S(h_i) = \beta T_p G(h_i) \Delta Rdf_i \quad (\text{A.5})$$

where β is the transpiration fraction or crop factor (-), the value of which is provided in Table 5; T_p (mm d^{-1}) (Eq. (A.2)) is the potential transpiration estimated for short grass; ΔRdf_i is the vertical fraction of the root density function per cell i (%) (Eq. (A.6)); and $G(h_i)$ is the reduction of root water uptake at pressure head h per cell i (-) (Eq. (A.8)). All these variables except for T_p are dimensionless.

7.2.1 The root-density distribution

In SWAP the vertical fraction of the root density function per cell i (ΔRdf_i), which defines the general shape of the roots, is entered manually in tabular form. In SWAP_{inv}, the root distribution is modeled with an empirical function of Gale and Grigal [1987] that was modified further by Pollacco et al. [2008a]. The model requires the rooting depth and the percentage of root density in the top 30 cm (ΔRdf_{30}). It is to be noted that in this literature the percentage of root density is often stated for the top 30 cm, but the user can specify any other depth. The values of the parameters for the two contrasting scenarios used in this study, composed of shallow and deep rooted plants, are provided in Table 4. For each cell i , the fraction of roots ΔRdf_i between the top depth z_{up} and the bottom depth z_{down} is computed as:

698
$$\Delta Rdf_i = \frac{E_c^{|z_{down}|} - E_c^{|z_{up}|}}{1 - E_c^{|z_{root}|}} \text{ with } \sum_1^{i=i_{max}} \Delta Rdf_i = 1 \quad (\text{A.6})$$

699 where z_{up} and z_{down} are respectively the top and bottom depth of each cell which is positive downwards (cm).
700 E_c is the “extension coefficient” parameter, z_{root} is the rooting depth (cm) and i_{max} is the last cell of the root-
701 zone. E_c varies between 0.700 and 0.9999, such that when E_c is close to 0.7 all the roots are distributed in the
702 top cell, and when E_c is close to 1, the roots are distributed evenly within the root-zone.

703
704 The value of E_c is computed from the percentage of roots. For example, in the top 30 cm, ΔRdf_{30} is
705 estimated by solving the following equation:

705
$$\Delta Rdf_{30} = \frac{E_c^0 - E_c^{30}}{1 - E_c^{|z_{root}|}} = \frac{1 - E_c^{30}}{1 - E_c^{|z_{root}|}} \quad (\text{A.7})$$

706 where E_c is the “extension coefficient” parameter, and z_{root} is the rooting depth (cm).

707 **7.2.2 Root water uptake**

708 When the capillary pressure head h_i per node i is reduced, the vegetation closes their stoma and
709 decreases transpiration, by using the Feddes et al. [1978] stress function computed as follows:

710
$$G(h_i) = 0, \text{ if } |h| > |h_4| \text{ or } |h| < |h_1|$$

711
$$G(h_i) = 1, \text{ if } |h| > |h_2| \text{ and } |h| < |h_3| \quad (\text{A.8})$$

712 Water uptake below $|h_1|$ (oxygen deficiency) and above $|h_4|$ (wilting point) is set to zero. Between $|h_2|$
713 and $|h_3|$, $g(h_i) = T_p$ maximal. The value of h_3 varies with T_p . For different values of T_p , h_3 is linearly
714 interpolated between h_{3low} and h_{3high} . The values of h_1 , h_2 , h_{3high} , h_{3low} and h_4 are provided in Table 5.

715 **7.3 Evaporation from bare soil**

716 The evaporation module of SWAP was simplified. Under wet soil conditions, the actual soil evaporation
717 E [mm d⁻¹] equals the potential soil evaporation E_p . During inter-storm period SWAP computes E by using the
718 empirical evaporation method of Black et al. [1969] that requires two fitting parameters. Nevertheless

719 Eagleson [1978], Milly [1986], Simmons and Meyer [2000] and Romano and Giudici [2007; 2009] showed
 720 that good results can be achieved by relating evaporation with θ . We therefore used the Romano and Giudici
 721 [2007; 2009] evaporation model that does not require any extra parameters:

$$722 \quad E = \frac{\text{MAX}\theta_{15}^0 - \theta_r}{\theta_s - \theta_r} E_p \quad (\text{A.9})$$

723 where the maximum θ is taken from the highest soil moisture between the surface and the depth to 15 cm; θ_r
 724 and θ_s are residual and saturated water contents ($\text{L}^3 \text{L}^{-3}$) respectively defined earlier by Eq. (3).

725 **7.4 Rainfall interception model**

726 SWAP computes rainfall interception following Braden [1985] and Von Hoyningen-Huene [1981]. These
 727 interception models require extra parameters and do not use potential evaporation of a wet canopy E_{pw} (mm
 728 d^{-1}). We introduced in SWAP_{inv} a physically-based interception model, following the work of Noilhan and
 729 Lacarrere [1995] and Varado et al. [2006] described in Pollacco and Mohanty [2012]. In this model, E_{pw} is
 730 used as a predictor, while the Leaf Area Index LAI (-) and the extinction coefficient of solar radiation K_g (-)
 731 are assumed as parameters. The values of the LAI and K_g are provided in Table 5. The gross precipitation P_g
 732 (mm d^{-1}) defined as the amount of water which reaches the canopy is computed following Rutter et al.
 733 [1971]:

$$734 \quad P_g = P_{\text{int}} + P_{\text{free}} \quad (\text{A.10})$$

735 where P_{free} (mm d^{-1}) is the free throughfall that is the fraction of precipitation that reaches the ground
 736 surface through gaps in the canopy; P_{int} (mm d^{-1}) is the intercepted precipitation.

737 The foliage of the canopy is considered as a water reservoir filled up to a depth of W_r (mm), with a maximum
 738 storage capacity W_{max} (mm). When the canopy is fully saturated ($W_r = W_{\text{max}}$) than any excess of P_{int} overflows
 739 P_{over} (mm) to the ground such that according to Valante et al. [1997]:

$$740 \quad P_{\text{over}} = \max \{P_{\text{int}} + W_r - W_{\text{max}}, 0\} \quad (\text{A.11})$$

741 The amount of water that reaches the ground is the net precipitation P_{net} (mm d^{-1}):

$$P_{\text{net}} = P_{\text{over}} + P_{\text{free}} \quad (\text{A.12})$$

A fraction of the water from the reservoir W_r will be evaporated at the rate of the actual evaporation of a wetted canopy EA_w (mm d^{-1}) during and after a rainfall event. W_r is calculated following Deardorff [1978]:

$$\partial W_r / \partial t = P_{\text{int}} - P_{\text{over}} - EA_w \quad (\text{A.13})$$

The maximum quantity of water which can be evaporated during a time step is computed as:

$$EA_w = \min \{E_{\text{pw}} F_w, W_r / dt\} \quad (\text{A.14})$$

where E_{pw} is the *potential transpiration of a wet canopy*.

According to Rutter et al. [1971], evaporation from wet canopies is assumed to be proportional to the fraction of the canopy that is wet F_w (0-1) that is computed following Deardorff [1978]:

$$F_w = (W_r / W_{\text{max}})^{2/3} \quad (\text{A.15})$$

W_{max} is related to LAI based on the empirical relationship of Varado et al. [2006] and Von Hoyningen-Huene [1981]. Varado et al. [2006] assumes that the interception of water of a canopy is similar to the interception of solar radiation F_s (0-1)(Eq. (A4)). Combining Varado et al. [2006] and Von Hoyningen-Huene [1981], W_{max} is computed as:

$$W_{\text{max}} = (0.935 + 0.498\text{LAI} - 0.00575 \text{LAI}^2) (1 - F_s)$$

(A.16)

W_{max} increases with increasing LAI and K_g . The partitioning of P_g and P_{free} is computed as:

$$P_{\text{free}} = F_s P_g \quad (\text{A.17})$$

$$P_{\text{int}} = (1 - F_s) P_g \quad (\text{A.18})$$

$$F_s = e^{-K_g \text{LAI}} \quad (\text{A.19})$$

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1076 **Acknowledgments**

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1086

LIST OF CAPTIONS

List of tables:

Table 1. Expected parameter space of the van Genuchten hydraulic parameters computed by taking the 90% confidence interval of the combined datasets of GRIZZLY [Haverkamp et al., 2005] and UNSODA [Leij et al., 1996]. The minimum range of θ_s is computed from the maximum value of reference θ .

Table 2. Contrasting 22 scenarios composed of three soil types, two rooting depths and five climates. To maintain the simulations more realistic deep roots were not assigned to subtropical climates and shallow roots were not allocated to arid climate.

Table 3. Reference values of the Mualem [1976] - van Genuchten [1980] hydraulic parameters.

Table 4. Contrasting scenarios of the percentage of roots in the top 30 cm, ΔRDF_{30} [Jackson et al., 1996], and maximum rooting depths, Z_{root} [Schenk and Jackson, 2002].

Table 5. Values of vegetation parameters that remains constant. Where $h_1, h_2, h_{3h}, h_{3b}, h_4$ are the capillary pressure head that regulate the water uptake model, LAI is the Leaf Area Index, β is the crop factor and K_g is the extinction coefficient of solar radiation [-]. Refer to Appendix A for further information.

Table 6. Sources of reference hydroclimate data compiled from AmeriFlux (<http://public.ornl.gov/ameriflux/>).

Table 7. Detailing the different scenarios used in Fig. 6.

Table 8. Empirical relationship for the 3 texture classes which relates w with average $\overline{ET_f}$ (ET/ET_p) and w with average $\overline{\theta}$.

List of Figures:

Fig. 1. Graphical example illustrating the objective space, the Pareto front and characteristic solutions of a hypothetical problem of simultaneous minimization of two criteria (in the specific case OF_θ and OF_{et}). Vector $\mathbf{e} = [e_1, e_2]$ indicates limits of acceptability (in the specific case uncertainty bounds), for distinguishing feasible solutions. Shown are the extreme solutions of the Pareto front (corresponding to $w = 0$ and $w = 1$), the solution that has the minimum distance from the origin and the solution provided by WOFSA, corresponding to $w = 0.75$.

Fig. 2. The 22 hydroclimatic scenarios depicted by average yearly groundwater recharge Q , transpiration T , evaporation E , interception P_{int} computed from SWAP_{inv} . For visualization, the gross precipitation $P_g = Q + T + E + P_{\text{int}}$ with the long-term storage computed to 0. The acronyms are provided in Table 3 for the soil texture, in Table 4 for the roots and in Table 6 for the climate.

Fig. 3. Examples of relationships between a normalized weighted objective function (WOF*) with the normalized uncertainty of the water flux (ΔWF^*) error, represented by ΔQ^* . The ideal is a linear correlation between WOF* and ΔQ^* .

Fig. 4. Flowchart of the *Weighted Objective Function Selector Algorithm* (WOFSA) where $\text{HYDRAU}_{\text{ref}}$ and

VEGETATION_{ref} are a known set of reference parameter values; **WF_{ref}** are the modeled reference water fluxes outputs which are computed from the SVAT hydrological model requiring a priori known sets of hydraulic parameters (**HYDRAU_{ref}**) and gross precipitation (**P_g**) and potential evapotranspiration (**ET_p**) as forcing data; **HYDRAU_{sim}** are trial set of parameter values that are obtained from the **OPTIMIZATION ALGORITHM**; **WF_{sim}** are simulated fluxes and **ΔWF** is their residuals, derived by a posteriori estimated hydraulic parameters (**HYDRAU_{sim}**) by minimizing the weight **w** (between the fitting criteria based on soil moisture **θ** and evapotranspiration **ET**) and the decoupling threshold θ_d of **WOF**. All the trials are stored in the **STORAGE** which are filtered such that the uncertainties in θ_{sim} and ET_{sim} are not greater than the uncertainties of retrieving θ and ET from remote sensing ($\Delta\theta_{rs}$ and ΔET_{rs}). WOFSA is performed in two separate parts: **Part A** generates uncertainties in the fluxes **ΔWF** as if they were available from independent measurements, while **Part B** optimizes **w** and θ_d by minimizing the **OF_{lin}** such that to ensure the maximum linearity between the normalized **WOF*** and the normalized maximum uncertainty **ΔWF_{max*}**. The different loops are colored coded with blue for loop 1, red for loop 2 and green for loop 3.

Fig. 5. Different steps of the WOFSA given as an example for loamy sand, temperate climate and short rooting depth. **(A)** An ensemble of generated parameter sets **HYDRAU_{sim}** with the relationship between **WOF** and the residuals between reference and simulated **WF_{sim}** given as an example for groundwater recharge ΔQ ; **(B)** From each generated **WOF_i**, described in **(A)** the maximum corresponding error ΔQ_{max} is selected; **(C)** Selection of feasible parameter sets ΔQ_{max} to reproduce the uncertainties in retrieving θ_{ref} and ET_{ref} from remote sensing; **(D)** Correlation between normalized **WOF*** and normalized **WF_{max*}** for top soil moisture **SM** (θ), root-zone soil moisture **SM_{rz}** (θ_{rz}) evapotranspiration **ET**, evaporation **E**, transpiration **T**, and groundwater recharge **Q**.

Fig. 6. Relationships between normalized optimized **WOF*** and normalized **ΔWF_{max*}**, for the scenarios described in Table 7.

Fig. 7. Reference time series θ plotted at different depths: **(A)** for coarse soils, showing that the top layer is decoupled from the deeper layer when θ is drying and $\theta < \theta_d$, and **(B)** for fine texture soils under dry climate, showing that the top layer gets gradually decoupled from the deeper layer.

Fig. 8. For all hydroclimatic conditions a relationship is obtained between average **ET** divided by the standard deviation of **ET** (σ_{ET}) with $(\theta_d / \theta)^{0.3}$. The scenarios are wetter as ET / σ_{ET} increases.

Fig. 9. For the three soil texture class subdivided climatically: **(A)** relationship of **w** with average evaporative fraction **ET_f**, and **(B)** correlation of optimal **w** with measured average θ . The empirical linear equations of each texture classes are described in Table 8. The enclosed hydroclimates are those for which a single **OF_{et}** can be used instead of a **WOF**. These hydroclimates are depicted by arrows which represent threshold values of θ and ET_f . The **(C)** schematizes the Feddes et al., [1978] plant water stress response function (**ET_f**) as a function of soil water pressure. The position of the parameter h_3 depends on the intensity of the potential transpiration ($T_p < 1 \text{ mm d}^{-1}$ or $T_p \geq 5 \text{ mm d}^{-1}$). The interpolation of h_3 is between the interval h_{3low} , h_{3high} for which their values are provided in Table 5.

LIST OF TABLES

Table 1. Expected parameter space of the van Genuchten hydraulic parameters computed by taking the 90% confidence interval of the combined datasets of GRIZZLY [Haverkamp et al., 2005] and UNSODA [Leij et al., 1996]. The minimum range of θ_s is computed from the maximum value of reference θ .

	θ_s	h_{ae}	n	K_s
	[m ³ m ⁻³]	[cm]	[-]	[cm d ⁻¹]
Minimum	MAX(θ_{ref})	7.6	1.09	0.48
Maximum	0.54	375	2.3	465

Table 2. Contrasting 22 scenarios composed of three soil types, two rooting depths and five climates. To maintain the simulations more realistic deep roots were not assigned to subtropical climates and shallow roots were not allocated to arid climate.

		Temp. Arid	Semi-Mediter.	Temp. Continental	Temperate	Subtropical
Shallow Roots	Loamy Sand		✓	✓	✓	✓
	Silt Loam		✓	✓	✓	✓
	Silty Clay		✓	✓	✓	✓
Deep Roots	Loamy Sand	✓	✓	✓	✓	
	Silty Loam		✓	✓	✓	
	Silty Clay		✓	✓	✓	

Table 3. Reference values of the Mualem [1976] - van Genuchten [1980] hydraulic parameters.

Texture	Acronym	θ_s	θ_r	L	h_{ae}	n	K_s	Sources
		[m ³ m ⁻³]	[m ³ m ⁻³]	-	[cm]	-	[cm d ⁻¹]	
Loamy Sand	LS	0.41	0.057	0.5	8	2.28	350.2	[Carsel and Parrish, 1988]
Silty Loam	SiL	0.43	0.061	0.5	83	1.39	30.5	[Ines and Mohanty, 2008b]
Silty Clay	SiC	0.36	0.07	0.5	200	1.09	0.48	[Carsel and Parrish, 1988]

Table 4. Contrasting scenarios of the percentage of roots in the top 30 cm, ΔRDF_{30} [Jackson et al., 1996], and maximum rooting depths, Z_{root} [Schenk and Jackson, 2002].

Description	Acronym	Z_{root}	ΔRDF_{30}	Vegetation type
		[cm]	[%]	
Shallow roots	SR	40	80	Meadows
Deep roots	DR	130	50	Semi-desert

1176 **Table 5.** Values of vegetation parameters that remains constant. Where $h_1, h_2, h_{3h}, h_{3l}, h_4$ are the capillary pressure
 1177 head that regulate the water uptake model, LAI is the Leaf Area Index, β is the crop factor and K_g is the
 1178 extinction coefficient of solar radiation [-]. Refer to Appendix A for further information.

h_1 [cm]	h_2 [cm]	h_{3h} [cm]	h_{3l} [cm]	h_4 [cm]	LAI [m ³ m ⁻³]	K_g [-]	β [-]
-1	-22	-1000	-2200	-16000	2	0.5	0.9
		[Singh et al., 2006] wheat			[Brutsaert, 2005] scrubland	[Varado et al., 2006] universal	[J. A. P. Pollacco, 2005] grassland

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1180

1181 **Table 6.** Sources of reference hydroclimate data compiled from AmeriFlux (<http://public.ornl.gov/ameriflux/>).

CLIMATE	ACRONYM	SITE	STATE	LAT.	LONG.	IGBP CLASSIF.
Temperate semi-arid	Tsa	Kendall Grassland	AZ	32	-110	Grasslands
Mediterranean	M	Tonzi Ranch	CA	38	-121	Woody Savannas
Temp. Continental	Tc	Walnut river	OK	37	-97	Cropland
Temperate	T	Mead Rainfed	NE	41	-96	Croplands
Subtropical	S	Kennedy Space Center Scrub Oak	FL	29	-81	Closed Shrublands

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1183 **Table 7.** Detailing the different scenarios used in Fig. 6.

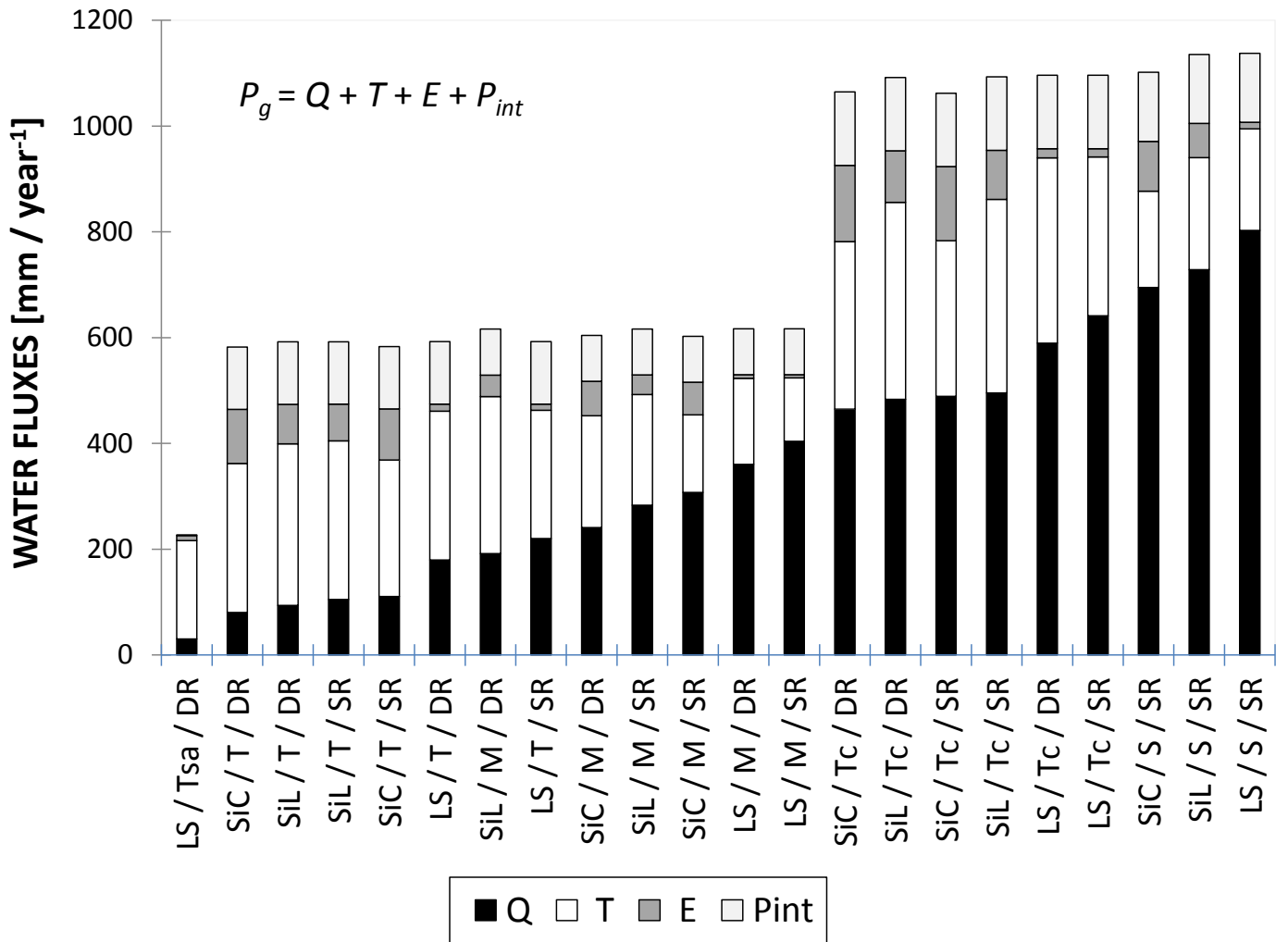
TEXTURE	SPECIFICATION	OF _{lin}	Fig. 6
Loamy sand	Decoupling equation	21%	A1
	No decoupling	17%	A2
Sandy clay	Shallow roots	13%	B1
	Deep roots	10%	B2
Silty clay	Calibrated with OF _{et}	13.9%	C1
	Calibrated with WOF	14.5%	C2

1184

1185 **Table 8.** Empirical relationship for the 3 texture classes which relates w with average $\overline{ET_f}$ (ET/ET_p) and w with
 1186 average $\bar{\theta}$.

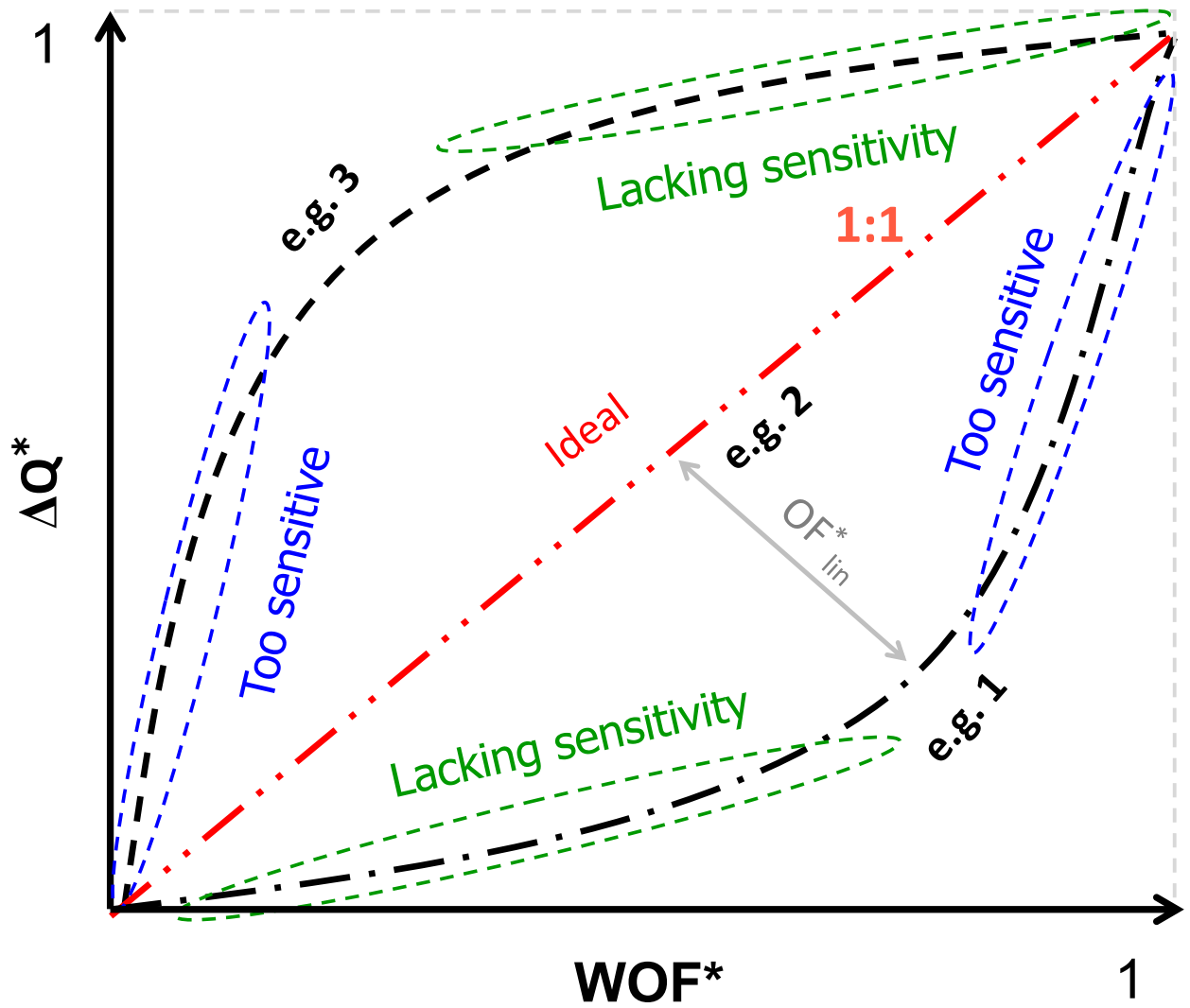
TEXTURE	$w =$	
	Fig. 10a	Fig. 10b
Loamy sand	$-0.91 \overline{ET_f} + 1.31$	$-13.06 \bar{\theta} + 1.04$
Sandy clay	$-0.59 \overline{ET_f} + 1.20$	$-3.10 \bar{\theta} + 1.5$
Silty clay	$1.15 \overline{ET_f} - 0.28$	$9.63 \bar{\theta} - 2.52$

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Fig. 2. The 22 hydroclimatic scenarios depicted by average yearly groundwater recharge Q , transpiration T , evaporation E , interception P_{int} computed from $SWAP_{inv}$. For visualization, the gross precipitation $P_g = Q + T + E + P_{int}$ with the long-term storage computed to 0. The acronyms are provided in Table 3 for the soil texture, in Table 4 for the roots and in Table 6 for the climate.



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Fig. 3. Examples of relationships between a normalized weighted objective function (WOF^*) with the normalized uncertainty of the water flux (ΔWF^*) error, represented by ΔQ^* . The ideal is a linear correlation between WOF^* and ΔQ^* .

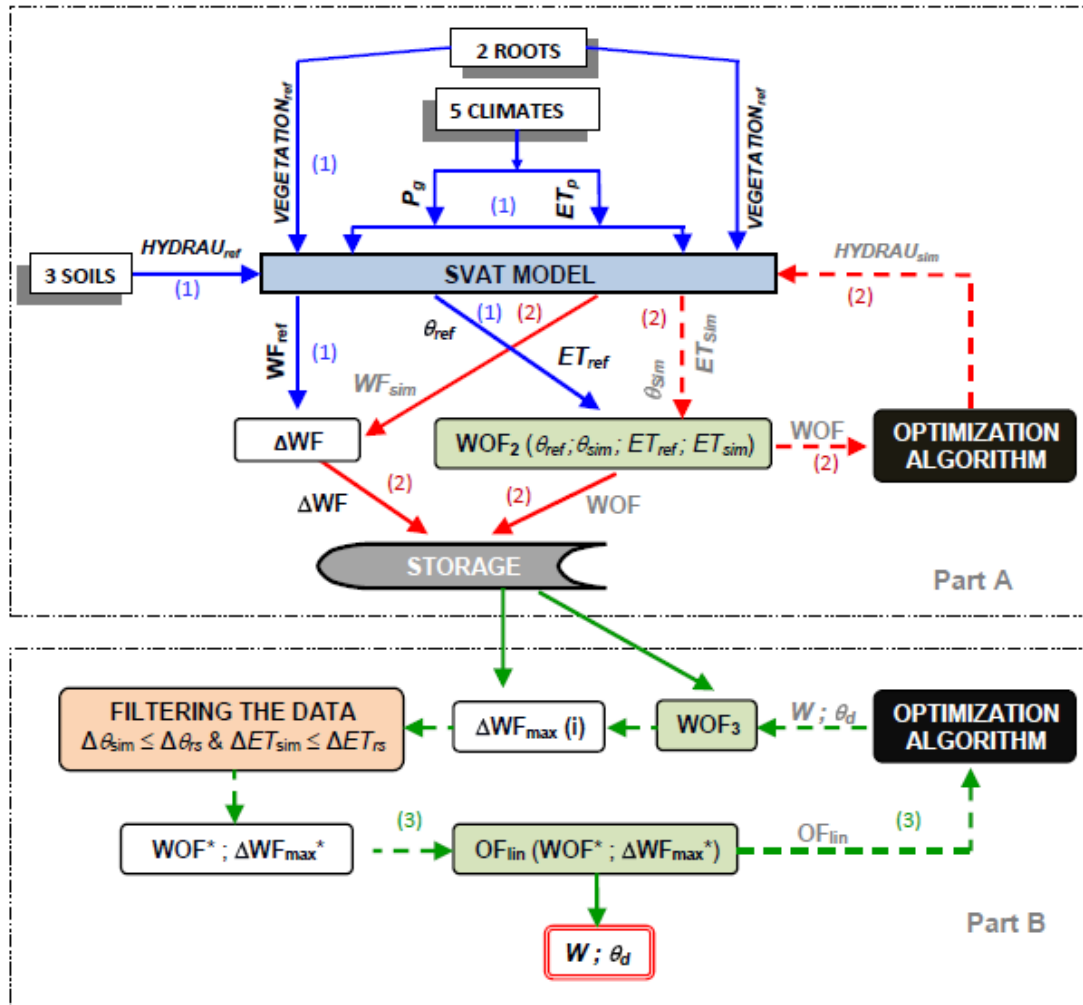


Fig. 4. Flowchart of the *Weighted Objective Function Selector Algorithm* (WOFSA) where **HYDRAU_{ref}** and **VEGETATION_{ref}** are a known set of reference parameter values; **WF_{ref}** are the modeled reference water fluxes outputs which are computed from the SVAT hydrological model requiring a priori known sets of hydraulic parameters (**HYDRAU_{ref}**) and gross precipitation (**P_g**) and potential evapotranspiration (**ET_p**) as forcing data; **HYDRAU_{sim}** are trial set of parameter values that are obtained from the **OPTIMIZATION ALGORITHM**; **WF_{sim}** are simulated fluxes and **ΔWF** is their residuals, derived by a posteriori estimated hydraulic parameters (**HYDRAU_{sim}**) by minimizing the weight **w** (between the fitting criteria based on soil moisture **θ** and evapotranspiration **ET**) and the decoupling threshold **θ_d** of **WOF**. All the trials are stored in the **STORAGE** which are filtered such that the uncertainties in **θ_{sim}** and **ET_{sim}** are not greater than the uncertainties of retrieving **θ** and **ET** from remote sensing (**Δθ_{rs}** and **ΔET_{rs}**). WOFSA is performed in two separate parts: **Part A** generates uncertainties in the fluxes **ΔWF** as if they were available from independent measurements, while **Part B** optimizes **w** and **θ_d** by minimizing the **OF_{lin}** such that to ensure the maximum linearity between the normalized **WOF*** and the normalized maximum uncertainty **ΔWF_{max}***. The different loops are colored coded with blue for loop 1, red for loop 2 and green for loop 3.

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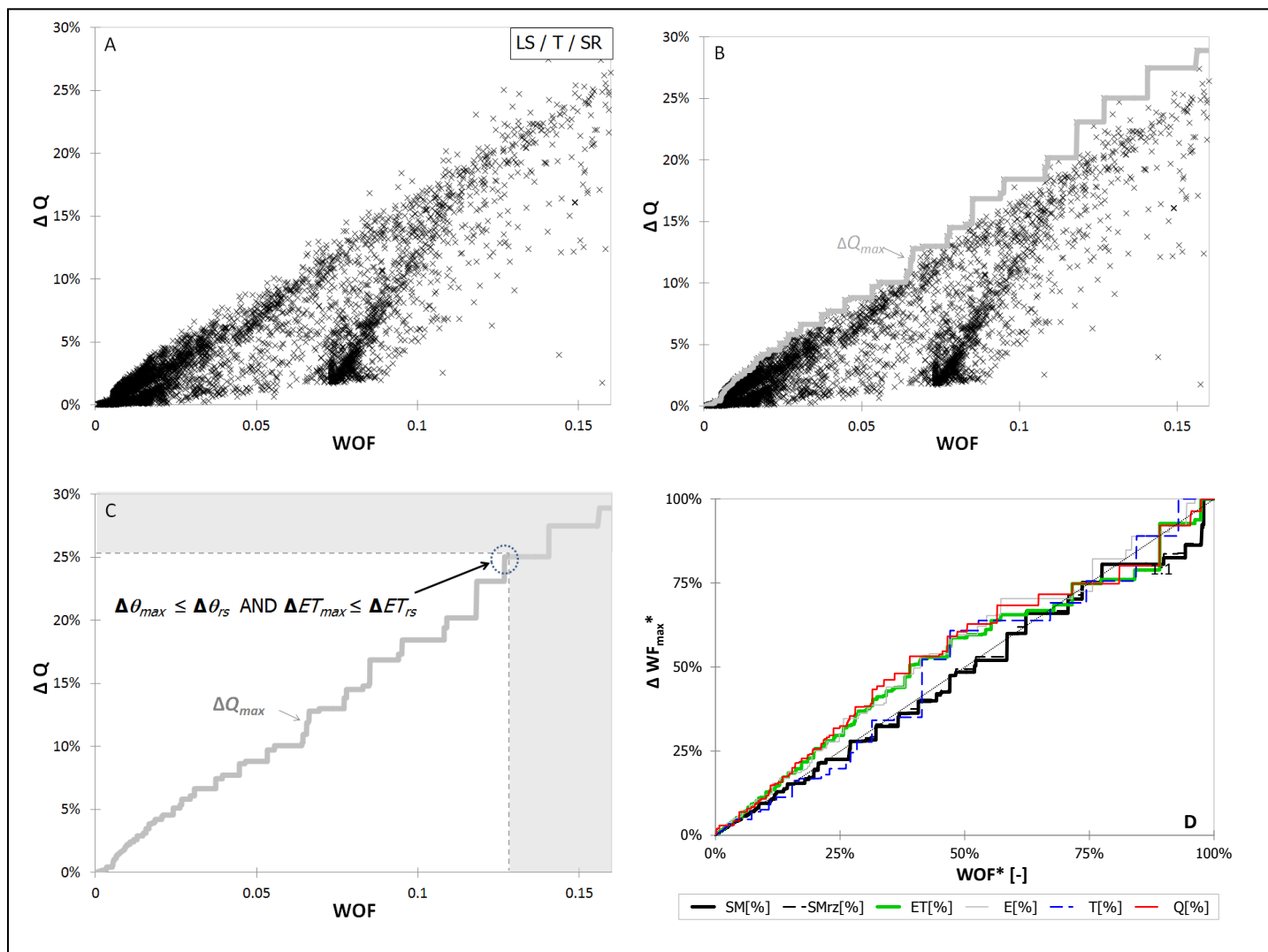
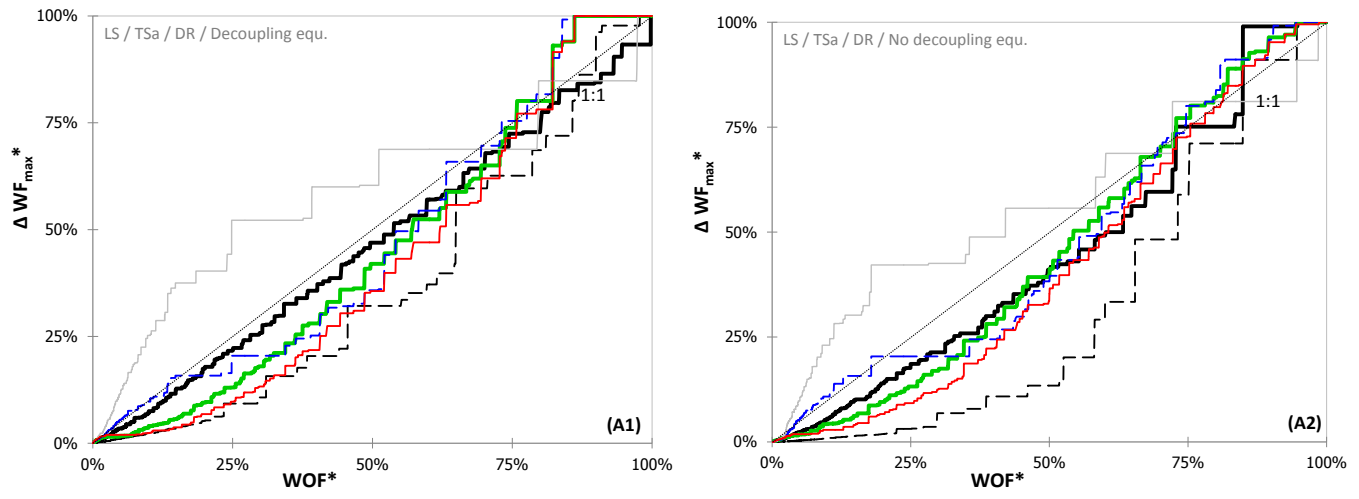
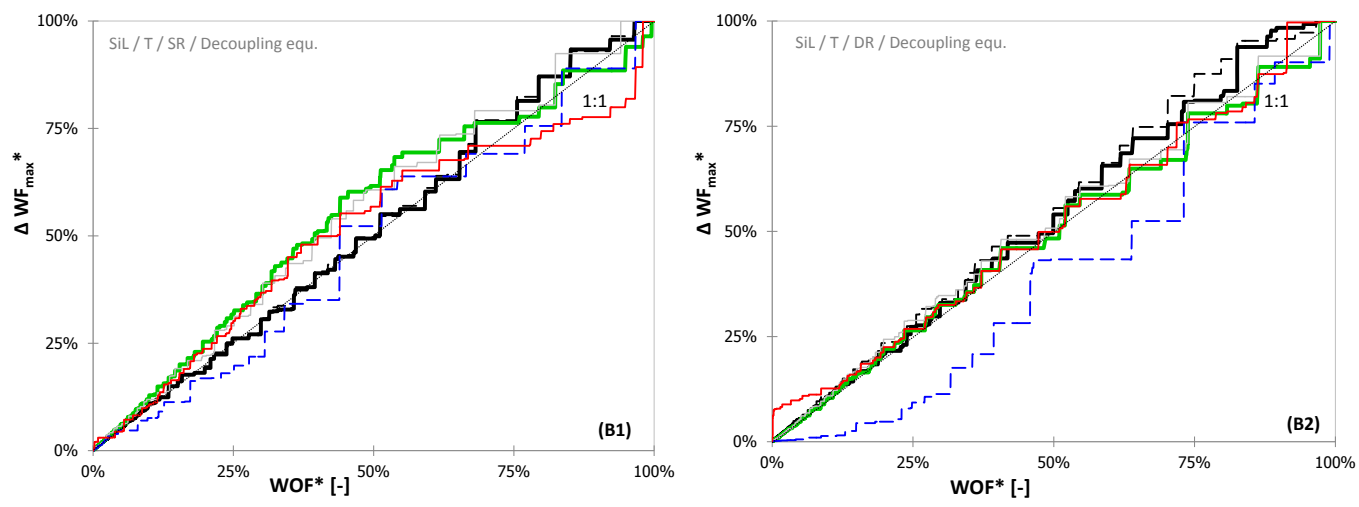


Fig. 5. Different steps of the WOFSA given as an example for loamy sand, temperate climate and short rooting depth. (A) An ensemble of generated parameter sets $HYDRAU_{sim}$ with the relationship between WOF and the residuals between reference and simulated WF_{sim} given as an example for groundwater recharge ΔQ ; (B) From each generated WOF_i , described in (A) the maximum corresponding error ΔQ_{max} is selected; (C) Selection of feasible parameter sets ΔQ_{max} to reproduce the uncertainties in retrieving θ_{ref} and ET_{ref} from remote sensing; (D) Correlation between normalized WOF^* and normalized WF_{max}^* for top soil moisture SM (θ), root-zone soil moisture SM_{rz} (θ_{rz}) evapotranspiration ET, evaporation E , transpiration T , and groundwater recharge Q .

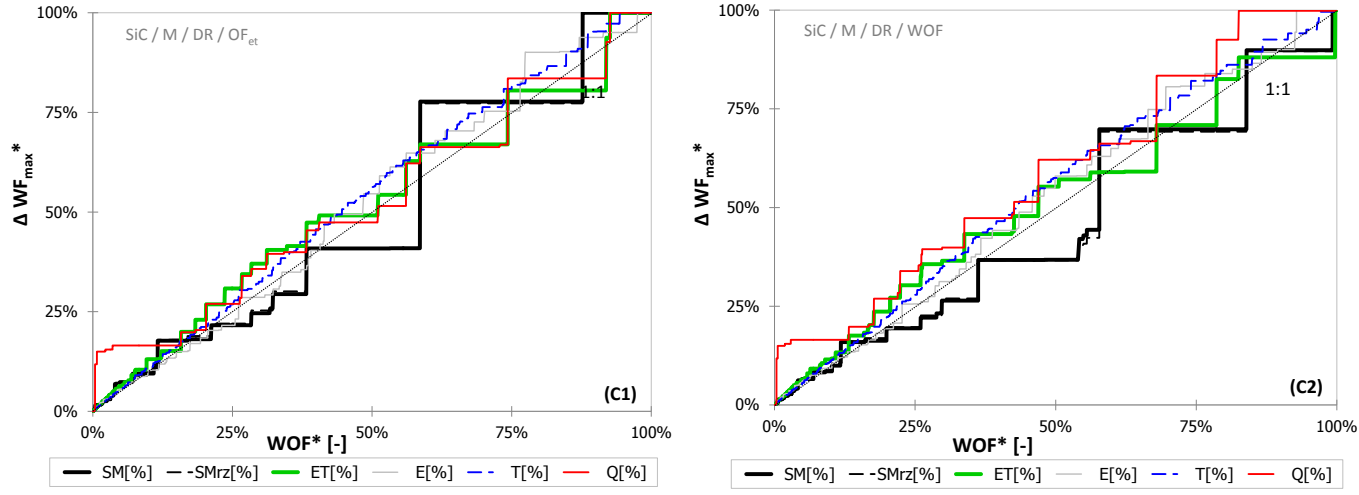
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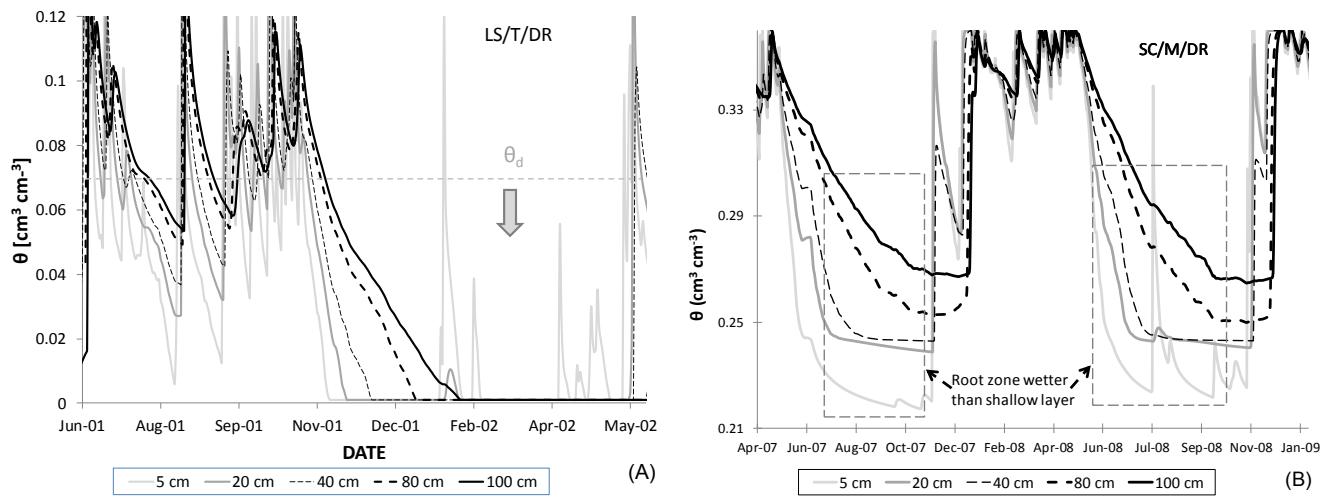
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Fig. 6. Relationships between normalized optimized WOF* and normalized ΔWF_{max}^* , for the scenarios described in Table 7.

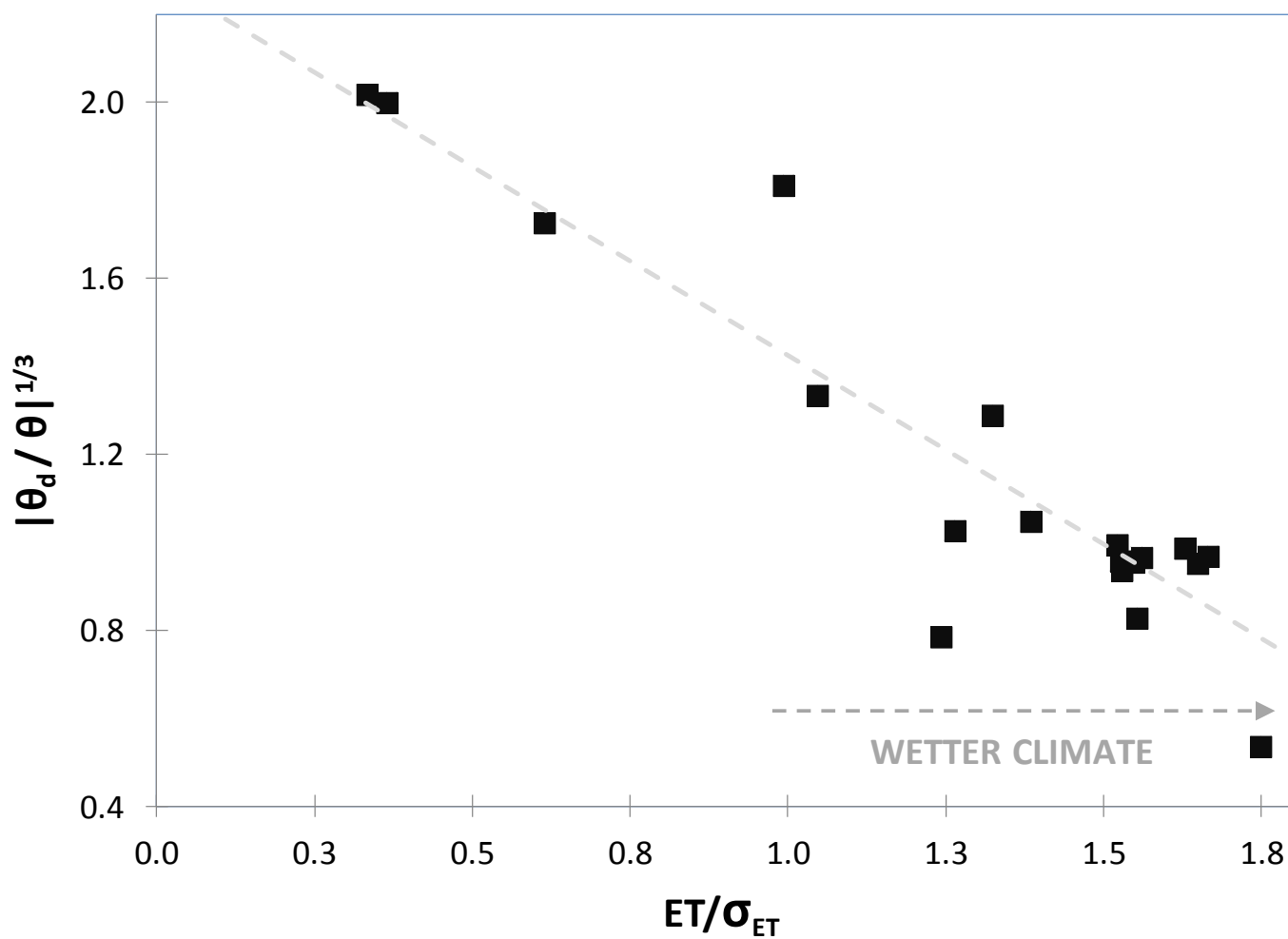
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Fig. 7. Reference time series θ plotted at different depths: **(A)** for coarse soils, showing that the top layer is decoupled from the deeper layer when θ is drying and $\theta < \theta_d$, and **(B)** for fine texture soils under dry climate, showing that the top layer gets gradually decoupled from the deeper layer.

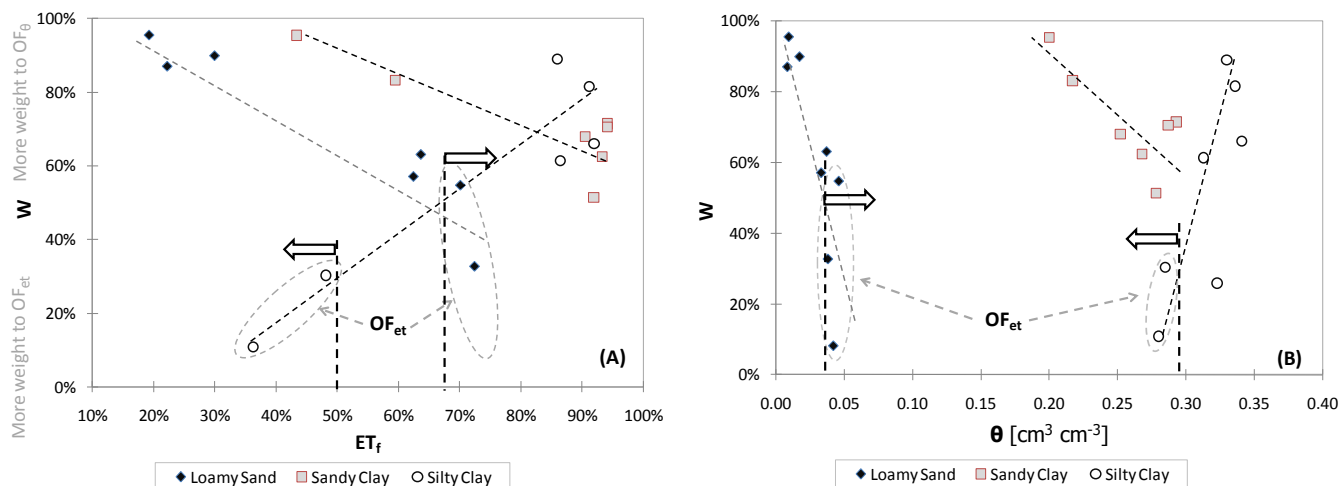
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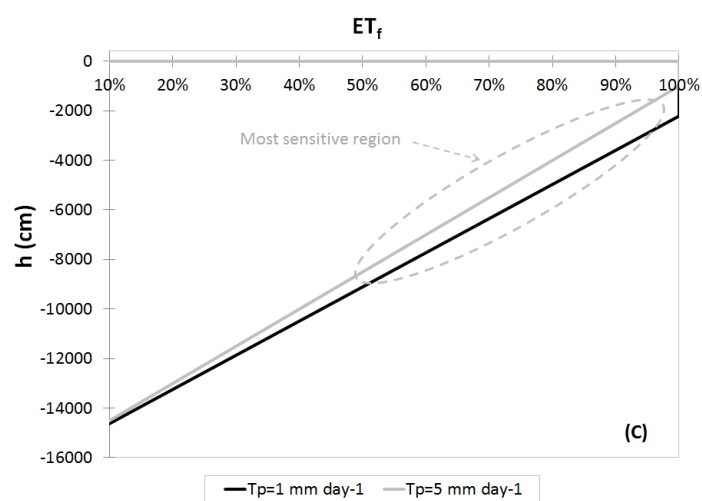
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Fig. 8. For all hydroclimatic conditions a relationship is obtained between average ET divided by the standard deviation of ET (σ_{ET}) with $(\theta_d / \theta)^{0.3}$. The scenarios are wetter as ET / σ_{ET} increases.

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Fig. 9. For the three soil texture class subdivided climatically: **(A)** relationship of w with average evaporative fraction ET_f , and **(B)** correlation of optimal w with measured average θ . The empirical linear equations of each texture classes are described in Table 8. The enclosed hydroclimates are those for which a single OF_{et} can be used instead of a WOF. These hydroclimates are depicted by arrows which represent threshold values of θ and ET_f . The **(C)** schematizes the Feddes et al., [1978] plant water stress response function (ET_f) as a function of soil water pressure. The position of the parameter h_3 depends on the intensity of the potential transpiration ($T_p < 1 mm d^{-1}$ or $T_p \geq 5 mm d^{-1}$). The interpolation of h_3 is between the interval h_{3low} , h_{3high} for which their values are provided in Table 5.