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Estimation of soil properties using observations and the crop model STICS. Interest of global sensitivity analysis and impact on the prediction of agro-environmental variables

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1. Introduction

Dynamic crop models are very useful to predict the behaviour of crops in their environment and are widely used in a lot of agro-environmental work such as crop monitoring, yield prediction or decision making for cultural practices (Batchelor et al., 2002; Gabrielle et al., 2002; Houlès et al., 2004). These models usually have many parameters and their estimation is a major problem for agro-environmental prediction (Tremblay and Wallach, 2004; Makowski et al., 2006). For spatial application, the knowledge of soil parameters is crucial since they are responsible for a major part of the variability of the crop model output variables of interest (Irmak et al., 2001; Launay and Guérif, 2003; Ferreyra et al., 2006). These parameters may be estimated from different techniques: either with soil analysis at the different points of the study area, from a soil map and the application of pedotransfer functions (Reynolds et al., 2000; Murphy et al., 2003), from remote sensing images (Lagacherie et al., 2008) or by using electrical resistivity measurements (Golovko and Pozdnyakov, 2007). The choice of the first method is difficult because of practical limitations, as well as time and financial constraints. Detailed soil maps adapted to the scale of precision agriculture and even to the scale of catchment are scarcely available (King et al., 1994), while the use of remote sensing images or electrical resistivity is still hampered by a lack of robust interpretation of the signal (Lagacherie et al., 2008). Moreover, these techniques do not permit to access the values of all the soil parameters required to apply a complex crop model. Fortunately, techniques derived from remote sensing images (Weiss and Baret, 1999; Houborg and Boegh, 2008) or yield monitoring (Blackmore and Moore, 1999; Pierce et al., 1999) allow soil parameters being estimated through the inversion of crop models.
Estimating parameters of complex models such as crop models may be not so easy (Tremblay and Wallach, 2004; Launay and Guérif, 2005). One of the reasons for the difficulties encountered may be a lack of sensitivity of the observed variables to the parameters, making the estimation process inefficient. Another reason may be that the influence of the parameters on the observed variables takes place mainly through

interactions, making it difficult to identify the relevant factors (Saltelli et al., 2000). For complex non-linear models such as crop models, global sensitivity analysis (GSA) methods are able to give relevant information on the sensitivity of model outputs to the whole range of variation of model inputs. Many studies have focused on this subject, namely, how to choose the main parameters to be estimated for the model calibration (Campolongo and Saltelli, 1997; Ruget et al., 2002; Gomez-Delgado and Tarantola, 2006; Makowski et al., 2006) and ranked the importance of the parameters by calculating global sensitivity indices: first-order indices (the main effect of the parameter on the output) and total indices (sum of all effects involving the parameter, including the interactions with other parameters). The common practice is consistent with the principles expressed by Ratto et al. (2007). Small total sensitivity indices indicate a negligible effect of the parameter on the model output concerned. These parameters can be fixed at a nominal value ("Factor Fixing setting"). High first-order indices reveal a clearly identifiable influence of the parameter on the model output concerned, and therefore the parameters need to be determined accurately ("Factor Prioritization setting"). Small first-order indices combined with large interaction indices result in a lack of identification. In practice, the two first rules are commonly used to select the set of parameters to be estimated in a calibration problem. GSA can also be used to evaluate the quantity of information contained in a given set of observations for estimating parameters and thus to determine which is the best observation set for estimating the parameters (Kontoravdi et al., 2005). Although the results of GSA are often used to design the estimation process, the link between GSA indices and the quality of parameter estimation has never been quantified.

Our objectives in this study are twofold. Firstly, we propose to use GSA results in order to measure the quantity of information contained in different sets of observations and to illustrate the link between this measurement and the quality of parameter estimates. Secondly, we propose to study the impact of the quality of parameter estimates on the prediction of variables of interest for agro-environmental work. As the performance of the estimation process is supposed to depend on several conditions such as soil type, cropping conditions (preceding crop and climate) or available observations, we chose to conduct the study on synthetic observations in order to be able to generate variability in parameter retrieval performance as well as in sensitivity structure of the observed model outputs to soil parameters and in the prediction performance. This choice also allows eliminating the impact of model errors, which may complicate the interpretation of the results. Finally, we considered in this study the STICS-wheat crop model and various synthetic observations on wheat crops: derived from remote sensing images (LAI and absorbed nitrogen) as well as grain yield.

2. Material and methods

2.1 The crop model, output variables and soil parameters

2.1.1 The STICS model

The STICS model (Brisson et al., 2002) is a nonlinear dynamic crop model simulating the growth of various crops. For a given crop, STICS takes into account the climate, type of soil and cropping techniques to simulate the carbon, water and nitrogen balances of the crop-soil system on a daily time scale. In this study, a wheat crop is simulated. The crop is

essentially characterized by its above-ground biomass carbon and nitrogen, and leaf area index. The main outputs are agronomic variables (yield, grain protein content) as well as environmental variables (water and nitrate leaching). Yield, grain protein content and nitrogen balance in the soil at harvest are of particular interest for decision making, especially for monitoring nitrogen fertilization (Houlès et al., 2004). Nitrogen absorbed by the plant and leaf area index are also important to analyze the health and growth of the plant during the crop's growing season.
The STICS model includes more than 200 parameters arranged in three main groups: those related to the soil, those related to the characteristics of the plant or to the genotype, and those describing the cropping techniques. The values of the last group of parameters are usually known as they correspond to the farmer's decisions. The parameters related to the plant are generally determined either from literature, from experiments conducted on specific processes included in the model (e.g. mineralization rate, critical nitrogen dilution curve etc.) or from calibrations based on large experimental database, as is the case for the STICS model (Hadria et al., 2007). The soil parameters are difficult to determine at each point of interest and are responsible for a large part of the spatial variability of the output variable. That is why the sensitivity analysis and parameter estimation processes described in this study only concern soil parameters.

2.1.2 Output variables considered

In this study, we focus on two types of STICS output variables. First, those corresponding with observations that may be done on wheat canopy by automated measurements. They consist in:
- the leaf area index (LAI_t) and the nitrogen absorbed by the plant (QN_t) at various dates t during the crop season - as potentially derived from remote sensing image inversion (Weiss and Baret, 1999; Houborg and Boegh, 2008),
- the yield at harvest (*Yld*) as potentially provided by yield monitoring systems.

These output variables, hereafter referred to as "observable variables" can be observed at different dates during the growing season.
Second, a main objective of this study, beyond the estimation of soil parameter values, lies in the prediction of some output variables of interest, and its improvement as compared to the prediction obtained with a lack of precise values on soil parameters. They consist in:
- yield at harvest (*Yld*),
- protein in the grain at harvest (*Prot*),
- nitrogen contain in the soil at harvest (*Nit*).

Yield, grain protein content and nitrogen balance in the soil at harvest are of particular interest for decision making, especially for monitoring nitrogen fertilization (Houlès et al., 2004). Nitrogen absorbed by the plant are also important to analyze the health and growth of the plant during the crop's growing season (Baret et al., 2006).

2.1.3 The soil parameters estimated

The STICS model contains about 60 soil parameters. In our case, in order to limit the problems of identifiability, the number of soil parameters to be estimated has been reduced. First, among the available options for simulating the soil system, the simplest was chosen, by ignoring capillary rise and nitrification. These assumptions define the domain of validity of the model considered and hence, of the results that are found. We then considered the soil as a succession of two horizontal layers, each characterized by a specific thickness parameter. From the observation of the tillage practices in the region around our experimental site of Chambry (49.35°N, 3.37°E) (Guérif et al., 2001), the thickness of the first layer was set at 0.30 m. We performed a first sensitivity analysis on the 13 resulting soil parameters. This allowed us to fix those whose effects on the observed variables were negligible: for each parameter we computed the values of its effects on all the observed variables considered for a lot of soil, climate and agronomic conditions, and dropped the parameters for which all these values were less than 10% of the total effects generated by the 13 parameters. We thus restricted the study to 7 parameters.

The 7 soil parameters considered (Table 1) characterize both water and nitrogen processes. They refer to permanent characteristics and initial conditions. Among the permanent characteristics, clay and organic nitrogen content of the top layer are involved mainly in organic matter decomposition processes and nitrogen cycle in the soil. Water content at field capacity of both layers affects the water (and nitrogen) movements and storage in the soil reservoir. Finally, the thickness of the second layer defines the volume of the reservoir. The initial conditions correspond to the water and nitrogen content, *Hinit* and *NO3init*, at the beginning of the simulation, in this case the sowing date.

Parameter	Definition	Range	Unit
argi	Clay content of the 1rst layer	14-37	%
Norg	Organic nitrogen content of the 1rst layer	0.049-0.131	%
epc(2)	Thickness of the 2nd layer	0-70 or 50-130*	cm
HCC(1)	Water content at field capacity (1rst layer)	14-30	g g-1
HCC(2)	Water content at field capacity (2nd layer)	14-30	g g-1
Hinit	Initial water content (both layers)	4-29	% of weight
NO3init	Initial mineral nitrogen content (1rst layer)	4-21.5 or 25-86**	kg N ha-1

* the first range is for a shallow soil and the second for a deep soil; ** the first range is for a wheat cultivated after sugar beet and the second for a wheat cultivated after pea

Table 1. The 7 soil parameters and ranges of variation.

2.2 Global sensitivity analysis

In this study, we chose a variance-based method of global sensitivity analysis which allows calculating the sensitivity indices for a non-linear model such as STICS. More precisely, the method we chose is Extended FAST.

2.2.1 Variance decomposition and sensitivity indices

We denote a given output variable of the STICS model as Y. The total variance of Y, $V(Y)$, caused by variation in the 7 selected soil parameters θ, can be partitioned as follows (Chan et al., 2000):

$$V(Y) = \sum_{i=1}^{7} V_i + \sum_{1 \le i < j \le 7} V_{ij} + \cdots + V_{1,2,\cdots,7} \quad (1)$$

where $V_i = V\left[E\left(Y|\theta_i\right)\right]$ measures the main effect of the parameter θ_i, $i = 1,\cdots,7$, and the other terms measure the interaction effects. Decomposition (2) is used to derive two types of sensitivity indices defined by:

$$S_i = \frac{V_i}{V(Y)} \quad (2)$$

$$ST_i = \frac{V(Y) - V_{-i}}{V(Y)} \quad (3)$$

where V_{-i} is the sum of all the variance terms that do not include the index *i*.

S_i is the first-order (or main) sensitivity index for the i^{th} parameter. It computes the fraction of *Y* variance explained by the uncertainty of parameter θ_i and represents the main effect of this parameter on the output variable *Y*.

ST_i is the total sensitivity index for the i^{th} parameter and is the sum of all effects (first and higher order) involving the parameter θ_i.

S_i and ST_i are both in the range (0, 1), low values indicating negligible effects, and values close to 1 huge effects. ST_i takes into account both S_i and the interactions between the i^{th} parameter and the 6 other parameters, interactions which can therefore be assessed by the difference between ST_i and S_i. The interaction terms of a set of parameters represent the fraction of *Y* variance induced by the variance of these parameters but that cannot be explained by the sum of their main effects. The two sensitivity indices S_i and ST_i are equal if the effect of the i^{th} parameter on the model output is independent of the values of the other parameters: in this case, there is no interaction between this parameter and the others and the model is said to be additive with respect to θ_i.

2.2.2 Extended FAST

Sobol's method and Fourier Amplitude Sensitivity Test (FAST) are two of the most widely used methods to compute S_i and ST_i (Chan et al., 2000). We have chosen here to use the extended FAST (EFAST) method, which has been proved, in several studies (Saltelli and Bolado, 1998; Saltelli et al., 1999; Makowski et al., 2006), to be more efficient in terms of number of model evaluations than Sobol's method. The main difficulty in evaluating the first-order and total sensitivity indices is that they require the computation of high dimensional integrals. The EFAST algorithm performs a judicious deterministic sampling to explore the parameter space which makes it possible to reduce these integrals to one-dimensional ones using Fourier decompositions. The reader interested in a detailed description of EFAST can refer to (Saltelli et al., 1999).

We have implemented the EFAST method in the Matlab® software, as well as a specific tool for computing and easily handling numerous STICS simulations. The uncertainties considered for the soil parameters are assumed independent and follow uniform distributions. These uncertainties are based to the measurements made in Chambry and correspond to the ranges of variation presented in Tab. 1. A preliminary study of the convergence of the sensitivity indices allowed us to set the number of simulations per parameter to 2000, leading to a total number of model runs of 7×2 000=14 000 to compute the main and total effects for all output variables and parameters considered here. One run of the STICS model taking about 1s with a Pentium 4, 2.9 GHz processor, the overall simulation process takes about 4h.

2.2.3 Criteria based on GSA indices

GSA provides main and total indices per parameter for each output variable considered. In order to summarize this information, we propose to create different criteria.
(i) The first one is a global measure of the information contained in a set of observations to estimate each parameter:
The Global Mean Sensitivity (GMS_i) computes the mean of the main effect of parameter θ_i minus its interactions with the other parameters for all observed variables, each component being weighted by the degree of dependence of the corresponding output variable with the other variables:

$$GMS_i = \frac{1}{K}\sum_{k=1}^{K}(1-\alpha_k)(S_i^k - R_i^k) \quad (4)$$

where k is a given observed output variable in a subset composed of K variables among {LAI_t, QN_t, t=1,…,T and Yld}, $R_i^k = ST_i^k - S_i^k$ is the sum of all interaction terms including parameter θ_i for the observed variable k, $0 \le \alpha_k \le 1$ is the mean of the absolute values of the correlation coefficients $|r_{kk'}|$ between the variable k and the other variables k' (calculated on the model simulations required for GSA): $\alpha_k = \frac{1}{K-1}\sum_{k'\neq k}|r_{kk'}|$, K>1.

The GMS_i criterion is based on the following rules:
- if ST_i is low (and thus S_i), observation k is assumed not to contain enough information to estimate parameter θ_i: in this case the corresponding part of the criteria should be low,
- if S_i is high (and thus ST_i), observation k is assumed to contain sufficient information to estimate parameter θ_i: in this case the corresponding part of the criteria should be high,
- if S_i is low and ST_i is high, then the model is over-parameterized and difficulties in identifying parameter θ_i are expected (Ratto et al., 2007): in this case the corresponding part of the criteria should be low,
- high correlation between output variables indicates that the information contents of these variables are redundant: in this case the weights of the corresponding sensitivity indices should be reduced.

GMS_i varies within the range [-1, 1]. It tends to 1 when S_i is close to 1 for all observed variables and when all the observed variables are perfectly uncorrelated: in this case the model has an additive structure for the parameter θ_i and this parameter has a clearly identifiable influence on the K observed variables. GMS_i tends to -1 when S_i and R_i^k are close to 0 and 1 respectively for all observed variables and when all the observed variables are perfectly uncorrelated: in this case problems of identification of the parameter θ_i are expected.
(ii) The second criterion is calculated at the whole parameter set level.
The Total Global Mean Sensitivity (*TGMS*), is the sum of the GMS_i for all parameters:

$$TGMS = \sum_{i=1}^{7} GMS_i = \sum_{i=1}^{7} \frac{1}{K} \sum_{k=1}^{K} (1-\alpha_k)(S_i^k - R_i^k) \tag{5}$$

The *TGMS* criterion varies within the range [-7, 1]. It tends to 1 when R_i^k is close to 0 for all parameters and all observed variables and when all the observed variables are perfectly uncorrelated: in this case the model is additive. *TGMS* tends to -7 when R_i^k is close to 1 for all parameters and all observed variables and when all the observed variables are perfectly uncorrelated: in this case the model is expected to be unidentifiable.

2.3 Parameter estimation

We chose a bayesian method which allow to take into account existing information on the parameters to be estimated (this improves the quality of the estimation process) and to compute an estimate of the posterior probability distribution of parameter values (Makowski et al., 2002; Gaucherel et al., 2008). More precisely, the method we chose is Importance Sampling.

2.3.1 The Importance Sampling method

The posterior parameter distribution is given by Bayes' theorem:

$$\pi(\theta / Y) = \frac{\pi(Y/\theta)\pi(\theta)}{\pi(Z)} \tag{6}$$

where Y is the vector of total observations of size K, $\pi(\theta / Y)$ is the posterior parameter distribution, $\pi(\theta)$ is the prior parameter distribution, $\pi(Y)$ is a constant of proportionality determined by the requirement that the integral of $\pi(\theta / Y)$ over the parameter space equals 1, and $\pi(Y/\theta)$ is the likelihood function. The likelihood is the probability of the data Y given the parameters θ. Its value is determined from the probability distribution of the errors of modelled and observed data. It is readily seen that both the prior distribution and the new data affect the posterior parameter distribution.

The principle of the Importance Sampling method (Beven and Binley, 1992; Beven and Freer, 2001) is to approximate the posterior parameter distribution $\pi(\theta / Y)$ given in (7) by a discrete probability distribution (θ_n, p_n), *n=1,...,N*, $\sum_{n=1}^{N} p_n = 1$, where p_n is the probability associated with the parameter vector θ_n. In our case, the method proceeds as follows:

(1) Randomly generate *N* vectors θ_n, *n=1,...,N*, from the prior parameter distribution $\pi(\theta)$,

(2) Calculate the likelihood values $\pi(Y/\theta_n)$ for *n=1,...,N*, associated with the different generated parameter vectors,

(3) Calculate $p_n = \dfrac{\pi(Y/\theta_n)}{\sum_{m=1}^{N} \pi(Y/\theta_m)}$

The pairs (θ_n, p_n), *n=1,...,N*, can be used to determine various characteristics of the posterior distribution, including the mean of the posterior joint distribution of θ, $\overline{\theta}^{post} = \sum_{n=1}^{N} p_n \theta_n$.

In this study, we assume that the errors of simulated and observed data are independent between dates and variables and follow normal distributions of zero mean and standard deviation σ_k. Thus, we use the following likelihood function:

$$\pi(Y/\theta) = \prod_{k=1}^{K} \frac{1}{\sqrt{2\pi\sigma_k^2}} \exp\left\{ -\frac{1}{2\sigma_k^2} \left[y_k - f_k(\theta, x) \right]^2 \right\} \tag{7}$$

The parameters are assumed to be independent in our case. The prior distribution $\pi(\theta)$ is thus the product of the different marginal prior distributions. Accordingly to the distributions based on the experimental fields of Chambry we assumed them to be uniform and correspond to the uncertainties given in Tab. 1.

We have implemented the Importance Sampling method in the Matlab® software. A preliminary study of the convergence of the estimates allowed us to set the total number of generated parameter vectors *N* at 100 000.

2.3.2 Criterion expressing the quality of parameter estimation

(i) For each parameter, we created a criterion noted RE_i (for Relative Error of the parameter *i*), to quantify the quality of the parameter estimation. It computes the ratio between the error of the estimated parameter $\overline{\theta}_i^{post}$ and the error of the prior information $\overline{\theta}_i^{prior}$:

$$RE_i = \frac{RMSE(\overline{\theta}_i^{post})}{RMSE(\overline{\theta}_i^{prior})} \tag{8}$$

where $RMSE(\overline{\theta}_i^{post}) = \sqrt{\frac{1}{P}\sum_{p=1}^{P}\left(\theta_{i,p}^{true} - \overline{\theta}_{i,p}^{post}\right)^2}$, $\theta_{i,p}^{true}$ is the true value of soil parameter θ_i for a given vector p and $\overline{\theta}_{i,p}^{post}$ is the corresponding estimation given by the Bayesian method. RE_i quantify how much the estimation given by the Bayesian method improves (RE_i<1) or not (RE_i≥1) the prior knowledge about the parameter value.
(ii) For all parameters, the criterion called Total Relative Error (*TRE*), is defined by the mean of the 7 values of RE_i:

$$TRE = \frac{1}{7}\sum_{i=1}^{7} RE_i = \frac{1}{7}\sum_{i=1}^{7}\frac{RMSE(\overline{\theta}_i^{post})}{RMSE(\overline{\theta}_i^{prior})} \tag{9}$$

2.3.3 Criterion expressing the quality of prediction

We created a criterion to quantify the quality of the prediction of the 3 agro-environmental variables defined above. This criterion computes the ratio between the error of prediction obtained from the mean of the posterior distributions of the parameters, $\overline{\theta}^{post}$ and the one obtained from the mean of the prior distributions, $\overline{\theta}^{prior}$. It is called Relative Error of Prediction and is defined as follows:

$$REP_j = \frac{RMSEP_j(\overline{\theta}^{post})}{RMSEP_j(\overline{\theta}^{prior})} \tag{10}$$

where $RMSEP_j(\overline{\theta}^{post}) = \sqrt{\frac{1}{P \times Q_j}\sum_{p=1}^{P}\sum_{q=1}^{Q_j}\left(f_j^q(\theta_p^{true}) - f_j^q(\overline{\theta}_p^{post})\right)^2}$, θ_p^{true} is the true values of soil parameters θ for a given vector p, $\overline{\theta}_p^{post}$ is the corresponding estimation given by the Importance Sampling method, and $f_j^q(\theta_p^{true})$ is assumed to be one of the Q_j observations of the predicted variable j, for the p^{th} vector of true values of soil parameters.

2.4 Numerical experiments

2.4.1 Generation of observations for parameter estimation

The STICS model output variables depend on the soil, climate and agronomic conditions for which the wheat crop is simulated. In view of this, we use different configurations in our study, as presented in Table 2: 4 contrasting climates, 2 different soil depths (shallow and deep), and 2 preceding crops (sugar beet and peas). The climatic data used were obtained from the meteorological station of Roupy (49.48°N, 3.11°E). Four different sets of data were chosen to characterize a dry climate (1975-1976), a wet climate (1990-1991), a medium-dry climate (1979-1980) and a medium-wet climate (1972-1973). The distributions of soil parameters used in our study (GSA, creation of observations and prior information for GLUE) are independent and uniform and deduced from the experimental data acquired in Chambry (see Tab. 1). In this application, we assume that the type of soil depth (shallow or deep) and the preceding crop (sugar beet or pea) are known. As a consequence, two different ranges were considered for the depth of soil *epc(2)* and for the mineral nitrogen content at the beginning of the wheat crop simulation *NO3init*.

Climatic conditions	Soil depth	Preceding crop	Configuration label
Dry	Shallow	Sugar beet	*dry-beet*
Medium-dry	Shallow	Sugar beet	*mdry-beet*
Medium-wet	Shallow	Sugar beet	*mwet-beet*
Wet	Shallow	Sugar beet	*wet-beet*
Dry	Deep	Sugar beet	*dry+beet*
Medium-dry	Deep	Sugar beet	*mdry+beet*
Medium-wet	Deep	Sugar beet	*mwet+beet*
Wet	Deep	Sugar beet	*wet+beet*
Dry	Shallow	Pea	*dry-pea*
Medium-dry	Shallow	Pea	*mdry-pea*
Medium-wet	Shallow	Pea	*mwet-pea*
Wet	Shallow	Pea	*wet-pea*
Dry	Deep	Pea	*dry+pea*
Medium-dry	Deep	Pea	*mdry+pea*
Medium-wet	Deep	Pea	*mwet+pea*
Wet	Deep	Pea	*wet+pea*

Table 2. Description of the 16 configurations based on soil, climatic and agronomic conditions.

We consider observations on wheat crops obtained for the different configurations described before. These observations consist of LAI_t and QN_t available at 10 dates t, distributed through the wheat growing season: November 15, December 12, January 15, February 16, March 15, April 05, April 19, May 03, May 17 and June 07; and Yld. Three possible sets of observations (see Table 3) were considered for the parameter estimation experiments and the computation of the criteria based on the GSA and GLUE results. In order to compute observations, 50 vectors of true values θ^{true} were randomly generated from the distributions defined above. The number P is thus equal to 50. Corresponding values of STICS-wheat model output variables were simulated for each configuration leading to 50x16 simulations. Observations $y_{q,t}$ were then computed by adding a random error term to the simulated values of the variables and dates defined above:

$$y_{q,t} = f_{q,t}\left(\theta^{true}, x\right) + \varepsilon_{q,t} \tag{11}$$

where $f_{q,t}$ is the STICS model output q (*Yld*, LAI_t or QN_t) calculated on date t (harvest for *Yld* or $t=1,\ldots,T$ for *LAI* and *QN*), x is the vector of explanatory variables and $\varepsilon_{q,t}$ is the observation error term. Following the assumptions made in Section 2.3.1 to compute the likelihood function of the GLUE method, the vector of observation error is given by: $\varepsilon_{q,t} \sim N\left(0, \sigma_{q,t}^2\right)$ where $\sigma_{q,t} = \sigma_q^0 f_{q,t}\left(\theta^{true}, x\right)$, σ_{Yld}^0=9%, σ_{LAI}^0=17% and σ_{QN}^0=30% according to measurements realized in agricultural plots (Machet et al., 2007; Moulin et al., 2007).

Set number	Variables used	Size K
1	LAI_t on dates $t=1,...,10$	K=10
2	LAI_t and QN_t on dates $t=1,...,10$	K=20
3	LAI_t and QN_t on dates $t=1,...,10$, and Yld	K=21

Table 3. Description of the 3 sets of observations.

2.4.2 Generation of observations for prediction

The prediction of variables of interest is performed on independent wheat crop seasons from those used in the estimation process. From each of the 50 vectors defined above, 120 configurations of prediction were studied and are composed by the corresponding type of soil depth, 10 climatic data, 3 different sowing dates and 4 different cropping techniques (2 amount of fertiliser and 2 types of preceding crops). The number Q_j is thus equal to 120 The climatic data were obtained from the meteorological station of Roupy (49.48°N, 3.11°E) and are different from those used in the parameter estimation process.

From each vector θ^{true}, type of soil depth and configuration, the values of synthetic observations of the predicted variables of interest (*Yld*, *Prot* and *Nit* at harvest) are simulated with STICS-wheat. The values of the permanent properties (*argi*, *Norg*, *epc(2)*, *HCC(1)* and *HCC(2)*) of θ^{true} are the same as those used to create the synthetic observations in the estimation step and the initial conditions (*Hinit* and *NO3init*) are randomly generated from the distributions defined in Tab. 1: we assume that the values of the initial conditions are not known for the predicted season. For each parameter estimation experiment defined above, each estimated values of the permanent properties are used to predict the output variables of wheat crop through the STICS model. Assuming that the initial conditions are unknown for the predicted season, they are fixed at the mean of their distribution.

3. Results

3.1 Relationship between criteria based on GSA results and the quality of estimates

3.1.1 At a single parameter level

For each soil parameter, we present here the results about the relationship between the criterion based on GSA results and the criterion related to the quality of the parameter estimate, for the three sets of observations and the 16 soil, climatic and agronomic conditions.

Figure 1 shows that a good link exists between GMS_i and RE_i: the relationship seems to be linear, the higher the GMS_i criterion, the lower the RE_i and the better the quality of estimation of the i^{th} parameter. The results show clusters of parameters: *h* (*Hinit*) at high GMS_i and low RE_i values, *e* (*epc(2)*) at intermediate GMS_i and RE_i values, and the other parameters all grouped in the same cluster at low GMS_i and high RE_i values. Within the scattering around the relationship, the position of the parameter depends on the configuration and especially the soil depth.

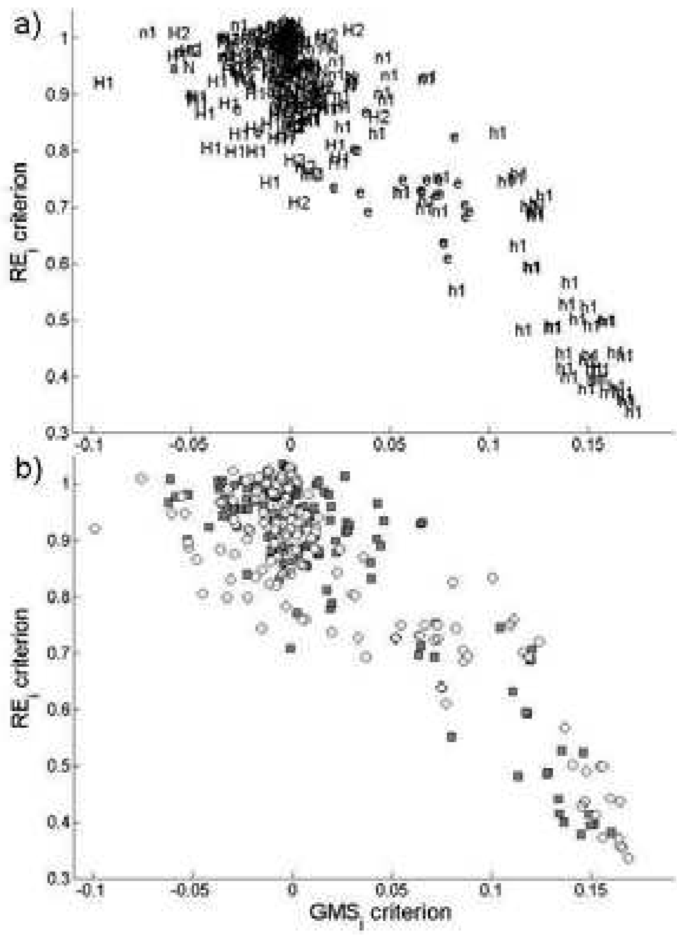

Fig. 1. Scatter diagrams of the criteria RE_i and GMS_i of the 7 soil parameters for the 3 sets of observations and the 16 configurations. a) Label *a* corresponds to *argi*, *N* to *Norg*, *e* to *epc(2)*, *H1* to *HCC(1)*, *H2* to *HCC(2)*, *h* to *Hinit* and *n* to *NO3init*. b) Symbol ○ corresponds to shallow soils and □ corresponds to deep soils.

The case of parameters for which the observations contain enough information to estimate them precisely can be illustrated by the parameter *Hinit*. For example, for the *dry-beet* configuration and the observation set #1, *Hinit* has a big main effect (equal to 0.582 on average), leading to a high value of GMS_i=0.155. In this case, the parameter *Hinit* has a low value of RE_i (RE_i=0.499) meaning a good improvement of its uncertainty through the parameter estimation process (see Figure 1a). In general, the results show that for high values of GMS_i, the reduction of the estimation error is large: a high GMS_i indicates good parameter estimation.

Small first-order indices combined with a large interaction are thought to induce problems of identification. In our case, this applies to most of the parameters. For example, *HCC(1)* has a small main effect (0.089 on average) and a large interaction (equal to 0.251 on average) for the *wet-beet* configuration and the first observation set, leading to a negative value of GMS_i=-0.099. In this case, the parameter *HCC(1)* has a high value of

RE_i (RE_i=0.921), meaning a poor improvement in parameter estimation (see Figure 1a). In general, the results show that for negative values of GMS_i, the reduction of the estimation error is small: a negative value of GMS_i reveals a bad quality of the parameter estimation.

The values of both criteria for parameter *epc(2)* vary a lot between the different configurations and especially between the types of soil depth. As it is shown is Figure 1b, only configurations with a shallow soil (with the symbol○) allow retrieving the parameter *epc(2)*. For shallow soil the observed variables are quite sensitive to *epc(2)*, leading to a quite good estimate, while for deep soil the observed variables are no longer sensitive to *epc(2)*, leading to a poor estimate. For example, the configuration *dry-beet* and the set #3 leads to intermediate GMS_i and RE_i values (GMS_i=0.073 and RE_i=0.724), while *dry+beet* and set #3 leads to lower (resp. higher) GMS_i (resp. RE_i) values (GMS_i=-0.008 and RE_i=0.871).

In order to quantify the quality of the relationship illustrated in Figure 1, we propose to compute the Spearman rank correlations coefficient (Spearman, 1904) between GMS_i and RE_i, for each configuration and observation set. This coefficient allows comparing the relationship between two ranking lists. The analysis is made after discarding the parameters having a negative GMS_i which have always a poor quality of estimation and whose rank would still be high. The results displayed in Table 4 show that the averaged Spearman's correlation between GMS_i and RE_i is satisfactory (about 75.4 %). The GMS_i criterion is thus considered to be effective for ranking the accessible parameters (for which the criterion is positive) with respect to their quality of estimates.

	Parameters*		Climates	Observation sets
(RE_i, GMS_i)	75 %	(*TRE*, *TGMS*)	72 %	91 %

* calculated for parameters having a positive value of GMS_i.

Table 4. Averaged Spearman's rank correlation coefficient of criteria (RE_i, GMS_i) and (*TRE*, *TGMS*). The first pair of criteria is involved in the parameter ranking and the second pair is involved in the climates and observation sets ranking.

3.1.2 At the whole parameter set level

In Figure 2 the values of *TRE* and *TGMS* have been averaged for each observation set and climate over the two soil depths and the two preceding crops. The relationship between *TRE* and *TGMS* appears satisfactory. The *TRE* criterion never reaches low values (the minimum value is about 0.8) even for high *TGMS* values (about 0.21), due to the relatively large number of parameters which are not easily retrievable. The effect of climate is striking. Configurations with a dry climate have the higher values of *TGMS* (between 0.16 and 0.2) and they correspond to the best quality of estimation of the parameter set (*TRE* between 0.81 and 0.86), unlike configurations with a wet climate (*TGMS* below 0.03 and *TRE* above 0.89).

The greater the number of observations considered in the estimation process (from set #1 to set #3), the lower is the *TRE.* As expected and seen in Figure 2, *TGMS* often decreases when the number of observations increases. Although some of the observed variables are mutually correlated (the average correlation coefficient between set #1 and set #2 is about 61 % while it is about 37 % between set #2 and set # 3), they each improve the quality of the parameter set estimation.

Finally, the Spearman's correlation coefficients between *TGMS* and *TRE* were computed for each type of soil depth, preceding crop and observation set, in order to quantify the ranking of the 4 climates given by both *TGMS* and *TRE*. The averaged Spearman's correlation presented in Table 4 between *TGMS* and *TRE* is satisfactory (about 72 %). Secondly, the Spearman correlations between *TGMS* and *TRE* were computed for each soil depth, preceding crop and climate, in order to quantify the ranking of the three observation sets given by both *TGMS* and *TRE*. The averaged Spearman's correlation between *TGMS* and *TRE* is very satisfactory (about 91 %).

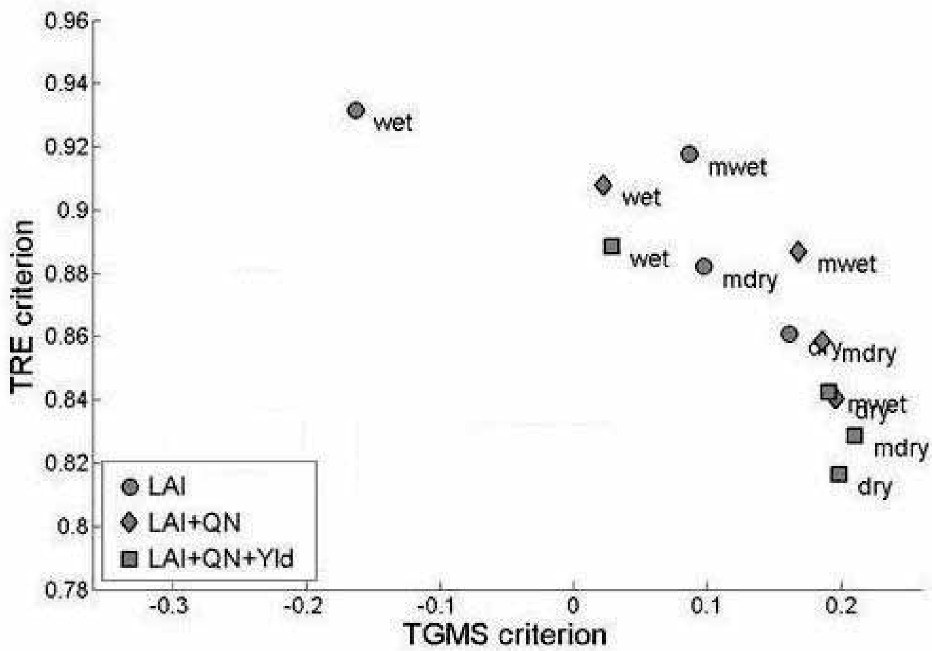

Fig. 2. Scatter diagrams of the criteria *TRE* and *TGMS* at the whole parameter set level, for the 3 sets of observations and the 4 types of climate. Each of the 12 points is an average of the 2 soil depth and the 2 preceding crop configurations. The symbol ○ corresponds to the set #1, ◊ to set #2 and ■ to set #3.

This study shows that the quality of parameter estimation can be explained by the results of GSA. Suitable empirical criteria have been proposed to summarize the results of GSA which allow ranking (i) the parameters with respect to their quality of estimate and (ii) the configurations (particularly the climate and the observation set) with respect to the quality of estimation of the whole parameter set. These criteria are thus shown in our case to be useful tools for estimating the potential of given configurations of observations for retrieving soil parameter values. They may be used also for optimizing the type of observations to be acquired and the dates of acquisition.

3.2 Impact of the quality of estimates on the quality of prediction

The quality of the prediction in now analysed. Figure 3 and 4 shows the results in term of REP_j for the prediction of the variables of interest concerning wheat crop, by using the estimated values of the permanent soil parameters (*argi*, *Norg*, *epc(2)*, *HCC(1)* and *HCC(2)*) in place of their prior values. The initial conditions (*Hinit* and *NO3init*) are assumed to be unknown for the prediction and are fixed at the mean of their distributions. The values of REP_j are calculated for the 2 types of soil depth and the 3 sets of observations.

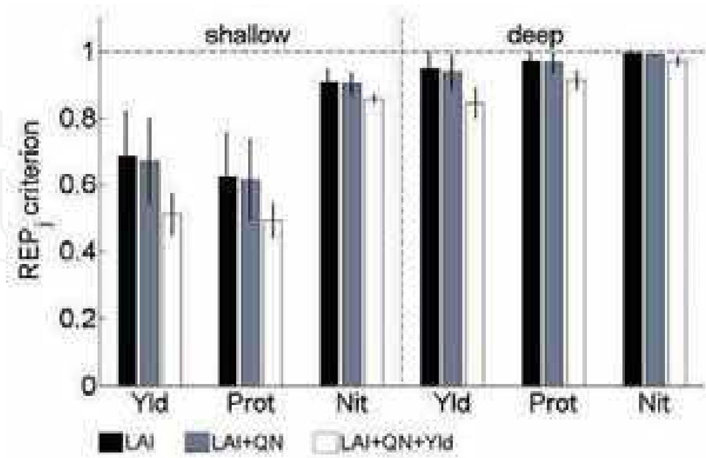

Fig. 3. Results of the prediction of the variables of interest. The results are presented for the 2 types of soil depth and the 3 sets of observations and averaged on the 4 climates.

In Figure 3, REP_j values are averaged on the 4 climates. It can be seen that 2 of the 3 variables of interest (*Yld* and *Prot*) have a significant lower REP_j and therefore a greatly improved quality of prediction when using the estimated values of the permanent parameters, as compared to when using prior information on the parameters. In that case, *Yld* and *Prot* seem to be quite sensitive to the permanent soil parameters. The output variable *Nit* is not or slightly affected by the estimation of the soil parameters because it is sensitive to the initial conditions, which are fixed at a nominal value for the prediction, and not to the permanent parameters. Through the estimation of the permanent soil properties, the size of the observation set slightly improves the quality of prediction: the bigger the observation set size the better the permanent parameter estimates and the better the prediction. The most important improvement between two sets of observations concerns the output variable *Yld* in a shallow soil: REP_j is about 0.66 for set #2 and about 0.52 for set #3. In that case, a lot of information is provided by the observation of *Yld*.

The type of soil depth affects a lot the quality of the prediction and especially for the output variables *Yld* and *Prot*, which have a lower REP_j when the type of soil is shallow. It is not surprising, accordingly to the results of parameter estimation, because the parameter *epc(2)* has a better quality of estimates in the case of shallow soil and because *Yld* and *Prot* are also quite sensitive to this parameter, as well as the observed variables (see Section 3.1.1). The output variable *Nit* is not affected by the soil depth because of its lack of sensitivity to *epc(2)*.

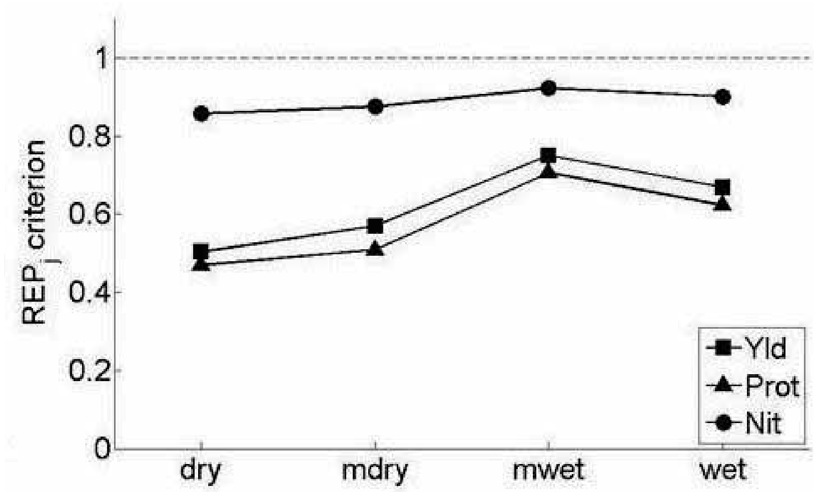

Fig. 4. Results of the prediction of the variables of interest. Effect of the climates on prediction of the variables of interest. The results are averaged on the 3 observation sets for a shallow soil.

The effect of climate on the quality of prediction of the variables of interest is illustrated in Figure 4 on a shallow soil and averaged over the 3 sets of observations. The dryer the climate the better the quality of the prediction. As the observed variables are more sensitive to the soil parameters in dry climatic conditions (see Section 3.1.2), that allows a better quality of the parameter estimates in that case. The results of the prediction are thus affected by the quality of the estimates and are better in dry climatic conditions, because of their sensitivity on the parameters. The REP_j value of the output variables *Yld* and *Prot* significantly decreases from 0.71 to 0.5 and 0.65 to 0.47. As previously, the output variable *Nit* is not accurately predicted and slightly affected by the climate: REP_j decreases from 0.92 to 0.86.

It was shown in this study that some soil parameters can be retrieved by considering observations on crops and that the estimated values of the permanent soil parameters allow reducing the uncertainty on the prediction, because of the sensitivity of the predicted variables on these parameters. The quality of the prediction is manly affected by two factors: the soil depth and climate. These results are closely linked to the quality of the parameter estimates.

4. Conclusion

In our results the link between the quality of parameter estimation and GSA results was illustrated through three types of behavior: high first-order indices are associated with good quality of estimation, low total indices are associated with bad quality of estimation, and high total indices combined with low first-order indices are associated with poor estimates because of interactions between parameters. Many other studies show that the parameter estimation performance can be explained by the results of GSA (Tremblay and Wallach, 2004; Gaucherel et al., 2008; Manache and Melching, 2008). Given the large number of output variables and dates considered in this application, the GSA indices had to be summarized to study the link between GSA and parameter estimation results. We proposed the GMS_i criterion and show its relation with the criterion RE_i which measures the quality of estimation of parameter *i*. The criterion GMS_i proves to be effective for ranking the accessible parameters with respect to their quality of estimation. For a given configuration, GSA is able to provide information on which parameters can be estimated and which can be fixed as they do not deserve an accurate determination (Ratto et al., 2007). We show in this work that the parameters having GMS_i close to zero are not accessible from the observations and the STICS model.

The total criterion *TGMS* can be used to predict the ranking of the configurations with respect to their ability to retrieve the whole set of parameters, and in particular the ranking of the climates and the observation sets: it is possible to predict which type of climate and observation set will lead to the better estimation of the whole parameter set. These results are particularly interesting for screening the possibility of estimating parameters from a given set of available observations in a given agro-environmental context, and, following Kontoravdi et al. (2005), promote GSA as an excellent precursor to optimal experimental design.

From observations on crop status, it is possible to retrieve the soil parameters and the estimated values allow improving the quality of the prediction of agro-environmental variables. Among them, some variables are strongly affected by the quality of the parameter estimates, such as grain yield and protein of the grain, because of their large sensitivity on the permanent soil parameters. This result is particularly interesting for agro-environmental work because the criteria based on GSA also allow screening the possibility of a given set of available observations to predict, through soil parameter estimates, the variables of interest for crop management.

Finally, it would be helpful to conduct such a study on real data to assess the impact of model errors on both soil parameter retrieval and link between the proposed criteria.

5. Acknowledgements

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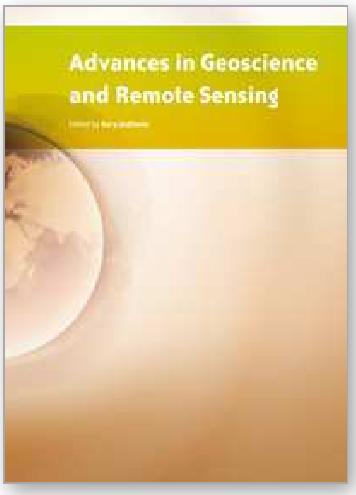

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