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# Uncertainty assessment of the agro-hydrological SWAP model application at field scale: A case study in a dry region

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ABSTRACT

Uncertainty analysis can provide useful insights into the sources and effects of uncertainty for decision makers to achieve the goals of reliability and sustainability in water management. This study presents parameters uncertainty of a physically based soil–water–atmosphere–plant (SWAP) model and its effect on model prediction within the generalized likelihood uncertainty estimation (GLUE) framework for two irrigated agricultural fields in a dry region of Iran. To simulate soil water dynamics of the two fields, the SWAP model is calibrated using soil moisture observation data. The results demonstrate that predictive uncertainty in soil moisture during the growing season in both fields is relatively small and a good model performance is achieved. Parameter uncertainty analysis of soil hydraulic parameters showed that in spite of similarity of soil texture in both the fields, the estimated parameters (i.e. posterior distribution) exhibit different behaviors. This was because of the dynamics of soil structure which varies considerably within cultivated fields during the growing season. Moreover, the simulated water balance fluxes (actual evapotranspiration and deep percolation) indicate that in irrigated agricultural fields in dry regions, the precision of actual evapotranspiration predicted by the SWAP model is high (i.e. a high degree of model reliability is achieved). However, deep percolation fluxes show higher variation (lower precision) and are more sensitive to soil hydraulic conductivity parameterization. Finally, this study reveals the importance of uncertainty analysis to estimate the degree of reliability associated with model predictions as an important first step for providing decision makers with realistic information about the models outputs.



## 1. Introduction

Agro-hydrological simulation models have been widely used for optimizing resources in agriculture for maximum crop growth and minimum environmental impact. In addition, these models describe the soil water fluxes, the soil vapor fluxes, and water and energy balances in the soil–crop–atmosphere system in detail (Van Dam, 2000). Numerous studies have applied agro-hydrological models to assess water balance or irrigation scheduling at field scale (e.g. Clemente et al., 1994; Droogers, 2000; Singh et al., 2006a,b). However, due to the inherent variability in natural processes and difficult or costly monitoring, the model input data and its internal parameters are rarely known with certainty (Wang et al., 2005). Thus, the parameters cannot be identified with ease. Assessment of parameter and predictive uncertainty of hydrologic models is essential for successful use of models in environmental management and a required assessment should be conducted before using its results in decision making processes (Ajami et al., 2008). Among agro-hydrological model applications, few studies have been conducted to investigate parameter uncertainty at field scale (e.g. Makowski et al., 2002; Lawless et al., 2008; He et al., 2009). The agro-hydrological SWAP (soil, water, atmosphere and plant) model based on the Richards' equation has been applied and tested under various conditions and has proven to produce reliable and accurate results (e.g. Droogers et al., 2000; Ahmad et al., 2002; Bonfante et al., 2010; Karimi et al., 2012). SWAP addresses the close interactions between soil water flow, surface water management, and vegetation development (Van Dam et al., 2008).

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More recently, inverse approaches have been increasingly used to estimate (calibrate) model parameters. Estimation of the model parameters is subject to uncertainty, which leads to uncertainty in model predictions. In most applications, this uncertainty needs to be quantified to provide meaningful prediction of model results. In many applications, according to our best knowledge, none of the SWAP model parameter estimates were conducted through uncertainty assessment. Among such inverse approaches for SWAP calibration, PEST (Doherty, 1994) has been intensively used to identify parameters of the soil hydraulic functions (e.g. Jhorar et al., 2002; Singh et al., 2006b; Vazifedoust et al., 2008). However, most optimization algorithms have the disadvantage of being very sensitive to the starting value of the parameters, while also being prone to converge to local minima (Abbaspour et al., 2001) (see Pande (2013a,b) for more examples of different algorithms to aid global convergence). There are also robust optimization techniques that attempt to search for the whole parameter space to find a global minimum. For example, Ines and Droogers (2002) used GA to inversely estimate the soil hydraulic functions in the unsaturated zone for SWAP model application. Hupet et al. (2003) also linked several global search algorithms to SWAP for parameter optimization, such as the global multilevel coordinate search (GMCS) algorithm (Huyer and Neumaier, 1999) and its combination with the classical Nelder–Mead simplex (NMS) algorithm. Yet another major problem in inverse modeling is Equifinality of models (e.g. Abbaspour et al., 1997; Beven and Freer, 2001); the condition in which different parameter sets can lead to a similar model response due to poorly constrained inverse problem formulation (Arkesteijn and Pande, 2013). It has been accepted that the process of calibration cannot lead to a single ‘optimal’ parameter set but one has to find a probability distribution of parameters that represents the knowledge about parameter values. Hence, the parameters cannot be identified easily and different parameter sets may result in similar prediction which is known as the equifinality (Beven, 2001). On the other hand, well-constrained inverse problems identify model parameters better and yield robust simulations (Pande et al., 2009, 2012).

Yet, the vast majority of SWAP model calibrations are still conducted by optimization algorithms and deterministic perspectives (e.g. Droogers et al., 2008; Singh et al., 2010; Noory et al., 2011). Indeed, previous studies on SWAP model applications have largely ignored quantifying the parameter and predictive uncertainty when the model is calibrated based on soil moisture data, especially its effect on the simulation of water balance components. One method that provides a reasonable framework for assessing uncertainty and the issue of equifinality is the generalized likelihood uncertainty estimation (GLUE; Beven and Binley, 1992). It is an informal Bayesian method that uses prior information about parameter values and estimates uncertainty in model parameters. This method, based on Monte Carlo simulation, transforms the problem of searching an optimal parameter set into searching a set of parameter values that provide reliable simulations for a range of model inputs (Beven, 2006; Sreelash et al., 2012). In GLUE, parameter uncertainty accounts for all sources of uncertainty (i.e. input uncertainty, structural uncertainty, and parameter uncertainty) and the likelihood measure value that is associated with a parameter set implicitly reflects all these sources of error on model performance (Beven, 2001). GLUE has been widely used for assessing uncertainty in hydrological models (Li et al., 2010) and various other fields of modeling (e.g. Zheng and Keller, 2007; Juston et al., 2010). For instance, Zhang et al. (2006) compared GLUE with a non-linear least square optimization method and indicated that GLUE can produce a wider range of potential outputs that are more robust in model predictions of pesticide transport in soils at field scale. They also suggested that the prediction uncertainties are useful in evaluating risk in decision making. He et al. (2009) applied GLUE in estimating CERES-Maize model parameters for sweet corn production.

So far, little effort has been made to analyze the uncertainty of agro-hydrological models applied at field scale. Due to various boundary conditions, management practices and spatiotemporal variability in soil hydraulic properties, it is of great importance to investigate the uncertainty in model parameters that affect agro-hydrological model outputs. The aim of the present paper is to assess the parameter uncertainties and their effect on model prediction, within GLUE framework, for two irrigated agricultural fields (maize and wheat) in a dry region in Iran. This study also aims at investigating SWAP model Equifinality and parameter identifiability – refers to whether the single true value of a model's calibration parameters can theoretically be inferred (Lancaster, 2004) based on available data – of soil hydraulic parameters calibrated based on soil moisture measurements, and further assessing their effects on water balance fluxes prediction. The SWAP modeling results and uncertainty analysis from this study are believed to make useful contributions toward agricultural water management decision making processes.

## 2. Materials and methods

### 2.1. Site description and data set

The study area, Borkhar district, is located in central Iran, north of the historic city of Isfahan. Borkhar district is characterized as having a predominantly arid to semi-arid climate. Long term average annual rainfall is 164.7 mm, most of which falls in the winter months from December to April, therefore profitable crop production without reliable irrigation is impossible in the area.

Two farm fields were selected for this study: a fodder maize field and a wheat field. Field measurements were made at the fodder maize field during the summer season and at the wheat field during the winter season (Table 1) of the agricultural year 2004–2005 (Vazifedoust, 2007). The soil texture in both fields is relatively heavy (52% clay and 38% silt in the maize field and 46% clay and 36% silt in the wheat field) and the bulk densities of the topsoil layer (0–60 cm) are 1.4 ($g\,cm^{-3}$) and 1.6 ($g\,cm^{-3}$) for the maize and wheat fields, respectively. Access to water with good quality in this area provides suitable growing conditions for wheat and maize. Groundwater levels are deep (>100 m) with low salinity ($EC < 2\,dS\,m^{-1}$).

Daily meteorological data, including minimum and maximum temperature, relative humidity, vapor pressure, sunshine hours, wind speed and rainfall were obtained from a meteorological station in the vicinity of the site. During the growing season, the irrigation depths were constant and the two study fields received heavy traditional irrigation. The irrigation depth in the wheat field was 17 cm for each of the six events and was 16 cm in the maize field for each of the eight events throughout the period of crop growth. The data on crop characteristics including plant height, leaf area index (LAI) and rooting depth were also obtained from the emergence stage to the maturity stage during crop development at the two study fields. The crop characteristics data are described in terms of crop growth by the measured characteristics as a function of crop development stage. During the growth period, volumetric soil moisture content was measured at three soil depths (i.e. 0–15, 15–30 and 30–60 cm). The data were used in the model calibration stage.

### 2.2. The agro-hydrological SWAP model

The soil–water–atmosphere–plant (SWAP) is an integrated physically based simulation model for one-dimensional vertical

**Table 1**
Overview of the data collected for SWAP model calibration and uncertainty analysis at farmer fields in Borkhar district (Vazifedoust, 2007).

| Data | Collection method | Frequency | Purpose |
|---|---|---|---|
| Meteorological data | Meteorological station | Daily | Input derivation |
| Soil properties | | | |
| Texture | International pipette method and USDA classification | Once | Input derivation |
| Bulk density | Core method | Once | Input derivation |
| Saturated percentage | Saturated paste method | Once | Input derivation |
| Organic carbon | Wet digestion method | Before sowing | Input derivation |
| pH | In soil–water suspension of 1:2 | Before sowing | General |
| Soil moisture | Gravimetric method | Weekly | Model calibration |
| Irrigation regime | | | |
| Discharge of irrigation source (i.e. canal water) | Volumetric method | Once | Input derivation |
| Duration of irrigation | Field observation | Once | Input derivation |
| Irrigation depth | Irrigation depth were calculated by multiplying the discharge and duration of irrigation and then divided by field area | Once | Input derivation |
| Crop growth data | | | |
| Crop development stage | Field observation | 4–5 times | Input derivation |
| Plant density and tillers | Field observation | 4–5 times | Input derivation |
| Plant height | Field observation | 4–5 times | Input derivation |
| Leaf area | Field observation | 4–5 times | Input derivation |
| Rooting depth | Field observation | 4–5 times | Input derivation |

water flow, solute transport and heat flow in agricultural fields. SWAP is based on the finite difference solution of Richards' equation extended with a sink term to account for root water uptake. Daily model outputs include simulated actual evaporation $E_a$; actual transpiration $T_a$; flow across the bottom of soil profile and moisture distribution in the soil profile (Van Dam, 2000). The SWAP 3.0.3 version that is used in this study is described by Kroes and van Dam (2003). The core part of the program is the vertical flow of water in the saturated–unsaturated zone, which can be described by the well-known Richards' equation:

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

where $\theta$ denotes the soil water content (cm$^3$ cm$^{-3}$), $t$ (day) is time, $h$ (cm) soil matric head, $z$ (cm) the vertical coordinate, assumed positive upwards, $K$ (cm day$^{-1}$) the hydraulic conductivity as a function of water content and $S$ (day$^{-1}$) represents the water uptake by plant roots. Eq. (1) is solved numerically, subject to specified initial and boundary conditions and using known relationships between $\theta$, $h$ and $K$. The relationships are described by the parametric relationships of Van Genuchten (1980) and Mualem (1976):

$$K(\theta) = K_s S_e^{\lambda}\left[1-\left(1-S_e^{n/(n-1)}\right)\right]^2 \quad (2)$$

$$S_e = \left(\frac{\theta-\theta_r}{\theta_s-\theta_r}\right) = \left[\frac{1}{1+|\alpha h|^n}\right]^{(n-1)/n} \quad (3)$$

where $\theta_r$ and $\theta_s$ are the residual and saturated volumetric water content (cm$^3$ cm$^{-3}$), respectively; $\alpha$ (cm$^{-1}$), $n$ and $\lambda$ are empirical parameters.

The upper boundary condition in SWAP is determined by the potential evapotranspiration, $ET_p$ (mm d$^{-1}$), irrigation, $I$ (mm d$^{-1}$) and precipitation, $P$ (mm d$^{-1}$). Crop growth simulation and crop yields can be computed by either using a simple crop module or by using a detailed crop growth simulation module. In the simple crop module, the user specifies leaf area index, crop height and rooting depth as a function of development stage. The simple model does not calculate the crop potential or actual yield. Detailed crop module or WOFOST (Supit et al., 1994) is a generic crop model, capable of simulating the growth and development of most crops. For this specific case, we used the simple crop module.

### 2.3. Uncertainty analysis and GLUE approach

There are different definitions of uncertainty that vary in different scientific disciplines (cf. Walker et al., 2003). In water management, as discussed by Refsgaard et al. (2007), the terminology that has been defined by Klauer and Brown (2004) is adopted as "a subjective interoperation of uncertainty in which the *degree of confidence* that a decision maker has about possible outcomes and/or probabilities of these outcomes is the central focus". Therefore, uncertainty assessment of model simulations is important in environmental modeling, especially when the models are used to support water management decisions (Beven, 2001; Refsgaard and Henriksen, 2004). There are numerous methods that assess uncertainty. The generalized likelihood uncertainty estimation (GLUE) method is one such method that can be used both as a calibration method and as an uncertainty propagation method based on the concept of equifinality (Beven and Binley, 1992).

In the GLUE method, parameter uncertainty accounts for all sources of uncertainty; i.e. input uncertainty (as a result of errors in input data such as rainfall), structural uncertainty (the conceptual uncertainty due to incomplete understanding and simplified description of modeled processes), and parameter uncertainty. Therefore, this method has found wide applications as an effective and general strategy for model calibration and uncertainty estimation. In the GLUE methodology, a prior distribution of parameter values is used to generate $n$ parameter sets to be used in the Monte Carlo simulation. The Latin hypercube sampling (LHS) method, a stratified-random procedure which provides an efficient way of sampling variables from their ranges (McKay et al., 1979), is used to sample the parameter space. The random parameter sets (samples) are then used to run the model $N$ times independently, and the output of the model for each run is evaluated against observed values using a performance measure (likelihood measure) criteria. A certain subjective threshold (a critical value) of the performance measure is defined, which is used to assess the acceptability of each parameter set. If the acceptability is less than the pre-defined threshold, the run is considered to be a non-behavioral solution and the corresponding parameter set is not considered for further analysis. The behavioral solutions are then weighted according to an appropriate likelihood measure. Finally, the acceptable or behavioral parameter sets are used to estimate the mean and uncertainty bounds for the estimated parameters and the predicted variables of interest.

The subjective choice of the likelihood measure is an important feature of the GLUE methodology (He et al., 2010; Li et al., 2010). In this study the inverse error variance, which is commonly used to measure the closeness between model predictions and observations (Beven and Binley, 1992), is chosen as the likelihood function.

$$L(\theta_i|O) = \left(\sigma_e^2\right)^{-T} = \left(\frac{\sum_{j=1}^{n}(O_j - Y(\theta_i))^2}{n-2}\right)^{-T} \quad (4)$$

where $O_j$ is the observed soil moisture content at time $j$, $Y_j(\theta_i)$ is moisture simulated by the $i$th parameter at time $j$, $n$ is the sample size and $T$ is a parameter chosen by the user. It is worth mentioning that, each simulation in Eq. (4) will have equal likelihood value when $T = 0$. However, more weight can be assigned to a single best solution with negligible weights assigned to other solutions by increasing the value of $T$ to $\infty$ (Vrugt et al., 2008b).

For determining behavioral parameter sets a choice of the threshold value is also crucial in the GLUE methodology (Beven et al., 2008). This threshold can be either defined by giving a certain allowable deviation of the highest likelihood value in the sample or as a fixed percentage of the total number of simulations, also called acceptable sample rate (ASR) (Li et al., 2010). The likelihood values of the retained solutions (behavioral parameter sets) are then rescaled to obtain the cumulative distribution function (CDF) of the output prediction and the associated uncertainty is derived from the CDF, normally chosen at the 5 and 95% prediction quintiles. In our case study, GLUE method can be tailored as follows:

Step 1: Determine a prior range for the parameters to be calibrated based on some field observations and/or pedotransfer functions.
Step 2: Sample $n$ parameter sets using Latin hypercube sampling.
Step 3: Run the SWAP model for each of the $n$ parameter sets and calculate the likelihood values based on Eq. (4).
Step 4: Define a cutoff threshold (or ASR) to collect the behavioral solutions as a fixed percentage of the total number of simulations.
Step 5: Normalize the likelihood values and calculate the probability ($p(\theta_i)$) or likelihood weight for each behavioral parameter set as follows:

$$p(\theta_i) = \frac{L(\theta_i|O)}{\sum_{i=1}^{N} L(\theta_i|O)} \quad (5)$$

where $N$ is the number of behavioral parameter sets.
Step 6: Sort the simulated soil moisture values by their corresponding probabilities to create a probability density function (PDF) of the model output prediction, and use these to generate 95% confidence interval (95CI).

For GLUE implementation, a sample size of $n$ = 100,000 is used with a value of $T$ = 1 in the likelihood function of Eq. (6) and ASR in step (4) is chosen as the best 1% of the samples. These are rather standard settings with GLUE (Vrugt et al., 2008a,b; Li et al., 2010) and in this context will result in a total of 1000 different behavioral solutions. Furthermore, in this study two indices are used to gauge the strength of calibration and uncertainty measures: the coverage (%) measures the percentage of soil moisture observations contained in the 95% confidence interval (95CI) whereas the spread ($cm^3\,cm^{-3}$) quantifies the width of the predictive uncertainty. The degree to which observations are bracketed by the 95CI indicates the degree to which the model and data uncertainties are being accounted for. The maximum value for the coverage is 100%, and ideally we would like to bracket all measured data, except the outliers, in the 95CI. The spread should also be as small as possible.

### 2.4. Model parameterization

In this study, the parameters of SWAP can be categorized into crop parameters and soil hydraulic parameters. The required crop parameters for maize and wheat are presented in Table 2 which were taken from literature (Doorenbos and Kassam, 1979; Wesseling et al., 1991) with some minor adaptations using local observations. The soil hydraulic properties are parameterized using six VGM parameters. It has been shown in recent SWAP model applications that soil hydraulic parameters are the most sensitive parameters (e.g. Ines and Droogers, 2002; Hupet et al., 2003; Jhorar et al., 2004; Singh et al., 2010; Ma et al., 2011). Many studies have revealed that computing the water balance components at the root zone using simulation models is quite sensitive to the soil hydraulic parameters of the soil profile (e.g. Wesseling and Kroes, 1998). Ines and Droogers (2002) analyzed the sensitivity of the six VGM parameters based on actual $ET$ and bottom flux and found that $\theta_r$ and $\lambda$ are non-sensitive parameters. Similar results were also obtained by Singh et al. (2010). Jhorar et al. (2002) found that the actual transpiration is sensitive to all VGM parameters. Hupet et al. (2003) showed that soil water content dynamics is much more sensitive to some hydraulic parameters (i.e. $\theta_s$, $n$, $\alpha$ and $K_s$) than to root water uptake parameter (RWUP) and the relative insensitivity of RWUP was due to relatively high unsaturated hydraulic conductivity values especially for fine-textured soil. On the other hand, the VGM parameters generally should be considered as fitting parameters (e.g. Šimůnek and van Genuchten, 1996; Mertens et al., 2005) since these parameters are generally poorly defined by direct measurements (Schaap and Leij, 2000). As the fitted parameters do not have a strict physical meaning, a possible correlation between them means that many combinations of the parameters could fit the data. Hence, fixing some of the soil hydraulic parameters during the calibration process may unfavorably influence on the estimates of other soil hydraulic parameters. Moreover, the choice of a parameter being fixed is usually rather arbitrary, without consideration of the actual information content of the data (Scharnagl et al., 2011). For example Assouline and Tartakovsky (2001) stated that unsaturated hydraulic conductivity for fine-textured soils is underestimated when $K_s$ in VGM equation is forced to match measured values during parameter estimation. Therefore, in the present study, all six VGM parameters are kept for subsequent parameter estimation and uncertainty analysis.

For the simulation of one-dimensional vertical water flow, a homogeneous soil profile of 200 cm depth is specified for the two study fields. Due to limitations of defining soil hydraulic functions for heterogeneous (layered) soil profiles and to keep the calibration simple, we consider a unique (homogeneous) soil profile for the simulations of soil water balance at the study sites. Moreover, several studies have shown that SWAP simulation results of water balance fluxes are quite similar under the homogeneous and heterogeneous soil layers (Jhorar et al., 2004; Singh et al., 2010). The soil profile is further discretized into 74 non-equidistant nodes (compartments). Nodal distance is shortest at the soil surface and is gradually increased with depth, with a distance of 0.5 cm at the upper and 5 cm at the lower boundary. This particular discretization scheme accommodates large gradients in pressure heads that occur close to the surface in response to atmospheric forcing (Kroes and van Dam, 2003). Furthermore, when the nodal spacing is too large, numerical solution of the Richards' equation becomes inaccurate due to linearization errors of pressure heads and averaging errors of hydraulic conductivity (Van Dam and Feddes, 2000; Downer and Ogden, 2004). It is worth mentioning that in our case study, the amount of ponded water is about 5 cm at the soil surface which was occasionally observed after heavy irrigation practices. So, the PONDMX parameter (maximum thickness of ponding water layer) in SWAP model is set to this value.

**Table 2**
Main crop parameters specified for the SWAP model.

| Parameter | Maize | Winter wheat |
|---|---|---|
| Temperature sum from emergence to anthesis, TSUMEA (°C) | 870.0 | 1300.0 |
| Temperature sum from anthesis to maturity, TSUMAM (°C) | 950.0 | 750.0 |
| Start value of temperature sum (°C) | 10.0 | 2.0 |
| Critical pressure heads, $h$ (cm) | | |
| $h_1$ (no water extraction at higher pressure heads) | −10 | −1 |
| $h_2$ (h below which optimum water uptake starts in the root zone) | −25 | −22.9 |
| $h_{3h}$ (h below which optimum water uptake reduction starts in the root zone in case of high atmospheric demand) | −400 | −1000 |
| $h_{3l}$ (h below which optimum water uptake reduction starts in the root zone in case of low atmospheric demand) | −500 | −2200 |
| $h_4$ (wilting point, no water uptake at lower pressure heads) | −14,000 | −16,000 |

**Table 3**
Mean values and standard deviations of the ROSETTA predicted soil hydraulic parameters.

| Parameter | Unit | Maize field | | Winter wheat field | |
|---|---|---|---|---|---|
| | | Mean | Standard deviation[a] | Mean | Standard deviation[a] |
| $\theta_r$ | $cm^3\,cm^{-3}$ | 0.098 | 0.0130 | 0.095 | 0.0092 |
| $\theta_s$ | $cm^3\,cm^{-3}$ | 0.470 | 0.0140 | 0.460 | 0.0097 |
| $\alpha$ | $cm^{-1}$ | 0.015 | 0.1070 | 0.014 | 0.0770 |
| $n$ | – | 1.320 | 0.0190 | 1.325 | 0.1500 |
| $K_s$ | $cm\,d^{-1}$ | 3.500 | 0.2580 | 3.500 | 0.2520 |
| λ | – | −1.070 | 1.1900 | −0.900 | 1.1300 |

[a] The standard deviation are given in logarithmic scale for $\alpha$, $n$ and $K_s$.

### 2.5. *Defining prior information for soil hydraulic parameters*

Determining soil hydraulic properties by field measurement have some limitations. Several researches have used PTFs or field measurements for defining prior distributions in soil hydraulic parameters estimation (e.g. Mertens et al., 2004), but they mostly applied it on non-arable land. Agricultural management practices in arable land such as our study area, specifically tillage and related management activities, can affect soil hydraulic properties and processes dynamically in space and time (Strudley et al., 2008). Additionally, there are limited PTFs for arable lands (more details can also be found in Sonneveld et al. (2003) and Haghighi et al. (2010)). Thus we chose to consider wide ranges for soil properties as the prior information in our inverse modeling (calibration) and uncertainty analysis. In this study, ROSETTA (Schaap et al., 2001), a numerical code for estimating soil hydraulic parameters with hierarchical pedotransfer functions, is used to define prior information for soil hydraulic parameters (e.g. Scharnagl et al., 2011). In the ROSETTA program, a bootstrap method (Efron and Tibshirani, 1993) is used to obtain independent calibration to different data sets and to calculate confidence intervals of neural network predictions. ROSETTA is used for defining prior information based on measured sand, silt, and clay fractions and bulk density of the topsoil layer (0–60 cm) at the study sites (Table 3). Uniform prior distributions are assigned to the six VGM soil hydraulic parameters. Lower and upper bounds of the estimated parameters ($p$) are specified as $p \pm 4u$, where $u$ denotes the standard deviation (Table 3). These wide prior ranges are physically reasonable. It should be noted that the calibrated soil hydraulic parameters represent *effective* soil properties, values of which cannot often be obtained by direct measurements (Feddes et al., 1993).

## 3. Results and discussion

The aim of uncertainty estimation is to assess the probability of a certain quantity (such as soil moisture in this study) being within a certain interval (Beven, 2001). Thus, by including uncertainty in model parameters, rather than using point estimations, more information about prediction error is available to the policy developers. In the following subsections, the results of the uncertainty analysis for the SWAP model application at the maize and wheat fields are discussed.

### 3.1. *Parameter uncertainty analysis*

Figs. 1 and 2 show the histograms of posterior distribution of parameters derived by the GLUE method for both fields. These histograms are derived from the behavioral solutions of the GLUE method. The posterior distributions represent the uncertainty in the parameters after combining prior information from ROSETTA with the information contained in the observational data, i.e. soil moisture values. Table 4 lists values of GLUE-derived statistical characteristics of the posterior distribution of each parameter.

The shape of the posterior distributions and their statistics (Table 4) are different for the two fields. For example the mean value of $K_s$ posterior of the maize field ($25.5\,cm\,d^{-1}$) is higher than that of the wheat field ($17.5\,cm\,d^{-1}$). Also the mean value of $n$ of the maize field (1.20) is lower than that of the wheat field (1.46). These indicate that although the soil textures of the two fields are similar (clay), their induced posterior parameter distributions are different. This is related to their different structures. In reality, soil structure varies considerably within agricultural fields during the growing season (Roger-Estrade et al., 2000; Strudley et al., 2008). The irrigation depth and its frequency in the two

**Table 4**
Summary statistics of the GLUE-derived parameter distribution ($Max_{LF}$: the parameter set that exhibits the highest value of likelihood, SD: standard deviation of the posterior, CV: coefficient of variation of the posterior).

| | Parameter | Unit | $Max_{LF}$ | Mean | SD | CV (%) |
|---|---|---|---|---|---|---|
| Maize field | $\theta_r$ | $cm^3\,cm^{-3}$ | 0.141 | 0.110 | 0.029 | 26.2 |
| | $\theta_s$ | $cm^3\,cm^{-3}$ | 0.421 | 0.420 | 0.008 | 2.0 |
| | $\alpha$ | $cm^{-1}$ | 0.007 | 0.018 | 0.009 | 47.4 |
| | $n$ | – | 1.270 | 1.201 | 0.060 | 5.0 |
| | $K_s$ | $cm\,d^{-1}$ | 25.20 | 26.10 | 6.943 | 26.6 |
| | λ | – | 3.51 | 0.210 | 0.212 | 101.0 |
| Wheat field | $\theta_r$ | $cm^3\,cm^{-3}$ | 0.077 | 0.086 | 0.020 | 23.8 |
| | $\theta_s$ | $cm^3\,cm^{-3}$ | 0.490 | 0.470 | 0.020 | 4.3 |
| | $\alpha$ | $cm^{-1}$ | 0.019 | 0.020 | 0.005 | 27.2 |
| | $n$ | – | 1.530 | 1.460 | 0.051 | 3.5 |
| | $K_s$ | $cm\,d^{-1}$ | 9.64 | 17.56 | 6.866 | 39.1 |
| | λ | – | −4.19 | −4.100 | 0.718 | 17.5 |

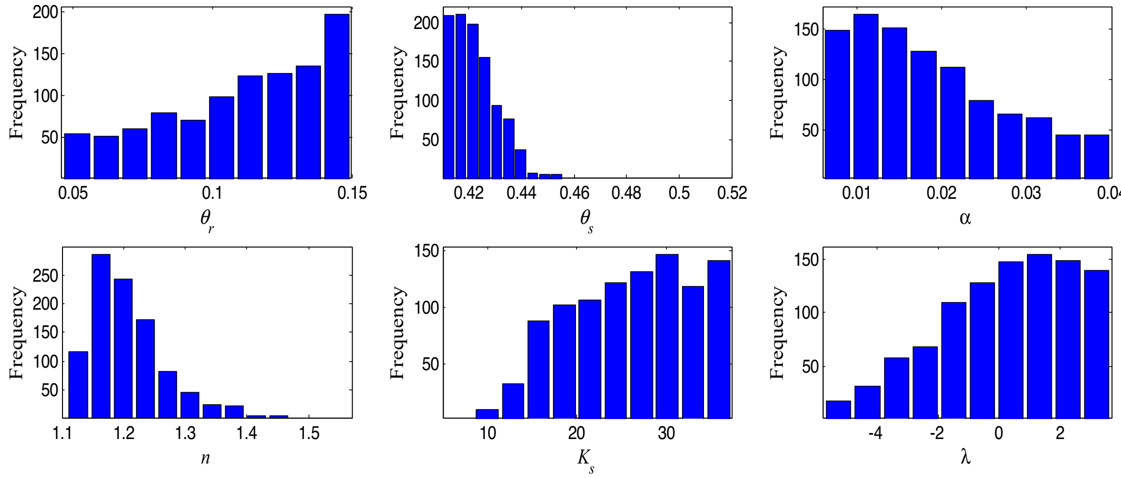


**Fig. 1.** Posterior distributions of soil hydraulic parameters at maize field ($x$-axis of each plot is fixed to the prior range of each parameter).

fields can affect the soil structure by changing its compaction. Furthermore, crop characteristics such as root system development and related management activities also affect the soil structure dynamics. Another affecting factor is the spatial variability of soil physical properties which are inherent within agricultural fields (Iqbal et al., 2005). Additionally, the maximum likelihood (best fit) parameter values (Table 4) are far different from the ROSETTA estimated parameters (Table 3), especially for $K_s$ and $\theta_s$, which suggests that direct use of PTFs estimated soil hydraulic parameters is not warranted.

The posterior distributions of some parameters such as $\theta_s$ and $n$ in maize field and $K_s$ and $\lambda$ in wheat field appear to be more sharply peaked than other parameters. This shows that the measured data contains sufficient information to estimate these parameters with more confidence (less uncertainty left). On the other hand, other parameters in both the fields (such as $\theta_r$ and $\alpha$) did not significantly change from their prior uniform distributions. These parameters tend to concentrate most of their density at their upper or lower bounds. This behavior may represent two types of error which are whether the systematic errors of input (forcing) data or compensating for structural deficiencies in the model (Vrugt et al., 2008a). In this study, the most important input data is the set of irrigation events since the area is arid and receives less amount of rainfall. In addition, as reported by Hupet et al. (2003), there is also a compensating effect in the calibration of SWAP model between the vertical unsaturated water fluxes and the root water uptake (sink term in Richards' equation, Eq. (1)).

In this study we used the coefficient of variation (CV) of the behavioral solutions for each parameter to assess their relative sensitivity. The values of CVs in Table 4 show that some parameters in both fields (such as $\theta_r$, $\alpha$, and $K_s$) have a higher value of CV that confirms low sensitivity to the soil water content dynamics in the study fields. In contrast, $\theta_s$ and $n$ are the most sensitive parameters (lowest value of CV) in the study fields which, in general, has also been confirmed by other investigators (e.g. Ines and Droogers, 2002; Hupet et al., 2003; Singh et al., 2010). The relative sensitivity of $\lambda$ is higher than $K_s$ and $\theta_r$ in the wheat field, while $\theta_r$ is relatively more sensitive than $\alpha$ in the maize field. These results indicate that the sensitivity of soil hydraulic parameters can vary with field conditions. Therefore, as also confirmed by Scharnagl et al. (2011) it is not realistic to fix some of the soil hydraulic parameters during calibration.

In order to provide more insight about parameter identifiability, scatter plots for the likelihood measure (given in Eq. (4)) of the behavioral solutions are shown in Figs. 3 and 4. These plots are the projections of the multidimensional parameter response surface onto single parameter axes (Beven, 2001). The presented scatter plots illustrate that the parameter response surface is rather complex, with many smaller peaks; hence no single optimum parameter set can be determined. This underlines the need to treat

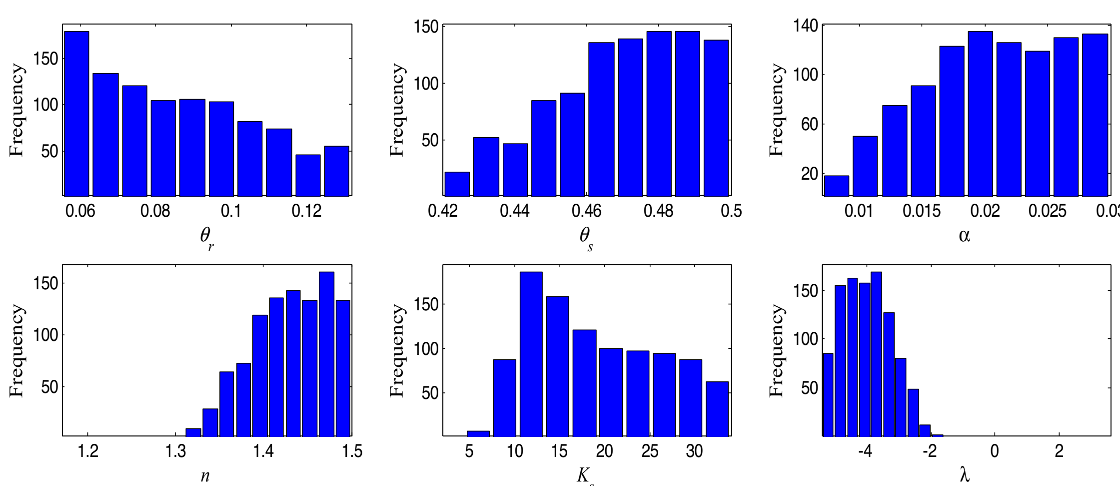


**Fig. 2.** Posterior distributions of soil hydraulic parameters at wheat field ($x$-axis of each plot is fixed to the prior range of each parameter).

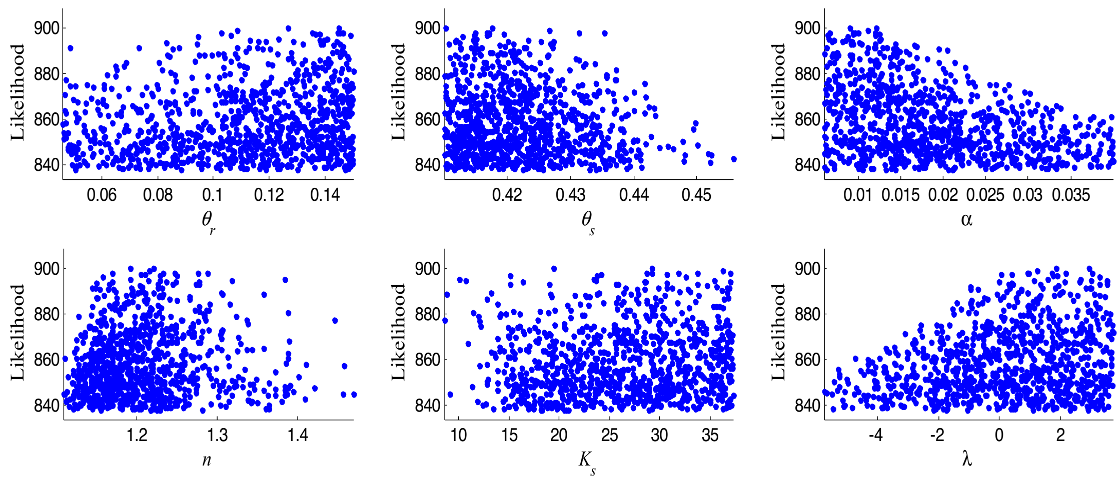


**Fig. 3.** Scatterplots of the likelihood measure versus the SWAP model soil hydraulic parameters at the maize field.

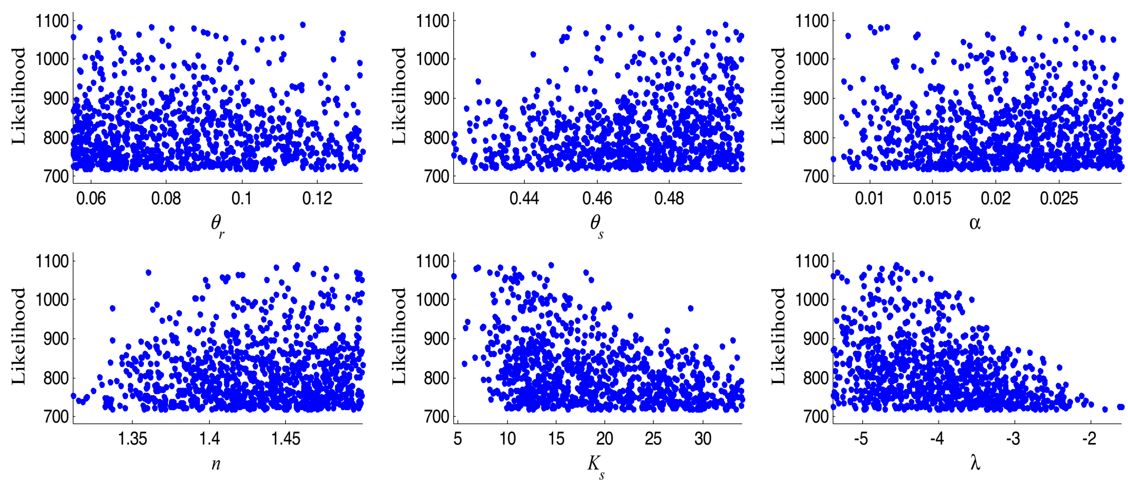


**Fig. 4.** Scatterplots of the likelihood measure versus the SWAP model soil hydraulic parameters at the wheat field.

parameters as sets of values (e.g. Brazier et al., 2000; Dean et al., 2008). Results suggest that $\theta_s$, $\alpha$, $n$, and $\lambda$ in the maize field and $n$, $K_s$ and $\lambda$ in the wheat field are more identifiable. As shown in Figs. 3 and 4, high probability parametric ranges can be specified for identifiable parameters that correspond to high likelihood values or low uncertainty levels. The ranges for maize field are: $\theta_s$ [0.41, 0.43] $cm^3\,cm^{-3}$, $\alpha$ [0.007, 0.014] $cm^{-1}$, $n$ [1.18, 1.28], $\lambda$ [0.1, 3.0] and for wheat field: $\theta_s$ [0.45, 0.48] $cm^3\,cm^{-3}$, $n$ [1.44, 1.50], $K_s$ [8,14] $cm\,d^{-1}$, $\lambda$ [−5.6, −4.2]. It worth mentioning that non-identifiability of some parameters may not indicate that the model is insensitive to those parameters. For example, $\theta_s$ in the wheat fields is a sensitive parameter but it is not well identifiable. Then this confirms that the poor identifiability of some sensitive parameters may be related to the inverse problem formulation (Arkesteijn and Pande, 2013).

### 3.2. Output uncertainty analysis

To determine how the uncertainty in soil hydraulic parameters translates into SWAP soil moisture predictive uncertainty, we study Figs. 5 and 6 that present soil moisture predictions for the two fields at three different depths of the soil profile. The degree of uncertainty in soil moisture predictions is expressed by 95CI (the shaded region), which is derived by sorting the behavioral solutions (step 6 in Section 2.3) and then considering the parameter sets within 2.5 and 97.5 percentile range. The uncertainty measures of 'coverage' and 'spread' are also shown in Table 5. It is clear that most of the measured values are bracketed by the 95CI in both the fields. The spread of 95CI is relatively thin, indicating good model performance. The measurements that are lying outside the 95CI either may be outliers or may be attributed to model structural inadequacy. The results presented in Figs. 5 and 6 and also in Table 5 highlight several interesting observations: (1) predictive uncertainties for different soil depths in each field are almost the same (note the spreads in Table 5). It is anticipated, however, because of the soil profile homogeneity assumption. (2) The uncertainty (the band thickness in Figs. 5 and 6) ranges at higher soil moisture values are mostly smaller than the ranges at lower soil moisture values. As soil moisture decreases, uncertainty increases possibly due to several influencing factors: (i) flow phenomena get

**Table 5**
Uncertainty measures for the two fields at different soil depth layers.

| | Soil depth (cm) | Coverage (%) | Spread ($cm^3\,cm^{-3}$) |
|---|---|---|---|
| Maize field | 0–15 | 80 | 0.037 |
| | 15–30 | 80 | 0.035 |
| | 30–60 | 60 | 0.034 |
| Wheat field | 0–15 | 100 | 0.054 |
| | 15–30 | 100 | 0.054 |
| | 30–60 | 90 | 0.056 |

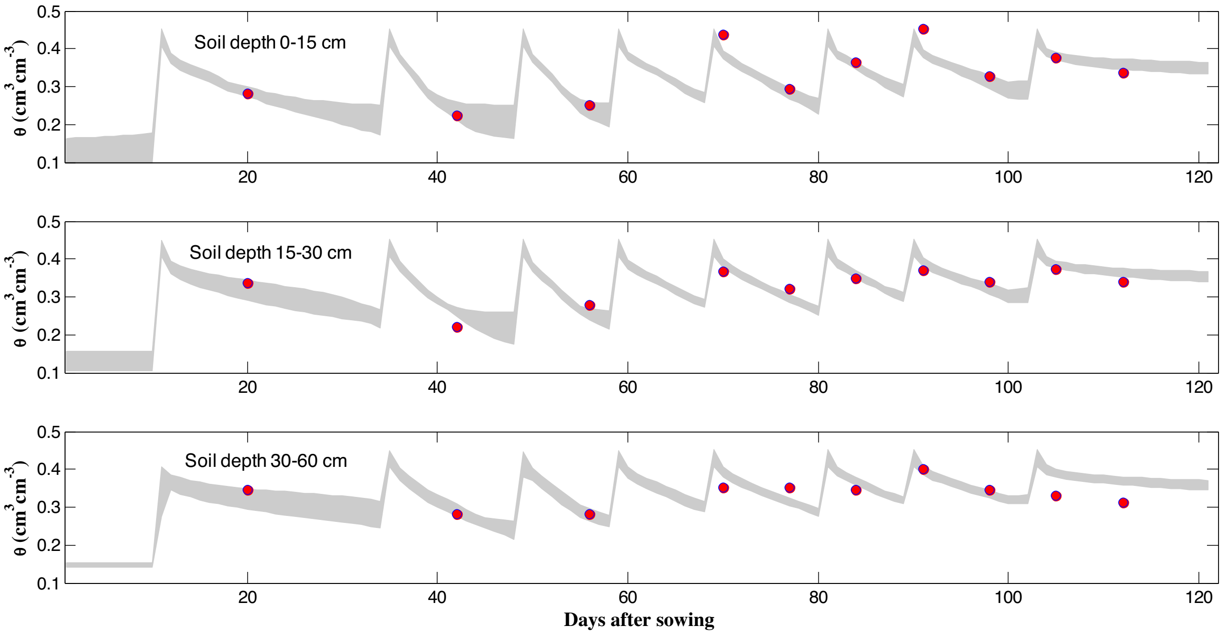


**Fig. 5.** Predictive uncertainty for simulated (in gray band) and measured (in red circle) soil moisture at maize field for different soil depth layers.

more complex as heat transfer, vapor flow, solute transport, and other related phenomena significantly influence water flow (Celia et al., 1995). (ii) Richards' equation – a special case of two-phase flow neglecting the non-wetting phase flow equation – becomes less valid and simultaneous flow of water and air in soil needs to be taken into account (Nitao and Bear, 1996; Tuller et al., 1999). (iii) Hydraulic models that assume the soil pore space as a bundle of cylindrical capillaries (e.g. VGM model) become less valid as the contribution of adsorptive surface forces and liquid films, neglected by these models, become more dominant (Tuller et al., 1999). (3) The predictive uncertainty in the wheat field is higher than maize field, one probable reason may be that the wheat growing season is longer than that of maize. The wheat field received higher amounts of rainfall than the maize field (33 mm vs. 0 mm), hence the wheat field study has one more source of input (forcing) uncertainty that may have resulted in higher predictive uncertainty.

Equifinality is another feature of model calibration presented here. As an example, Table 6 shows three parameter sets at the maize and wheat fields that yield the same performance measures (root mean square errors, RMSE). The so called equifinality, as defined by Beven (2006), is the inability to meaningfully distinguish one single "best" parameter set given inherent uncertainties and errors in available data and model structures and typical over-parameterization of model structures. Some authors have suggested equifinality can be reduced and the parameter identifiability can be improved by defining informative prior distribution of soil hydraulic parameters (Mertens et al., 2005; Scharnagl et al., 2011). Scharnagl et al. (2011) proposed an approach to provide

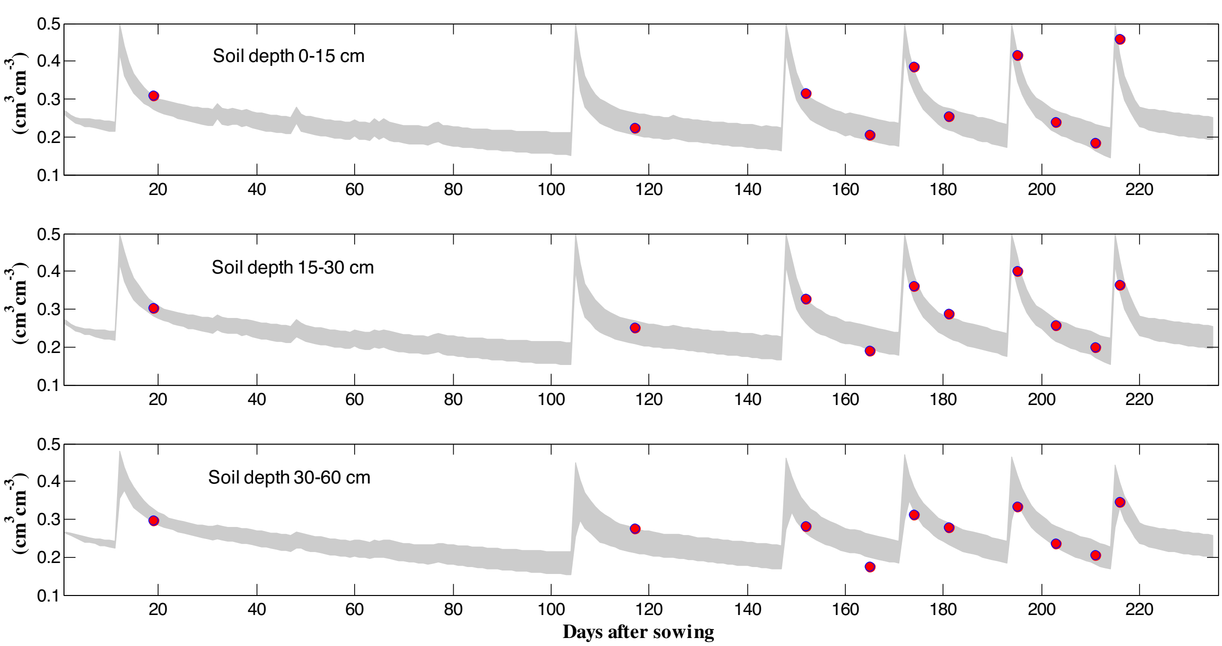


**Fig. 6.** Predictive uncertainty for simulated (in gray band) and measured (in red circle) soil moisture at wheat field for different soil depth layers.

**Table 6**
The equifinality in soil moisture simulations of SWAP model application.

| Parameter | Unit | Maize field | | | Wheat field | | |
|---|---|---|---|---|---|---|---|
| | | Parameter set 1 | Parameter set 2 | Parameter set 3 | Parameter set 1 | Parameter set 2 | Parameter set 3 |
| $\theta_r$ | $cm^3\,cm^{-3}$ | 0.125 | 0.138 | 0.148 | 0.089 | 0.078 | 0.092 |
| $\theta_s$ | $cm^3\,cm^{-3}$ | 0.412 | 0.416 | 0.428 | 0.462 | 0.491 | 0.491 |
| $\alpha$ | $cm^{-1}$ | 0.010 | 0.008 | 0.009 | 0.017 | 0.028 | 0.029 |
| $n$ | – | 1.186 | 1.312 | 1.264 | 1.490 | 1.416 | 1.398 |
| $K_s$ | $cm\,d^{-1}$ | 32.72 | 12.32 | 29.43 | 9.03 | 13.90 | 15.69 |
| $\lambda$ | – | 1.800 | 3.005 | 2.988 | −4.256 | −4.766 | −5.060 |
| RMSE | $cm^3\,cm^{-3}$ | 0.03202 | 0.03202 | 0.03202 | 0.02863 | 0.02864 | 0.02864 |

**Table 7**
The statistical characteristics of water balance fluxes for the two fields.

| | | $ET_a$ (mm/growing season)[a] | $Q_b$ (mm/growing season) |
|---|---|---|---|
| Maize field | Min | 599.7 | −233.6 |
| | Max | 749.1 | −105.5 |
| | Mean | 676.1 | −162.8 |
| | SD | 25.7 | 26.5 |
| | CV (%) | 3.8 | 16.3 |
| Wheat field | Min | 567.0 | −642.1 |
| | Max | 585.7 | −508.0 |
| | Mean | 576.6 | −552.9 |
| | SD | 3.8 | 23.5 |
| | CV (%) | 0.5 | 4.2 |

[a] Total amount of irrigation plus rainfall for maize and wheat were 1280 mm and 1350 mm, respectively. Total potential evapotranspiration are 1054 mm and 1018 mm.

prior distribution for soil hydraulic parameters that incorporates information on parameter correlation. We applied this approach (data not shown) but it proved unsuccessful. It may be due to different field conditions (agricultural fields) and high temporal variability of soil structure as discussed in the previous section. The improvement of the parameter identifiability (or decreasing the model equifinality) mainly depends on how the model structure interacts with each response, and less on the amount of observational data itself (Kuczera and Mroczkowski, 1998). There are some techniques for decreasing equifinality by adopting additional information, such as complementary measured data (Wagener et al., 2003; Fenicia et al., 2008) and using the scaled forms of Richards' equation which is soil-independent (e.g. Sadeghi et al., 2012a, 2012b) for achieving a better insight to the highly non-linear equation of Richards. However, such enough additional data was not available for the investigation undertaken here.

### 3.3. Assessment of the water balance fluxes

For irrigated agricultural fields in dry regions with a deep groundwater table, the components of root zone water balance are irrigation, rainfall, actual evapotranspiration ($ET_a$) and deep percolation ($Q_b$). Agro-hydrological models are usually used to simulate the soil water balance fluxes ($ET_a$ and $Q_b$) for analyzing water management scenarios (e.g. Nemes et al., 2006; Karimi et al., 2012) and increasing crop water productivity (e.g. Vazifedoust et al., 2008; Chen et al., 2010) in agricultural fields. In this study, since the SWAP model is calibrated based on soil moisture measurement data, it is interesting to analyze the effect of posterior parameters on the variation in soil water balance fluxes at field scale. This reveals the risk of using the calibrated model for flux prediction. Table 7 shows the statistical characteristics of the simulated soil water balance fluxes. Since the prediction of $ET_a$ may be much more accurate and reliable than that of the separate prediction of $E_a$ and $T_a$ (Jhorar et al., 2004), the values of $ET_a$ are shown in Table 6. It is notable that the posterior distributions of VGM soil hydraulic parameters, obtained based on soil moisture measurements, reflect all sources of uncertainty. The standard deviations (SD) in Table 7 display the impact of uncertainty in estimating soil moisture on the fluxes for maize and wheat fields. The simulation of $Q_b$ at the maize field appears to be more uncertain (larger CV) than at the wheat field. A reason behind it may be due to the effect of non-identifiability of $K_s$ in the maize field (Fig. 3) compared to the wheat field (Fig. 4). Such non-identifiability in $K_s$ translates into much uncertainty in $Q_b$ simulation. Since a unit hydraulic gradient (free drainage) condition was used at the bottom boundary of the soil profile in the two fields, thus $Q_b$ is only related to the hydraulic conductivity function ($K(\theta)$ in Eq. (2)) of the lowest compartment and because of high amount of percolation at saturation (or near saturation) condition the $K_s$ plays the major contribution in $Q_b$ simulation. In contrast to $Q_b$, the $ET_a$ fluxes are less uncertain because this flux is sensitive to all VGM parameters (Jhorar et al., 2002). Hence, the compensating effect of different parameters and/or different parameter combinations does not lead to higher uncertainty as compared to $Q_b$. Another reason may be that under full irrigation the $ET_a$ rate is generally close to the potential rate. Hence, in this situation the soil hydraulic parameters may have minor effects on the $ET_a$ flux, as also indicated by Baroni et al. (2010). Therefore, there is a high degree of SWAP model reliability in predicting $ET_a$ in irrigated agricultural fields in dry regions. Our results confirm that the hydrological behavior of the fitted soil hydraulic parameters have different effects on different soil water fluxes. Although, there are no flux measurements available for the study area, the results show that the calibration and uncertainty analysis of agro-hydrological models at field scale is complicated because of often uncertain boundary conditions, interaction between crop growth and the environment, and high rate of temporal and spatial variability in the root zone of soil profile.

## 4. Conclusions

It is generally accepted that uncertainty analysis should be included as part of model calibration and implementation. The knowledge of model uncertainty is crucial for interpretation of model results and reliable model predictions. This along with estimates of associated uncertainties can provide decision makers with useful information that allows them to incorporate risk in policy development for water management in agriculture. In this paper, we investigated the soil hydraulic parametric uncertainty and SWAP model predictive uncertainty within the GLUE framework for two agricultural fields located in a dry region. Results presented in this study showed that different boundary conditions, crop characteristics and model structure simplifications (such as homogenous soil profile assumption and the spatial and temporal variability of soil hydraulic parameter) can lead to quite different simulated soil moisture dynamics and parameter estimation at field scale. Moreover, results indicated that only a few parameters were distinguishable and non-identifiable parameters led to model equifinality. It is recommended to use complimentary information about the agricultural fields, such as water balance fluxes measurement and individual crop characteristics to achieve more precise ranges for parameters.

Another objective of this study was to assess the distributions of water balance fluxes when SWAP model is calibrated based solely on the soil moisture measurements. According to the results, it is concluded that in dry regions where agricultural fields are frequently irrigated, the precision in predicting actual evapotranspiration is rather high and a high degree of SWAP model reliability is achieved. However, the precision in estimating deep percolation was lower than that of actual evapotranspiration.

This study focused on SWAP model (with a simple crop module) calibration and output uncertainty. We envisage future study with SWAP-WOFOST (i.e. with a detailed crop module) model which is also capable of simulating water and salt limited crop yields.

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