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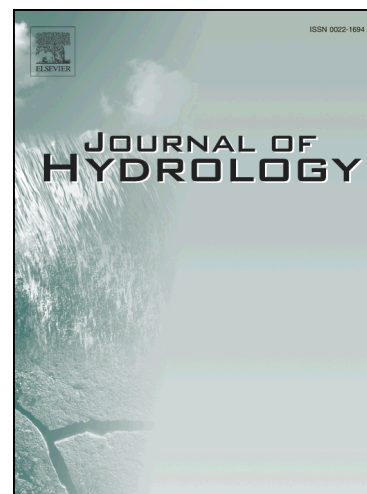
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Estimation of available water capacity components of two-layered soils using crop model inversion: Effect of crop type and water regime

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Abstract

Characterization of the soil water reservoir is critical for understanding the interactions between crops and their environment and the impacts of land use and environmental changes on the hydrology of agricultural catchments especially in tropical context. Recent studies have shown that inversion of crop models is a powerful tool for retrieving information on root zone properties. Increasing availability of remotely sensed soil and vegetation observations makes it well suited for large scale applications. The potential of this methodology has however never been properly evaluated on extensive experimental datasets and previous studies

suggested that the quality of estimation of soil hydraulic properties may vary depending on agro-environmental situations. The objective of this study was to evaluate this approach on an extensive field experiment. The dataset covered four crops (sunflower, sorghum, turmeric, maize) grown on different soils and several years in South India. The components of AWC (available water capacity) namely soil water content at field capacity and wilting point, and soil depth of two-layered soils were estimated by inversion of the crop model STICS with the GLUE (generalized likelihood uncertainty estimation) approach using observations of surface soil moisture (SSM; typically from 0 to 10 cm deep) and leaf area index (LAI), which are attainable from radar remote sensing in tropical regions with frequent cloudy conditions. The results showed that the quality of parameter estimation largely depends on the hydric regime and its interaction with crop type. A mean relative absolute error of 5% for field capacity of surface layer, 10% for field capacity of root zone, 15% for wilting point of surface layer and root zone, and 20% for soil depth can be obtained in favorable conditions. A few observations of SSM (during wet and dry soil moisture periods) and LAI (within water stress periods) were sufficient to significantly improve the estimation of AWC components. These results show the potential of crop model inversion for estimating the AWC components of two-layered soils and may guide the sampling of representative years and fields to use this technique for mapping soil properties that are relevant for distributed hydrological modelling.

Keywords: Soil Hydraulic Properties ; Available Water Capacity ; STICS ; soil water content ; GLUE ; Inverse modelling

1.0 Introduction

The capacity of the soil to store water available for plants, generally referred as available water capacity (AWC) is a key parameter for modelling the catchment-scale water balance. In particular, in tropical semi-arid contexts, where potential evapotranspiration equals or exceeds

rainfall, recharge to groundwater is difficult to estimate from vadose-zone water balance (De Vries et Simmers, 2002) and it is particularly sensitive to the size of the soil water storage (Anuraga et al., 2006 ; Sreelash et al. 2013). Therefore, accurate estimates of AWC and its spatial variability at the catchment scale are needed to improve the sustainable management of groundwater resources. The increasing availability of high frequency and high resolution remote-sensing data now allows retrieving precise soil hydraulic properties maps of the top few centimeters of the soil (Montzka et al., 2011) but estimating AWC of the entire root zone at the catchment scale remains a challenge.

AWC depends on soil hydraulic properties (SHPs), soil depth and plant rooting characteristics. It may be defined from different point of view - pedologists, soil scientists, ecophysicologists - with different approaches and different levels of complexity, considering one or several layers corresponding to pedological horizons. A common definition of the AWC is the difference between the soil water content at field capacity and wilting point (Bruand et al., 2003). Those parameters can be determined in the field, which minimize soil disturbance or in the laboratory which requires soil sampling and sample preparation that could distort the soil sample and increase the margins of errors. All methods are highly time-consuming and expensive (Steele-Dunne et al., 2010; Botula et al., 2012). Therefore, it is impractical to use them to obtain soil properties for catchments larger than a few hectares. For larger areas SHPs are generally estimated from soil characteristics that are easily available from soil maps (mainly textural properties) using pedotransfer functions (PTFs). However, PTFs are often site-specific and may lead to crude estimates of SHPs with large uncertainties when extrapolated over large areas (Vereecken et al., 1989, 1990, Wösten, 2001, Stump et al., 2009) or beyond the specific context (geomorphic regions or soil type) under which they are developed (McBartney et al., 2002). A more recent technique is Digital Soil Mapping (DSM) that couple field and laboratory observational methods with spatial and non-spatial soil

inference systems (Lagacherie and McBratney, 2007). DSM makes an extensive use of technological and computational advances such as remote sensing and geostatistics for producing digital maps of soil types and soil properties (Lagacherie et al., 2008; Vaysse and Lagacherie, 2015). However, approaches based on DSM estimates basic soil properties such as soil texture, bulk density, pH etc. and still rely on PTFs to translate them into more functional properties (McBratney et al., 2003). They are thus also limited by the quality of the PTFs and their adequacy to the studied situation.

As AWC components are important parameters for hydrological models, model inversion is another alternative for retrieving them. The principle is to use *in situ* or remotely sensed observations corresponding to model outputs strongly linked with AWC components to estimate them using parameter estimation or data assimilation methods. Such approach has been carried out in several studies for estimating SHPs and soils depth using various types of models: hydrological models (Ritter et al., 2003; Ines and Mohanty, 2008; Charoenhirunyingyos et al., 2011), crop models (Guérif et al., 2006, Varella et al., 2010a, 2010b; Sreelash et al., 2012), Land Surface Models (Bandara et al., 2013, 2014 and 2015) or SVAT (soil vegetation atmosphere transfer) models (Jhorar et al, 2002, 2004). Several studies have shown that SHPs of vertically homogeneous soils can be estimated through model inversion using surface soil moisture (see for example Montzka et al., 2011; Nagarajan et al., 2011). For multi-layered soils, profile soil moisture observations allow assessing SHPs (Ritter et al., 2003; Braga and Jones, 2004; Wohling et al., 2010; Li et al., 2011) but this requires large experimental settings which limits its spatial application. On the other hand, using only surface soil moisture measurements that can be spatially available from remote sensing, is not sufficient to provide unique and physically reasonable estimates of hydraulic properties for multi-layered soils through model inversion (Vereecken et al., 2008; Ines and Mohanty 2008; Charoenhirunyingyos et al., 2011) because of the poor connection in the hydraulic processes

between layers (Montzka et al., 2011), except in some particular situations (Shin et al., 2012; Bandara et al., 2013). Shin et al. (2012) also reported that the weakness of hydrological models in simulating plant root activities in the root zone results in relatively larger errors in the estimation of SHPs in crop land as compared to bare soil. As crop lands represent a large contribution to hydrologic processes within agricultural catchments, precise knowledge of AWC components is critical for managing water resources to maintain agricultural production. The known projections of climate change make this objective even more essential.

Recently, crop model inversion has been proposed by several authors to retrieve AWC components (Guérif et al., 2006; Varella et al., 2010a, 2010b; Sreelash et al., 2012). The main interest of using of crop models for retrieving AWC components in crop lands is that they are more efficient than hydrological models, Land Surface Models or SVAT models in describing the specificity of crop behavior with regards to water processes (effect of crop type on rooting system characteristics and water needs, effect of crop management practices on the water balance). This is partly because they account AWC components impacts not only on the soil water balance, but also on the coupled carbon and nitrogen cycling (Rugé et al., 2002; Satti et al., 2004; Breda et al., 2006). The increasing availability of high frequency and high resolution vegetation and soil moisture data from remote sensing makes crop model inversion approach a potentially powerful tool for spatial applications, especially for parameterizing catchment-scale hydrological models.

However, accuracy of the parameter estimates strongly depends on environmental conditions such as climate and crop type (Varella et al., 2010b). Charoenhirunyingyos et al. (2011) and Sreelash et al. (2012) show that combining surface soil moisture and vegetation measurements in model inversion, by bringing information on both surface and root zone SHPs, improves

substantially parameter estimation. However, these conclusions are based on synthetic experiments or very limited field datasets. In fact, few studies based on field data have been carried out to evaluate the potential of model inversion methods for estimating AWC components on multi-layered soils with observations potentially accessible from remote sensing and this problem is still considered as challenging (Mohanty 2013).

In this paper, we used an extensive field dataset from a tropical agricultural catchment in South India involving four types of crops across 3 years. The objectives are:

- (i) to analyze the potential of model inversion methods for estimating AWC components (water content at field capacity and wilting point, soil depth) on two-layered soils with observations potentially accessible from remote sensing on a large set of field situations; and
- (ii) to investigate the influence of the crop type and water regimes experienced by the crops on the accuracy of these estimations.

2.0 Materials and Methods

2.1 Site information

The experimental catchment of Berambadi (84 km²) is located in the Kabini river basin in South India (AMBHAS Site, www.ambhas.com, long term environmental observatory BVET <http://bvet.obs-mip.fr>; Braun et al., 2009; Ruiz et al., 2010; Violette et al., 2010). It is intensively used for agro-hydrological, remote sensing and hydrological investigations (Kumar et al., 2009). The land is used for agriculture and the crops are mostly rainfed or irrigated with groundwater. We used a total of 60 crop/soil/climate situations covering 4 crops across 3 years from May 2011 to Dec 2013 and 42 agricultural plots each approximately 1 ha in size, monitored for soil moisture and crop growth. Among them, 15 crop/soil/climate situations from 12 plots were used for the calibration of STICS plant parameters (see section

2.4). The inversions were performed on 45 crop/soil/climate situations from 33 plots. The results presented in the following will only concern the situations/plots used for the inversions.

The 4 crops studied have distinct characteristics (Table 1). Turmeric is an irrigated 8 months crop (May to December) while the 3 others are rainfed crops grown over 4 months (May to August for sunflower and sorghum and September to December for maize).

< Table 1 here please >

The climate is tropical semi-arid, dominated by south-west monsoon with a mean annual rainfall of 800 mm (coefficient of variation 0.28), and an annual Potential Evapotranspiration (PET Penman Method, Penman, 1948) of 1100 mm (coefficient of variation 0.05), computed over 2005-2015. Daily records of air humidity, wind velocity, maximum and minimum air temperatures, precipitation and global radiation were obtained from an automatic weather station (CIMEL, type ENERCO 407 AVKP) and a meteorological flux tower (Astra Microwave, India) located in the study area. Measurements from the closest station were considered for each plot.

< Table 2 here please >

For the study period, the amount and distribution of rainfall and (Rain+ Irrigation)/PET ratio varied across years and cropping seasons (Table 2). This led to a varying degree of crop water stress experienced by the crops. 2012 was relatively dry as compared to 2011 and 2013 which can be classified as “normal years”.

2.2 Crops: management and LAI measurements

Information on management activities such as date and dose of sowing, fertilizing, irrigation and date of harvest were obtained during field visits. Sowing dates (expressed as day of the year) vary between 130 to 150 for Sunflower and Sorghum, between 110 and 124 for turmeric and between 250 and 262 for maize. Fertilizer is applied once at the beginning of the season, the quantity varying between 20 to 30 kg.N/ha for sunflower, 30 to 50 kg.N/ha for sorghum, 100 to 200 kg.N/ha for turmeric and 25 to 50 kg.N/ha for maize.

LAI was measured using a Portable Leaf Area meter CI – 202 (CID Bioscience) and a LAI-2000 Plant Canopy Analyzer (LI-COR) every 10 days in 2011 and 2012, and every 20 days in 2013 concurrently with soil moisture measurements (see next section). Three measurements of LAI were taken in one representative sample area of 2 m² and the mean value was used as representative of the plot.

< Figure 1 here please >

Time series of LAI (Fig. 1) obtained by interpolation of the measurements using a parametric growth curve approach (Baret, 1986) revealed a large variability resulting mainly from interactions between crop, climate and soil type. It provides the basis for the determination of root zone soil water content properties from crop model inversion.

2.3 Soils: pedology, soil moisture measurements, reference AWC parameters values

Soils in the studied area are roughly classified as red soils (Alfisols, FAO) or black soils (Vertisols, FAO). According to the 1:50,000 scale soil map of the area prepared by Karnataka State Remote Sensing Application Center (KSRSAC), six categories are considered based on the particle size distribution of the top layer: Clay and Clay Loam for vertisols, Gravelly Loam Sand, Loamy Sand, Sandy Clay Loam and Sandy Loam for Alfisols. Sandy Clay Loam

is the major soil class, covering 50 % of the area. The soil is gravelly sandy loam at the hill slopes, sandy loam and sandy clay loam in the plains and clay loam and clay soil in the valley.

Surface soil moisture (SSM; typically from 0 to 10 cm deep) used for model inversion was measured using Theta Probe Soil moisture sensor – ML2x (Delta-T devices, sampling volume: 2.5 cm diameter, 6 cm long) and the mean of 3 measurements used as representative of each field plot. Additionally three soil samples per plot were collected for gravimetric soil moisture measurements. Theta Probe devices were calibrated twice a year using the gravimetric measurements: once during period of low soil moisture (before the start of the cropping season) and other during period of high soil moisture (during or at the end of the first cropping season). Profiles of soil moisture - used to determine in situ soil hydraulic properties – were also measured using soil moisture sensors (Trime-FM TDR, IMKO Micromodultechnik GmbH, sampling volume: 15 cm diameter, 18 cm long). The measurements were made at an increment of 10 cm from surface up to 1 m depth for shallow soils and up to a depth of 2 m for deeper soils. Both surface and profile soil moisture were measured throughout the year at a frequency of 10 days in 2011 to 2012 and 20 days in 2013. To capture the extreme values of soil moisture in both dry and wet conditions, surface and profile soil moisture were measured daily for a 30 day period once in October 2011 and once in August 2013.

< Table 3 here please >

To compare the estimated values of soil properties retrieved from model inversion to ‘observed values’, water content at field capacity (θ_{FC}), wilting point (θ_{WP}) and soil depth (D_L) were determined from in situ measurements on the monitored plots (Table 3). As proposed by Hunt et al. (2009) and Martinez-Fernandez et al. (2015), θ_{FC} and θ_{WP} were inferred from long term soil moisture data: θ_{FC} as the ‘minimum of maximum value’ of the layer soil

moisture in the growing season, while discarding soil moisture data immediately after a rainfall event (or irrigation event), and θ_{WP} as the '5th percentile of the minimum values' of soil moisture in the growing season. Our time series of soil moisture exhibited alternate wetting and drying cycles, thus capturing both maximum and minimum soil water content. Bulk density was determined as the ratio of volumetric soil moisture (from TDR measurements) to gravimetric soil moisture (measured on soil samples). The depth of soil layers was determined by soil augering. The depth of soil from surface to weathering zone varied from 70 cm to 150 cm and was independent of the soil type.

2.4 Model and Parameters

The STICS crop model (Brisson et al., 1998; Coucheney et al., 2015) is a daily time-step model which simulates the functioning of a soil-crop system over a single or several successive crop cycles. It has been successfully used for spatial applications and coupled with hydrological models at the catchment scale (Beaujouan et al., 2001). The upper boundary conditions are governed by standard climatic variables (radiation, maximum and minimum air temperatures, rainfall, potential evapotranspiration) and the lower boundary condition is the soil/sub-soil interface. We used the Penman method to calculate potential evapotranspiration (PET; Penman, 1948). Crops are described by their LAI, above-ground biomass and nitrogen content and the number and biomass of harvested organs. The main processes described are carbon assimilation and allocation to different organs and water and nitrogen balances (for detailed description, see Brisson et al, 1998, 2008).

The different components of actual evapotranspiration (ET) are calculated from the potential evapotranspiration: soil evaporation (E_s), plant transpiration (T_p) and evaporation from the water intercepted by the foliage that contributes to reducing the evaporative demand at the plant level. For E_s , two stages are considered following rainfall: a first stage where the soil

evaporates at the potential rate, and a second stage where evaporation is lower and decreases according to climate and type of soil. Crop water requirements (or maximum transpiration) are determined according to a crop coefficient approach which is well adapted to the crops considered herein (Brisson, 1998, 2008). The actual plant transpiration T_p is based on the water physically available in the soil and the capacity of the plant to extract it, due to its root characteristics, corresponding to the concept of AWC (amount of water between field capacity θ_{FC} and wilting point θ_{WP}). The ratio of actual transpiration to maximal transpiration, is a bilinear function of the amount of water available in the rooting zone (with a minimum value of 0 when the soil water content is equal to θ_{WP} and a maximum value equal to $(\theta_{FC} - \theta_{WP})$). The soil water content regarded as being the threshold between the maximal transpiration stage and the reduced transpiration stage depends on root density, stomatal functioning of the plant and climatic demand. Water stress indices are derived from those calculations and affect different components of plant growth.

The soil is considered as a reservoir and is defined as a succession of up to five homogeneous layers characterized each by its retention capacity characteristics (θ_{FC} and θ_{WP} , bulk density and thickness). Water transfer downwards in the soil microporosity is simulated on a one-dimensional regular mesh discretized per 1cm step with a functional reservoir type model according to the tipping bucket concept. Incoming water fills the layers by downward flow, assuming that the upper limit of each single reservoir corresponds to the layer's field capacity.

The STICS model contains about 200 input parameters which are related to the characteristics of the plant, soil and crop management activities. The plant parameters for sunflower, sorghum, turmeric and maize related to leaf growth, biomass, yield, and root growth were calibrated with the OptimiSTICS software (Buis et al., 2011), using all the available data on a restricted number of plots that were therefore not used for inversions. With the calibrated

model, the crop specific parameters can be assumed constant for the given crop for the study area. The parameters related to the agricultural practices (sowing dates, fertilization dates and doses, irrigation dates and doses and harvest dates) were set in accordance with the information collected from farmers.

< Table 4 here please >

In order to reduce the number of soil parameters to be potentially estimated, we adopted the simplified representation of the soil proposed by Varella et al. (2010a): a surface layer and a second layer mainly representing the root zone. The first layer depth was set at 10 cm which is compatible both with our field measurements of SSM and the order of magnitude of SSM retrievals from radar remote sensing (Jackson et al., 1995, Baghdadi et al, 2006) for further applications at larger scale. Here we considered only the permanent soil properties related to water storage and transfers in the soil and restricted the estimation to five parameters: soil moisture at field capacity (θ_{FC}) and wilting point (θ_{WP}) of both layers and thickness of the second layer (D_{L2}) (Table 4). These parameters describe the maximum AWC (expressed in mm) of each layer which determines maximum water storage and available water for plant uptake as follow:

$$AWC = (\theta_{FC} - \theta_{WP}) \cdot BD \cdot D_L \cdot 10^{-1} \quad (1)$$

where BD is the bulk density (g/cm^3) and D_L is the thickness (cm) of the layer.

These parameters influence also other processes such as soil evaporation, carbon and nitrogen cycle in the soil (Brisson et al, 2008). They are involved separately in some of these processes which bring independent constraints for their estimation. The soil input parameters non-estimated in the inversion process were obtained from local soil maps, soil experiments and standard values for soil classes (details are provided in Appendix-A).

2.5 Inversion method

Generalized Likelihood Uncertainty Estimation (GLUE) approach is an informal Bayesian method using prior information of parameter values for estimating model parameters (Beven and Binley, 1992; Makowski et al., 2002). Based on Monte Carlo simulation, GLUE transforms the problem of searching an optimal parameter set into searching sets of parameter values which would produce reliable simulations of the variables of interest (Aronica et al., 2002). GLUE based approaches have been successfully applied to hydrological models (e.g. Li et al., 2010) and dynamic crop models (Makowski, 2004 ; Guérif et al., 2006 ; Varella et al., 2010a, 2010b ; Sreelash et al., 2012).

Sets of parameters values are randomly chosen in a prior distribution representing the potential parameter space. These sets are then used in model simulations, which produce multiple sets of values of output variables of interest. These outputs are compared with measured values with an appropriate likelihood measure. The parameters values corresponding to the highest likelihoods are called acceptable or “behavioural” values. The size of this ensemble is defined as a proportion of the total number of parameters values: the acceptable sample rate (ASR). The behavioural values are then used to determine the estimates of the parameters and their uncertainty bounds.

Prior information was defined here as independent uniform distributions with bounds as the minimum and maximum of the observed values measured on a wide set of 60 plots (larger than the 33 considered in this study) in different soil types of the Berambadi catchment (Table 4). These lower and upper bounds of the parameters were decreased/increased by 10 % to account for any errors in the measured soil moisture. The parameters sets were sampled in the prior distributions using Latin Hypercube Sampling (LHS; McKay et al., 1979). An initial sample of size 20000 was produced and then filtered to remove parameter combinations

which were considered as not reasonable. The sampled combinations in which $(\theta_{FC1} - \theta_{WP1}) \leq 7.0$ g/g and $(\theta_{FC2} - \theta_{WP2}) \leq 7.0$ g/g were removed since these situations were never observed in the field experimental data. The simulations were carried out for the 9500 remaining samples.

We used the sum of absolute errors (SAE), proposed by Brazier et al. (2000) as the likelihood metric. SAE was calculated for each variable considered in the inversion for each model run as,

$$SAE_i^k = \sum_{j=1}^{M_i} \left| \hat{y}_{i,j}^k - y_{i,j} \right|, i = 1 \text{ to } n \quad (2)$$

where, SAE_i^k is the sum of absolute errors for parameter set k , with $k = 1, \dots, N$ (N being the number of sets), variable i , with $i = 1$ to n (n being the total number of variables considered), and measurement date j , with $j = 1, \dots, M_i$ (M_i being the total measurements dates for the variable i), $\hat{y}_{i,j}^k$ is the simulated value of variable i at date j for the parameter set k and $y_{i,j}$ is the measured value of variable i at date j .

Observations used to estimate soil parameters were made of a combination of two STICS output variables: SSM and LAI. On average, 10 observations of LAI and SSM were used in case of turmeric plots and 7 observations in the case of sunflower, sorghum and maize plots (Table 1). The SAE values of SSM and LAI were normalized (RSAE) to take into account their varying units and magnitudes (Eq. 3). We used a combined likelihood function by assigning weights to RSAE of LAI and SSM so as to take into account in an appropriate way the relative influence of these variables (Eq. 4). Based on the results of the preliminary experiments carried out to study the influence of each variable on the parameter estimation (not reported here), we set w_1 to 0.4 and w_2 to 0.6.

$$RSAE_i^k = \frac{SAE_i^k}{\sum_{k=1}^N SAE_i^k} \quad (3)$$

$$CL^k = (w_1 * RSAE_{LAI}^k + w_2 * RSAE_{SSM}^k)^{-1} \quad (4)$$

where $w_1 + w_2 = 1$.

ASR was set to 4 % based on these preliminary experiments. The medians of the behavioural values were taken as the estimates of the parameters.

2.6 Statistical criteria for assessing inversion performance

Several criteria are used for assessing the performance of the inversion process:

- For each parameter and each inversion situation, a relative absolute error (RAE) was computed, based on the difference between estimated and observed values:

$$RAE_{i,p} = abs\left(\frac{(x_{i,p}^{obs} - \bar{x}_{i,p}^{post})}{x_{i,p}^{obs}}\right) \quad (5)$$

where $x_{i,p}^{obs}$ is the observed value of the soil parameter x_i for a given plot p and $\bar{x}_{i,p}^{post}$ is the corresponding value of the estimate obtained from the GLUE method.

A mean absolute error (MRAE) was computed as the mean of RAE of a given parameter x_i for the different plots.

$$MRAE_i = \frac{1}{p} \sum_{p=1}^p RAE_{i,p} \quad (6)$$

- A relative error (RE_i) was used to quantify the improvement brought by the inversion process with respect to prior information. RE_i was computed here as the ratio of the

MRAE calculated for the estimated parameter (\bar{x}_i^{post}) to that calculated for the prior information (\bar{x}_i^{prior}).

$$RE_i = \frac{MRAE(\bar{x}_i^{post})}{MRAE(\bar{x}_i^{prior})} \quad (7)$$

RE_i quantifies the improvement ($RE_i < 1$) or degradation ($RE_i \geq 1$) in the estimate of parameter x_i with respect to prior information (Varella et al. 2010a).

- As an alternative to RE, the information brought by the inversion process in the parameter estimate was also assessed, for each parameter and each inversion situation, by comparing the standard deviation of the prior and posterior parameter distributions, using a normalized standard deviation given in Eq. (8):

$$\sigma_{norm_{i,p}} = \frac{\sigma_{\bar{x}_{i,p}^{post}}}{\sigma_{\bar{x}_{i,p}^{prior}}} \quad (8)$$

$\sigma_{norm_{i,p}}$ quantifies the reduction ($\sigma_{norm_{i,p}} < 1$) or increase ($\sigma_{norm_{i,p}} > 1$) in the uncertainty associated to parameter estimation.

2.7 Sensitivity analysis

We performed a sensitivity analysis was performed to assess the information content of LAI and SSM observations for estimating SHPs (Varella et al, 2010a). Sobol' main sensitivity indices (Saltelli et al., 2008), which measure the part of variance of simulated outputs explained by the parameters independently from each other, were estimated using the EASI (effective algorithm for computing global sensitivity indices) method (Plischke, 2010). The main advantage of this method is that it does not require any specific numerical experiment design for the estimation of the indices. They have thus been computed at no extra cost using

all the simulations performed for the model inversions. Non-normalized Sobol' indices were used (i.e. Sobol' indices multiplied by the total variance of SSM / LAI) to visualize the variance explained by each parameter and not “just” the proportion of total variance they explain.

3.0 Results

3.1 Accuracy of estimated soil properties

The mean value of RAE on the 45 situations ranged between 0.13 and 0.21 depending on the estimated parameter (Fig. 2). Estimation of field capacity of both layers (θ_{FC1} and θ_{FC2}) showed relatively lower RAE (mean RAE < 0.15) as compared to the other parameters (0.19 for θ_{WP1} and D_{L2} , 0.21 for θ_{WP2}). The standard deviation of RAE varied between 0.1 and 0.24. θ_{FC1} and θ_{FC2} exhibited relatively lower error variability than the other parameters. However, the quality of estimation of all the parameters varied significantly depending on the situations and RAE inferior to 10% can be obtained for all parameters.

< Figure 2 here please >

The RE in the estimations was less than 1.0 for all parameters (Fig. 3), indicating that the inversion improved the accuracy of all the estimated parameters with respect to the mean of the joint prior distribution. The RE in the estimation was the lowest for θ_{FC1} (0.58) and similar for θ_{WP1} , θ_{FC2} and D_{L2} (mean value approximately 0.76). For all the parameters RE was less than 0.80, which is a substantial improvement in the estimation of the parameters with respect to their prior information.

< Figure 3 here please >

Normalized standard deviation (σ_{norm}) was largely inferior to 1 for θ_{FC1} and θ_{WC1} (Fig. 4), which means a significant reduction in the uncertainty of their estimated values as compared

to the uncertainty associated with the prior information. The reduction of uncertainty for the second layer parameters (θ_{FC2} , θ_{WP2} and D_{L2}) was not so significant. The relatively larger variability of σ_{norm} in the case of θ_{WP1} , θ_{FC2} and θ_{WP2} shows that under certain conditions the uncertainty in the estimates reduced significantly while in some cases the reduction in uncertainty is only marginal or nil. The level of uncertainty in D_{L2} is globally closer to that of prior information even if it can reach 70 to 80% of prior information uncertainty in some cases.

< Figure 4 here please >

3.2 Effect of crop type

The crop type used for inversion plays an important role in the quality of estimation of the parameters. This is evident from the consistently lower MRAE of the parameters, except for θ_{FC1} , obtained with maize crop as compared to those obtained with the other crops (Fig. 5).

< Figure 5 here please >

The MRAE in the estimation of all parameters except θ_{FC1} were nearly half for maize than that of the other crops, reaching values of about 10%. One of the main differences between maize and the other crops concerning the link between root zone hydraulic properties and crop growth is the water regime experienced by these crops. Due to both climatic conditions (sunflower and sorghum are grown in rainy season) and management options (irrigation is mainly devoted to turmeric as it is a cash crop), maize faces drier conditions than the other crops. Average (Rain+irrigation)/PET ratio was 0.87 for maize against 1.32 for sunflower and sorghum, and 1.3 for turmeric. STICS model simulations (Fig. 6) confirmed that maize experienced the maximum stress (both in intensity and duration) as compared to other crops. All maize plots experienced water stress, while for the other crops, the variability of water

stress index values is relatively higher, indicating that they experienced different levels of stress depending on year, soil type or farming practices.

< Figure 6 here please >

The quality of estimation of θ_{FC1} was on the contrary better with sunflower and sorghum as compared to turmeric and maize. Higher rainfall (and hence higher frequency of high moisture content conditions in the first layer) occurred during the cropping season of sunflower and sorghum which would have favored the estimation of θ_{FC1} since SSM observations can be seen as a proxy of θ_{FC1} in these conditions. For maize, soil moisture data used for inversion have not attained the actual values of field capacity for all situations (results not shown).

3.3 Effect of water regime

Figure 7 shows dynamics of sensitivity indices of LAI and SSM simulated by the STICS model to the estimated parameters for a maize plot, representative of the maize plots used in this study. The variance of SSM explained by the variations of θ_{FC1} clearly follows the dynamic of simulated SSM: the wetter is the first layer the more the simulated soil moisture is sensitive to θ_{FC1} . This confirms that SSM observed during wet situations contains more information to estimate this parameter.

< Figure 7 here please >

The influence of the other parameters (θ_{WP1} and second layer parameters) on simulated SSM starts with the first period of dryness faced by the crop (days 80-95) which coincide with the beginning of a long water stress period (Fig. 7a). It increases significantly during the senescence period (days 100-150) which is marked by a second period of dryness and a

continuous increase of water stress. In dry conditions the level of θ_{WP1} limits plant water uptake in layer one and thus directly affect its moisture content. Second layer parameters also affect SSM by limiting available water capacity and plant water uptake in second layer and thus by modifying the repartition of plant water uptake between both layers.

The dynamics of sensitivity indices of LAI to the estimated parameters follow that of the simulated water stress. In this case, LAI is only sensitive to parameters relative to the second layer indicating that AWC_2 (available water capacity of layer-2, which represent the major part of total AWC) plays a major role in the dynamic of LAI when the crop is affected by water stress, as it occurs in this case after the maximum LAI (days 100-150, Fig.7b). Before this period, the water stress is nil and the sensitivity of LAI to the estimated parameters is very low.

These results show that the levels of information content in LAI and SSM observations to estimate AWC components are strongly linked with the water regime and its interaction with the crop growth. This has been observed for all the situations although the dynamics and levels of sensitivity indices vary depending on the situations and crops (not shown here).

Impact of the water regime and its interaction with crop growth on the quality of AWC components estimation is illustrated and quantified in the following subsections.

3.3.3 Surface Layer Properties

As a consequence of the linked patterns of sensitivity of simulated SSM to first layer parameters and SSM value, the quality of estimation of θ_{FC1} and θ_{WP1} showed a high dependence on the status of water content in the first layer (Fig. 8).

< Figure 8 here please >

Inversions performed on dry situations (where SSM values were always far from θ_{FC1}) yielded poor estimates of θ_{FC1} . On the contrary, situations where at least 3 SSM observations were available when the first layer was wet (SSM values close to θ_{FC1}) provided particularly good estimates of θ_{FC1} with an error of about 5 % in mean and inferior to 10 % in most cases.

As expected, the opposite behavior was observed for θ_{WP1} since the sensitivity of simulated SSM to θ_{WP1} was found to be negatively correlated to SSM values (Fig. 7b). Situations in which at least one observation of SSM was available during period of dryness provided better estimates of θ_{WP1} than the other situations (Fig. 8b) with errors reduced by approximately half.

3.3.4 Second layer Properties

Figure 9 shows that the quality of estimation of the second layer properties was related to the water stress experienced by the crop. Better results were obtained on situations experiencing large water stress compared to those obtained on situations with no or limited water stress. The level of water stress experienced by the crop was quantified by S , the proportion of days in the crop cycle when the water stress index was less than 0.6 (1 corresponds to no stress and values tending to 0 to very high stress). The error, expressed as MRAE, was relatively lower in situations where $S > 20\%$ as compared to situations where $S < 20\%$. In situations where $S > 20\%$ there was a substantial improvement in the quality of estimation of θ_{FC2} and θ_{WP2} , while D_{L2} showed only a marginal improvement. The MRAE in the estimation of θ_{WP2} was reduced by more than half in case of $S > 20\%$ as compared to situations where $S = 0$, reaching a value inferior to 15%. MRAE of θ_{FC2} was about 10% for $S > 20\%$. Similar results were obtained when considering MRAE as a function of minimum stress values (not shown).

< Figure 9 here please >

Figure 10 shows that the RAE of the estimation of second layer properties was clearly negatively correlated with the number of observations of LAI available when the simulated water stress index was under 0.60. Situations in which at least one LAI observation was available during period of crop stress considerably improved the estimation of θ_{WP2} . For θ_{FC2} at least 2 observations of LAI during period of crop stress were necessary to obtain results significantly better than when using observations done during periods without stress. We still notice that the estimation of D_{L2} , even though it is slightly better when LAI observation are made during stressed periods, still remains poorer than that of θ_{FC2} and θ_{WP2} .

< Figure 10 here please >

4.0 Discussion

4.1 Accuracy of estimated soil properties

We have shown that in favorable conditions crop model inversion using observations potentially available from remote sensing may lead to reasonably accurate estimations of AWC components of two-layered soils and this even using limited number of observations. Most of the studies dedicated to the estimation of soil hydraulic properties or AWC components from model inversion using observations potentially available from remote sensing are based on synthetic dataset (Jhorar et al., 2002, 2004; Montzka et al., 2011; Bandara et al., 2013) or on very limited number of real cases (Charoenhirunyingyos et al., 2011; Sreelash et al., 2012; Shin et al., 2012; Bandara et al., 2014, 2015). However, assessing the interest of such methods requires their evaluation on large and diverse datasets. This study

represents a contribution toward this assessment and confirms the potential utility of this method.

Further improvements of the estimation errors are still attainable by increasing the level of information used for the inversion. In addition to observations of model outputs, prior information on estimated parameters may be used in the inversion process to better constrain the estimations. A few recent studies (Scharnagl et al., 2011; Scholer et al., 2011), mainly using hydrological models, have proposed to use soil maps or local texture measurements combined with hydraulic properties databases or pedotransfer functions to constrain the inversion problem by using informative prior distributions in Bayesian inversion systems. This may be particularly helpful for reducing equifinality problems. Thanks to the, sometimes independent, role played by AWC components in the model, the decoupling in space and time of the hydric processes affecting the two layers, and the availability of both SSM and LAI observations in humid and dry conditions, the potential compensation effects between AWC components were limited. However, compensative effects may still occur in some situations and this additional information could also help in estimating additional parameters such as bulk density. The evaluation of the potential of such approaches on large real dataset and using commonly available data as source of constraints constitutes one of the next key methodological challenges for the estimation of AWC components from crop model inversion.

4.2 Effect of hydric regime and its interaction with crop type

We found that the quality of estimation of AWC components was largely dependent on the hydric regime and its interaction with crop type: field capacity of surface layer was better estimated in wet conditions whereas wilting point of surface layer and deeper layer properties were better estimated in dry conditions and with crops facing hydric stress. This confirms on a

large set of real data what was partially suggested in (Jhorar et al., 2002; Varella et al., 2010b; Bandara et al., 2013) mostly on synthetic datasets. Our sensitivity analysis experiments suggested that this was due to the variation of the level of information content in LAI and SSM observations. If water inputs from rain or irrigation are not sufficient for ensuring optimal crop growth then crop growth is highly dependent to AWC and vegetation measurements bring significant information, particularly on the layers mostly representative of the root zone. On the contrary if SSM can be seen as a proxy of surface field capacity in wet conditions, its information content to estimate this property decreases in dry conditions. This sensitivity analysis also shed light on the results obtained by (Sreelash et al., 2012) about the complementarity of SSM and LAI observations. In a more general way, these results confirm the interest of using multiple remotely-sensed constraints for the estimation of root-zone soil moisture and associated soil properties in model-data fusion systems and the dependency of their information content on the vegetation state and soil moisture conditions (Barrett and Renzullo, 2009; Van Dijk and Renzullo, 2011).

Situations which experience large water stress and include wetting and drying cycles are thus optimal observational objects for estimating AWC components of multi-layered soils from crop model inversion. The complementary use of a few SSM observations in wet conditions and LAI observations during water stress period bring significant level of information for their estimation.

4.3 Impact of errors on the results

The results of the inversions presented in this study are also impacted by different types of error:

- (i) model errors (including both errors in the values set for model's input parameters that are not estimated in the inversions and errors in model's equations);
- (ii) observation errors, i.e. errors on measured LAI and SSM used in the inversions; and
- (iii) reference values errors, i.e. errors on the 'observed' values of the AWC components that are compared to the estimated parameters for assessing their quality.

Model errors may be linked with model complexity. Complex crop models have been built to mimic as realistically as possible the different processes involved in crop growth and its interaction with its environment but the resulting high number of parameters increases the degrees of freedom in model calibration process and the amount of information needed to feed the model. This may contribute to decrease model's robustness (Confalonieri et al., 2012). The crop model used in this study is representative of the most complex category of crop models (Jones et al., 2016) and the way parameters and input variables non estimated in the inversion process are set is conform to the usual practices. Obviously, the limits of the plant parameters calibration process and the errors on the information used to set its other entries impact the model simulations as well as do the errors in its equations. The inversions are based on the computation of the differences between simulated and observed values of SSM and LAI (SAE_{SSM} and SAE_{LAI} , eq. 2). This computation is affected in the same way by model and observation errors and these errors may be compensated by unrealistic values of the inversed parameters. Errors on SAE_{SSM} and SAE_{LAI} have been approximated for each situation by comparing the observed and simulated values of LAI and SSM, using the reference values of AWC components in simulations. As expected, large SAE errors on LAI and/or SSM often lead to large errors in the estimated parameters that are sensitive to these

variables (results not shown). As practical applications of the method are likely to include situations with large model and/or observation errors, we didn't remove such situations from our analysis, to evaluate as fairly as possible the performance we can expect from this method. Ensemble modelling has recently shown to be an efficient way of improving crop simulation (Martre et al., 2015). Although it would be cumbersome to implement, using several models could be considered in an inversion process to reduce the impact of model error.

Reference values errors may impact the evaluation of the quality of parameters estimate. Particularly, the lesser reliability of D_{L2} measurements in field conditions, as it is difficult to estimate by augering the precise depth of the base of the soil profile, may partly explain that its estimation still remains poorer than that of θ_{FC2} and θ_{WP2} . In addition, D_{L2} estimate from inversion represents an effective soil thickness that might be far from the value assessed in field conditions. Some particular situations may create such discrepancy between effective and measured values: presence of an obstacle that prevents the roots to attain the base of the soil profile and limits the effective AWC, or presence of a transient perched water table connected with the base of the profile that allows a larger effective AWC than observed.

4.4 Practical application of the method on agricultural catchments

The results presented in this study contribute to evaluate the potential of AWC components retrieval from crop model inversion and may help to define optimal configuration for the application of this method on agricultural catchments. This next step is challenging but necessary to bring solutions to the issue of monitoring water resources in irrigated agricultural catchments.

Application of this method for deriving soil maps of AWC components would require the use of SSM and LAI data retrieved from remote sensing. The method presented here is directly

applicable with remote sensed data and the benefit of using them has already been shown in other studies (Santanello, et al., 2007; Charoenhirunyngyos et al., 2011; Ines et al., 2013; Bandara et al 2015). In tropical regions, where cloudy conditions are frequent, SSM and LAI are attainable from radar remote sensing (e.g. Wagner et al., 1999; Tomer et al., 2015 for SSM ; Kim et al., 2012 ; Hirooka et al., 2015 for LAI).

Crop model inputs such as climate or farming practices are often less precisely known at the territory scale than at point scale. The level of precision of the available information on these inputs may impact crop models simulations (Jego et al., 2015). Additional studies would be required to assess the influence of these uncertainties on the results of the inversions to evaluate to what extent they impact the quality of AWC components retrieval.

Finally, systematic multi-local application of this method in its current configuration for deriving soil maps of AWC components in agricultural catchments may face the problem of vegetation types or crops non-represented in the model and of the dependence of its performance to the agro-pedo-climatic conditions on which it is applied. It may thus advantageously be combined with advanced geostatistical methods able to take into account in an optimal way all kind of existing soil information (McBratney et al., 2003). In this context, the results presented in this study may guide the sampling of representative fields over a territory to use this technique for soil mapping exercise.

5.0 Conclusion

In this study we evaluated on an extensive field experiment the potential of crop model inversion for estimating AWC components on two-layered soils with observations potentially accessible from remote sensing.

We have shown that:

- 1) the quality of estimation of AWC components varied depending on the situations on which it was estimated. These estimations were however systematically better than the prior information used although this prior information was already of relatively good quality;
- 2) the quality of estimation of AWC components was found to largely depend on the hydric regime and its interaction with crop type: field capacity of surface layer was better estimated in wet conditions whereas wilting point of surface layer and deeper layer properties were better estimated in dry conditions and with crops facing hydric stress;
- 3) using simultaneously LAI and SSM observations allowed to obtain mean relative absolute error of 5% for field capacity of surface layer, 10% for field capacity of root zone, 15% for wilting point of surface layer and root zone, and 20% for soil depth, in favorable conditions; and
- 4) a few observations of LAI and SSM available in favorable conditions were sufficient to largely improve the estimation of AWC components.

We confirmed the utility of the inversion of crop-models to provide realistic soil-water properties and further improvements such as inclusion of informative prior distributions or reduction of model error are still conceivable. Further studies are however still needed to apply this method for deriving soil maps of AWC components at agricultural catchment scale. Such improvements will allow deriving accurate maps of soil AWC at the catchment scale, which are essential for distributed hydrological models aimed at studying the impact of agriculture on water resource in tropical catchments.

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List of Tables

Table1

Crop	Number of situations monitored	Growing Season	Average length of the growing period	Avg. number of LAI/SSM Observations per situation
Turmeric	17	May to December	~240 days	10
Sunflower	11	May to August	~110 days	8
Sorghum	9	May to August	~110 days	8
Maize	8	September to December	~100 days	7

Table 1: Monitored plots and vegetation measurements from 2011 to 2013. (LAI – Leaf Area Index; SSM – Surface Soil Moisture)

Table2

Variable	2011			2012			2013		
	S1	S2	S1 + S2	S1	S2	S1 + S2	S1	S2	S1 + S2
Rain (mm)	520	321	841	302	282	584	557	301	858
Irrigation (mm)	0	0	170	0	0	165	0	0	90
PET (mm)	347	351	698	366	341	707	342	344	686
(Rain + Irrigation)/PET	1.50	0.91	1.45	0.83	0.83	1.06	1.63	0.88	1.38

S1 - Season-1: May to August (sunflower and sorghum)

S2 - Season-2: September to December (maize)

S1 + S2: May to December (turmeric).

Table 2: Cumulated Rain, Potential Evapotranspiration (PET Penman Method, Penman, 1948), Irrigation and (Rain+ Irrigation)/PET ratio over the corresponding growing season for turmeric, sunflower, sorghum and maize crops for 2011, 2012 and 2013 in the Berambadi catchment.

Table3

Soil Type/ Parameter	No of Plots	Soil moisture at Field Capacity θ_{FC} (g/g)	Soil moisture at Wilting Point θ_{WP} (g/g)	Available water Content AWC (mm)
Sandy Loam	11	14.0 to 19.5	4.5 to 7.5	127.0 to 215.0
Sandy Clay Loam	15	17.5 to 23.5	6.5 to 11.0	139.0 to 231.0
Clay Loam	7	22.5 to 30.0	10.5 to 12.5	129.0 to 198.0

Table 3: Range of observed values of Field Capacity and Wilting Point obtained from long term soil moisture observations (2011-2014) and AWC (computed using Eq. 1) for different soil types in the 33 plots. Field Capacity and Wilting Point values are presented in gravimetric unit, the unit used in the model STICS.

Table4

Parameter (name in STICS)	Definition	Unit	Initial Range
θ_{FC1} (HCC(1))	Water content at field capacity of layer 1	g/g	10 – 32
θ_{FC2} (HCC(2))	Water content at field capacity of layer 2	g/g	10 – 32
θ_{WP1} (HMINF(1))	Water content at wilting point of layer 1	g/g	5 – 15
θ_{WP2} (HMINF(2))	Water content at wilting point of layer 2	g/g	5 – 15
D_{L2} (EPC(2))	Thickness of layer 2	cm	70 – 150

Table 4: The soil parameters of STICS model selected for estimation along with their initial ranges of values used as prior information.

List of Figures

Figure 1

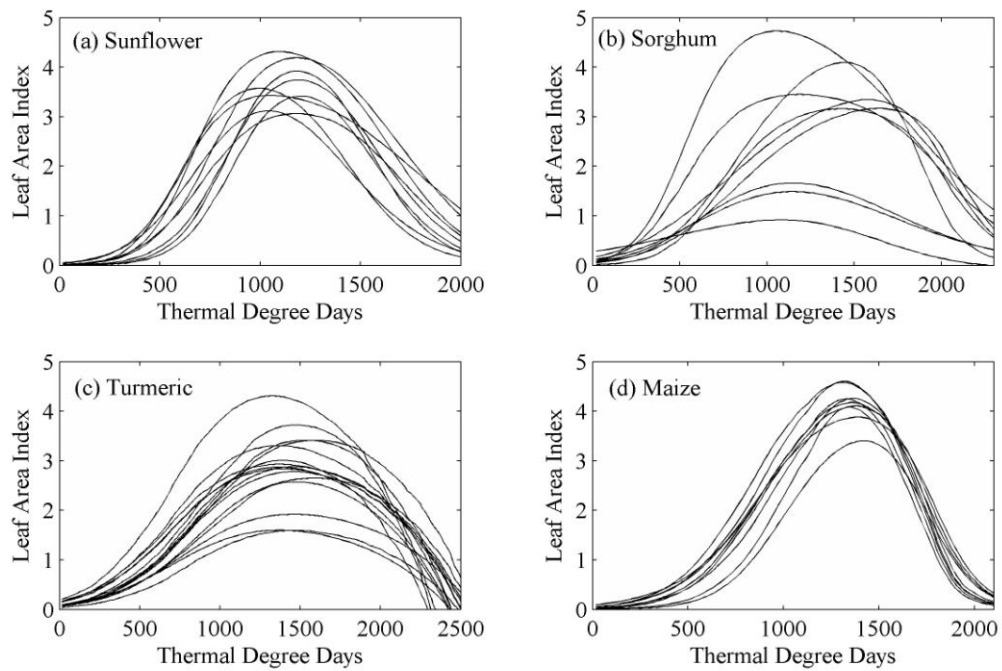


Figure 1: LAI curves for (a) Sunflower, (b) Sorghum, (c) Turmeric and (d) Maize showing the variability of LAI between plots and crops.

Figure 2

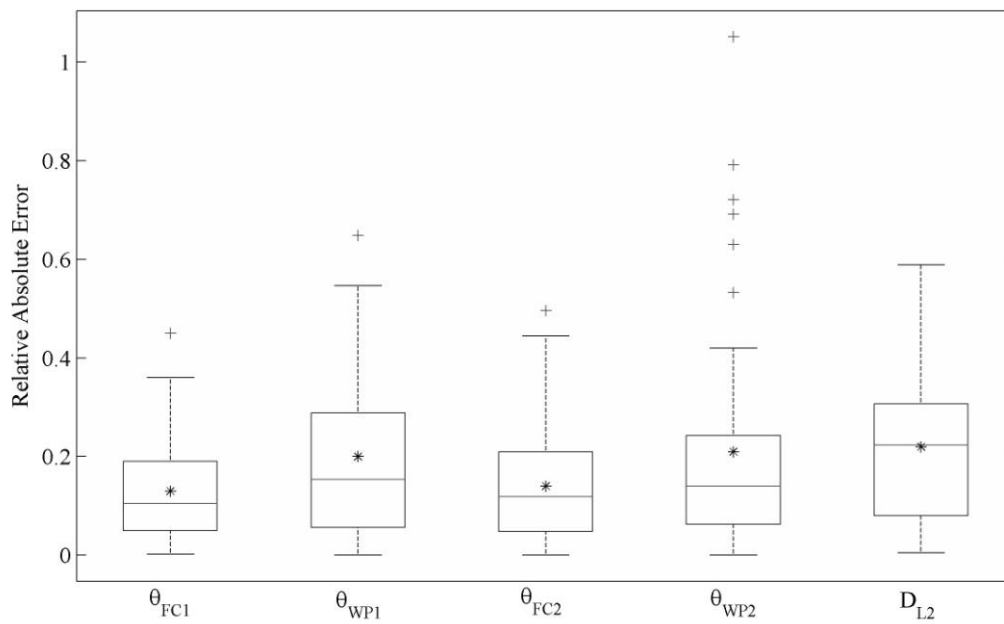


Figure 2: Boxplot of the Relative Absolute Error (RAE, Eq.5) in the estimation of soil parameters for 45 situations (All Crops), * is the mean value of the RAE (MRAE), + represent outliers.

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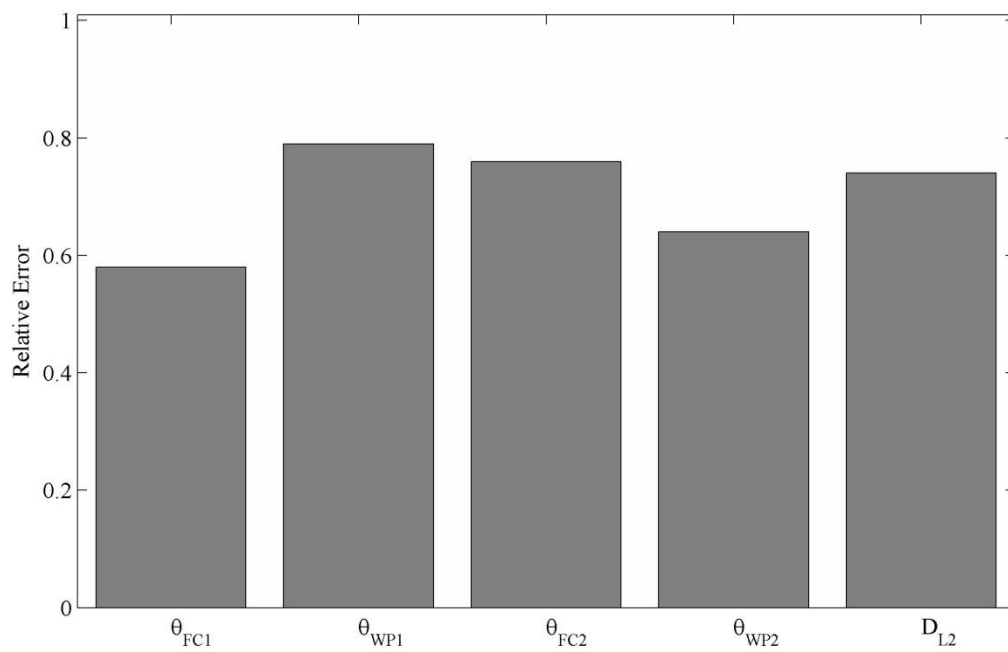
Figure 3

Figure 3: Relative error (RE, Eq.7) in the estimation of soil parameters.

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Figure 4

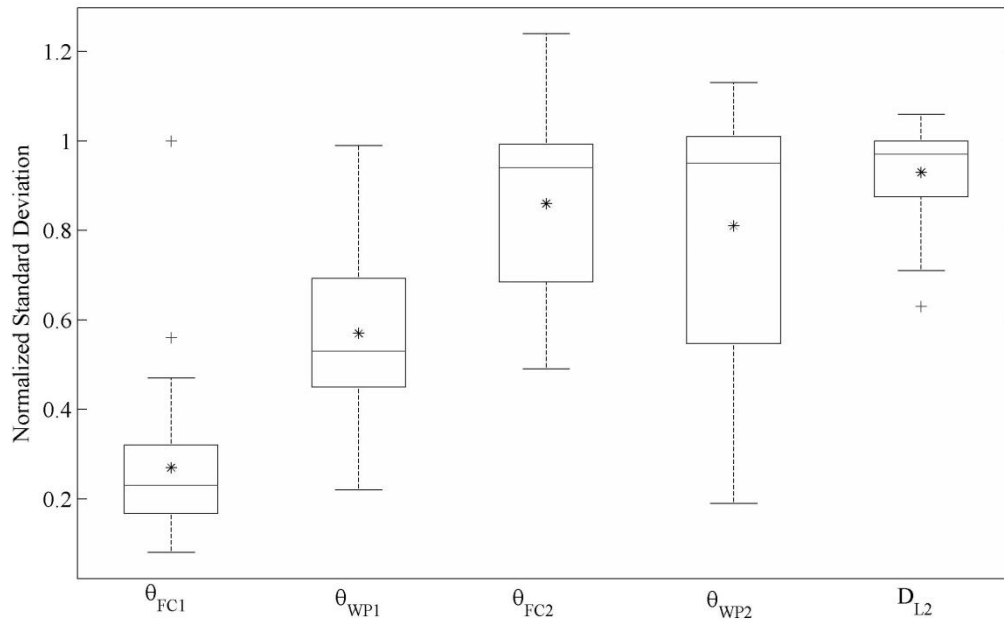


Figure 4: Boxplot of the normalized standard deviation (σ_{norm} , Eq.8) of the parameter estimates on the 45 situations, * is the mean value, + represent outliers.

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Figure 5

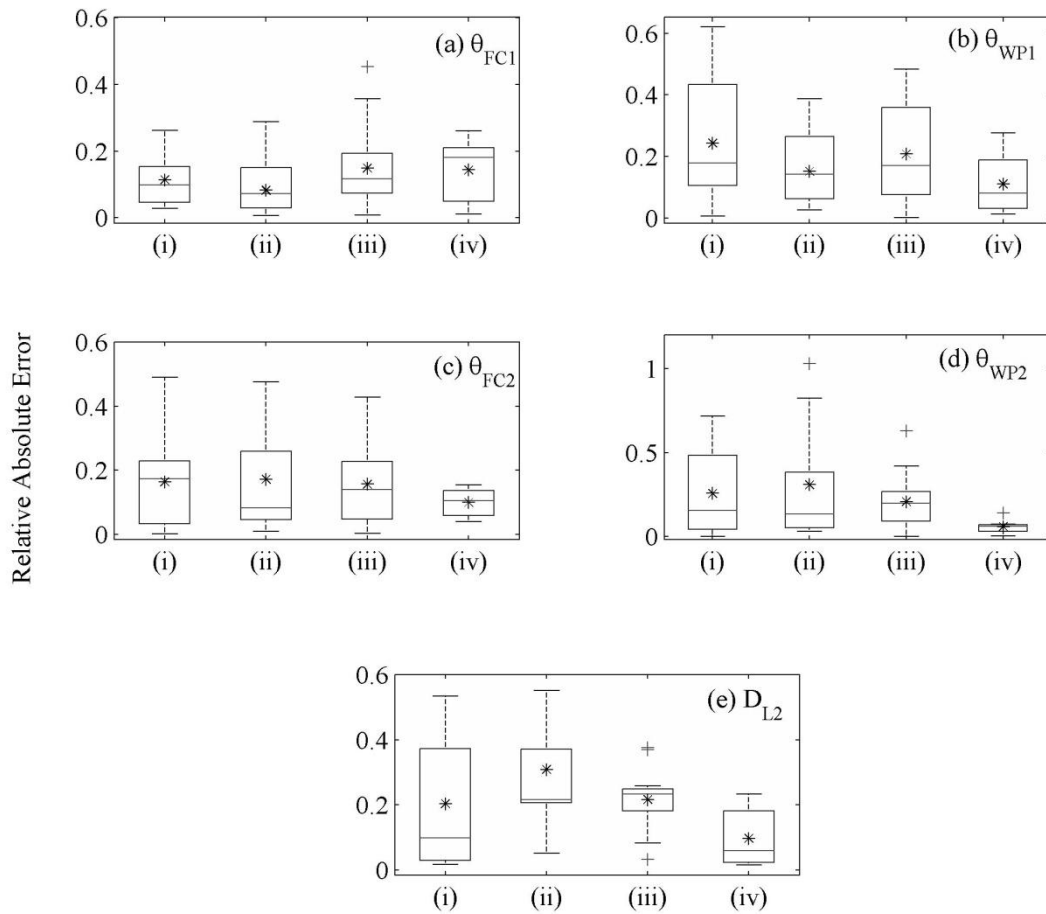


Figure 5: Boxplot of RAE in estimation of (a) θ_{FC1} , (b) θ_{WP1} , (c) θ_{FC2} , (d) θ_{WP2} and (e) D_{L2} , for (i) Sunflower, (ii) Sorghum, (iii) Turmeric and (iv) Maize, * is the mean value (MRAE), + represent outliers.

Figure 6

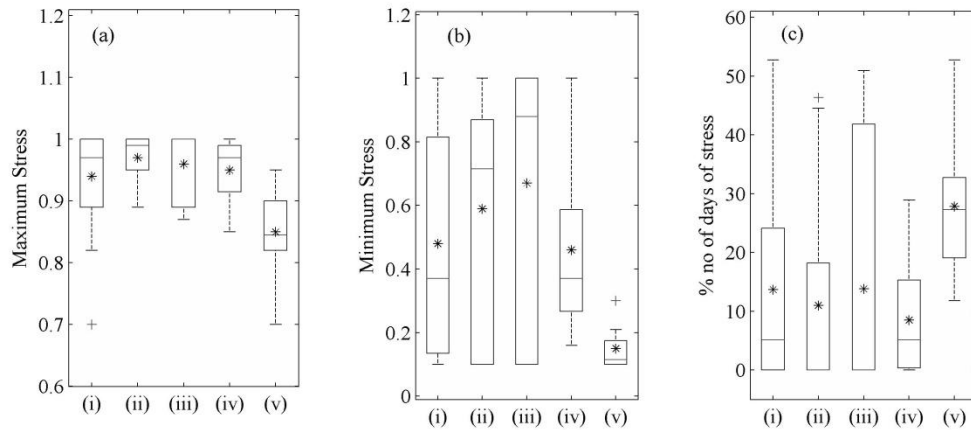


Figure 6: Variability of simulated water stress between plots in terms of (a) maximum water stress index during crop cycle, (b) minimum water stress index during crop cycle and (c) percentage number of days S of the crop cycle for which stress index is inferior to 0.6, for (i) All crops (45 situations), (ii) Sunflower, (iii) Sorghum, (iv) Turmeric and (v) Maize. The water stress index in STICS model expresses the reduction of plant transpiration as compared to a potential and varies from 0 to 1, 0 being the highest stress and 1 indicating no stress. * is the mean stress, + represent outliers.

Figure 7

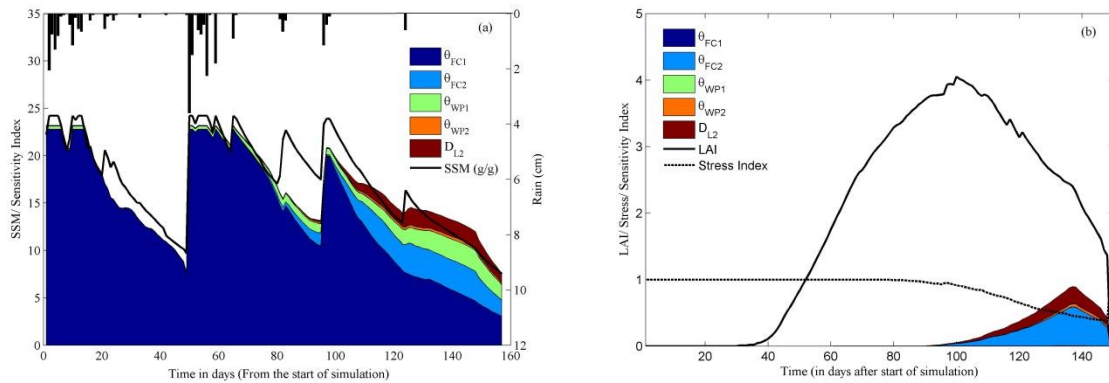


Figure 7: Temporal variations of (non-normalized) Sobol' main sensitivity indices of (a) SSM and (b) LAI to soil hydraulic parameters and 2nd layer depth during the entire simulation period for one plot of maize crop. Solid black curves represent the mean of simulated (a) SSM and (b) LAI. Bar chart in (b) represents the rainfall (in cm). Dashed black curve in (b) represents the mean of simulated water stress.

Figure 8

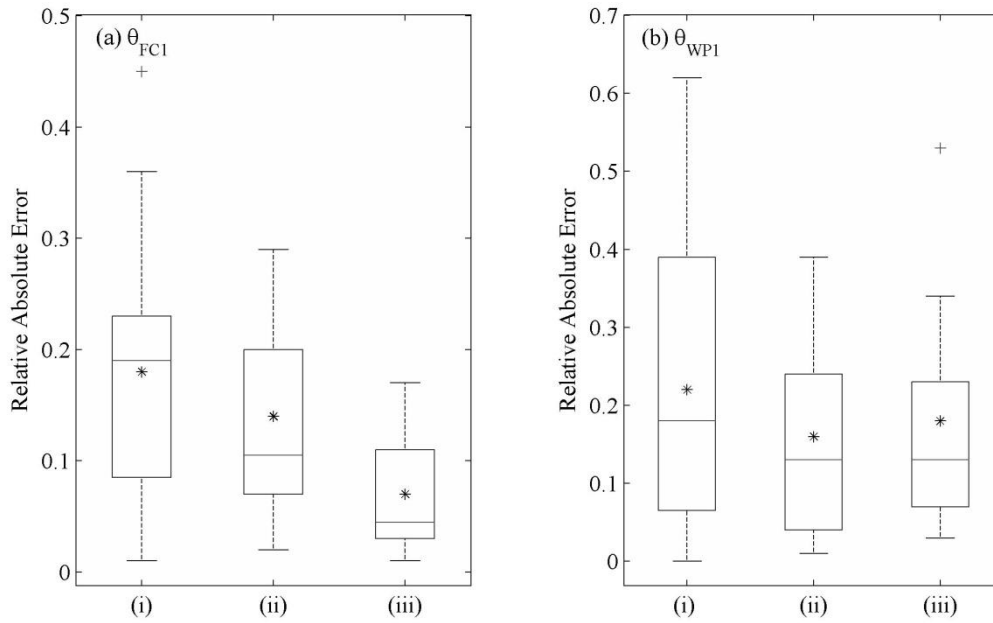


Figure 8: Box plot of RAE in the estimation of (a) θ_{FC1} for different situations of N , (i) $N = 0$ (17 Plots), (ii) $N = 1$ to 2 (14 Plots) and (iii) $N > 2$ (14 Plots), N being the number of observations of SSM measured when the first layer water content simulated by the model from measured SHPs falls within $\pm 10\%$ of θ_{FC1} values and (b) θ_{WP1} for different situations of N , (i) $N = 0$ (21 Plots), (ii) $N = 1$ to 2 (14 Plots) and (iii) $N > 2$ (10 Plots), N being the number of observations of SSM measured when the first layer water content simulated by the model from measured SHPs was less than half of θ_{FC1} . * is the mean value (MRAE), + represent outliers.

Figure 9

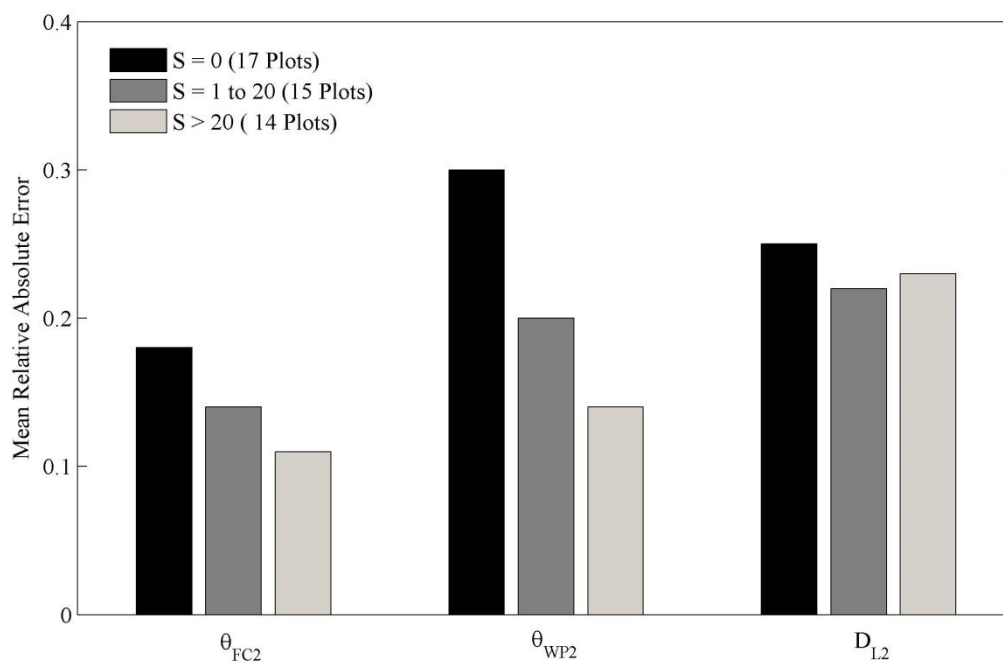


Figure 9: MRAE in the estimation of 2nd layer parameters (θ_{FC2} , θ_{WP1} and D_{L2}) for three levels of water stress experienced by the crops. 'S' is the percentage number of days of the cropping seasons that are under significant stress (stress index of 0.6).

Figure 10

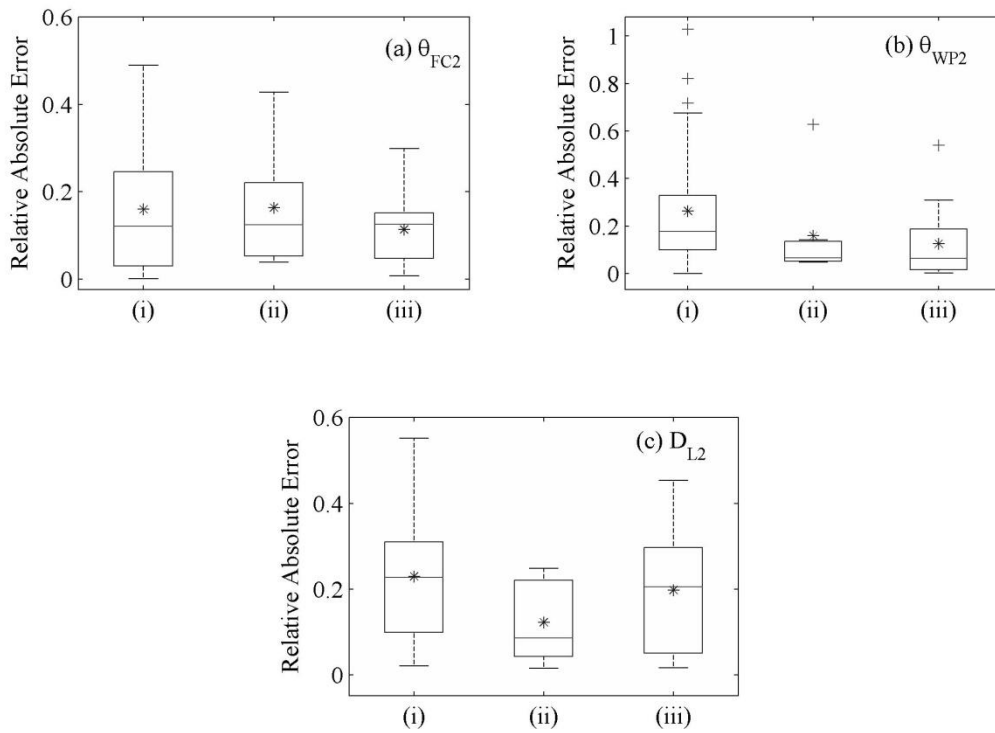


Figure 10: Box plot shows the RAE in the estimation of (a) θ_{FC2} (b) θ_{WP2} and (c) D_{L2} for different situations of N, (i) $N = 0$ (26 Plots), (ii) $N = 1$ (7 Plots) and (iii) $N > 1$ (12 Plots). N is the number of observations of LAI measured when simulated stress index is under 0.6. * is the mean value (MRAE), + represent outliers.

Appendix-A

Values and source of non-estimated soil parameters used in this study

Parameter	Source	Range	Remarks
pH	Soil Map	5.04 to 8.13	KRSAC*
Organic Nitrogen Content (% of dry soil)	Site specific relation between clay content and organic nitrogen content from laboratory analysis on soil cores sampled in the fields	0.06 to 0.16	Field Experiments
Albedo of bare soil (%)	Standard Values	0.18 to 0.28	Brisson et al., 2008
Rainfall-Runoff Ratio (%)	Estimated using profile soil moisture in bare soil conditions	0.05 to 0.15	Field Experiments
Bulk Density (g.cm ⁻³)	From ratio of volumetric and gravimetric soil moisture content	1.15 to 1.60	Field Experiments
Depth of tilling (cm)	Ploughing and tilling depth from field	5 to 30	Field Experiments

* Karnataka State Remote Sensing Application Center

Highlights:

- Crop model inversion is a powerful method for estimating available water content components
- It was evaluated on a large field experiment dataset (4 crops, 45 situations)
- Interaction between crop type and soil water regime highly impacted the quality of estimation
- Mean relative error of estimated properties varied between 5 and 20% in favorable conditions

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