L'analyse de sensibilité globale mesure qualité d'estimation des paramètres

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4.1. Objectif

Le sous-groupe de paramètres du sol sélectionné au Chapitre 3 est à estimer par inversion du modèle STICS avec des observations du couvert végétal. Cependant, les paramètres n'auront pas tous la même qualité d'estimation car le jeu d'observations utilisé pour faire l'inversion ne fournit par la même quantité d'information sur chacun d'entre eux. La qualité d'estimation des paramètres est définie ici comme étant l'amélioration de l'estimation par inversion, avec un jeu d'observations donné, par rapport à l'estimation issue de l'information a priori (sa valeur moyenne). La qualité d'estimation est étroitement liée à la quantité d'information apportée par le jeu d'observations sur les paramètres, dans le sens où plus cette quantité est grande meilleure est la qualité. Nous avons vu que dans le cas du modèle linaire (voir Chapitre 1.3.1), la matrice de Fisher permet de déterminer cette quantité d'information pour un jeu d'observations donné. Il n'existe pas de correspondance dans le cas de modèle non linéaire comme STICS, mais nous avons vu (dans le Chapitre 1.3.1) que dans ce cas, la quantité d'information peut être déterminée en fonction des résultats de l'analyse de sensibilité globale des variables observables du modèle aux paramètres à estimer. C'est l'objectif de l'article qui suit.

4.2. Méthodes

Dans l'article qui suit, nous proposons de déterminer la quantité d'information contenue dans les observations du couvert végétal à partir des indices de sensibilité calculés par la méthode Extended FAST. Nous proposons alors deux paires de critères, une au niveau du paramètre et une au niveau du sous-groupe de paramètres. Chaque paire est composée :

- d'un critère basé sur les indices principaux et totaux, qui permet de synthétiser les résultats de l'analyse de sensibilité afin de déterminer la quantité d'information fournie par le jeu d'observations sur le ou les paramètres du sol,
- d'un critère basé sur la *RMSE* (erreur moyenne d'estimation), qui définie la qualité d'estimation du ou des paramètres comme étant l'amélioration de l'estimation par inversion relativement à l'estimation issue de l'information a priori (sa valeur moyenne).

L'information a priori, utilisée par la méthode d'estimation de paramètres, ainsi que l'incertitude sur les paramètres, utilisée par la méthode d'analyse de sensibilité, sont déterminées à partir des gammes de variation des valeurs mesurées des paramètres du sol établies sur les deux parcelles de Chambry (voir Chapitre 2.4). L'estimation des paramètres du sol par inversion est réalisée en utilisant la méthode Importance Sampling (voir Chapitre 2.3) et des observations synthétiques du couvert végétal de blé d'hiver, dans différentes configurations composée de :

- quatre climats contrastés caractérisés comme sec, moyen sec, moyen humide et humide (parmi ceux présentés au Chapitre 2.4.3),
- deux gammes de profondeurs de sol (de 30 à 100 cm pour les sols peu profonds et de 80 à 160 cm pour les sols profonds),
- deux types de précédents culturaux (betterave et pois, ce qui affecte la gamme de variation de *NO3init*),
- trois types/tailles de jeux d'observations (*LAI*, *LAI*+*QN*, *LAI*+*QN*+rendement).

L'utilité des observations synthétiques réside dans le fait qu'il est possible d'analyser la pertinence des critères proposés, indépendamment d'éventuels biais dans le modèle STICS ou dans les observations.

4.3. Résultats

Précision d'estimation des paramètres

Tout d'abord, les précisions d'estimation des paramètres du sol seront présentées, à savoir non relativement à l'estimation issue des valeurs moyennes de l'information a priori (résultats non présentés dans l'article), même si la précision d'estimation reste liée à l'information a priori. Le Tableau 4-1 montre la précision moyenne d'estimation des paramètres du sol : seuls les paramètres *HCC(1)*, *HCC(2)* et *Hinit* (en conditions climatiques sèches) présentent une erreur *RRMSE* en deçà de 20% (entre 16.9 et 17.9% pour *HCC(1)*, entre 16.2 et 19.6% pour *HCC(2)* et 18.1% pour *Hinit* en conditions climatiques sèches). Ces trois paramètres sont donc ceux qu'il est possible d'estimer avec le plus de précision, avec des observations du couvert végétal de blé et compte tenu de l'information a priori utilisée. Notons que le paramètre *epc(2)* devient lui aussi estimable avec une précision du même ordre lorsque le type de profondeur de sol est profond.

	Condition	*argi*	*Norg*	*epc(2)*	*HCC(1)*	*HCC(2)*	*Hinit*	*NO3init*
RRMSE (%)	–	24.9	25.9	40.6	**17.9**	**18.6**	25.3	35.9
	+	24.2	26.3	23.4	**16.9**	**17.2**	23.9	36.3
	sec	25.8	26.8	31.4	**17**	**16.2**	**18.1**	33.7
	humide	23.4	25.4	32.6	**17.8**	**19.6**	31.2	38.5

Tableau 4-1. Précision moyenne d'estimation des paramètres du sol (*RRMSE*) avec des observations synthétiques de blé, sachant la condition agropédoclimatique : faible profondeur de sol (**–**), forte profondeur de sol (+), climat sec (sec) ou climat humide (humide). En gras les *RRMSE* inférieurs à 20%.

Amélioration de l'estimation des paramètres

A présent, nous allons présenter l'amélioration de l'estimation des paramètres du sol par inversion du modèle, calculée relativement à l'estimation issue des valeurs moyennes de l'information a priori (résultats non présentés dans l'article). Le Tableau 4-2 montre ces améliorations calculées par le critère *RE* : plus le critère est faible, plus l'amélioration est forte. Globalement, les améliorations les plus fortes concernent *Hinit*, *HCC(1)*, *epc(2)* et *HCC(2)*. Ces paramètres sont également ceux qui ont la meilleure précision d'estimation. Notons cependant qu'il est possible que l'estimation d'un paramètre soit améliorée même si sa performance d'estimation est faible. Par exemple, le paramètre *epc(2)* a un critère *RE* de 0.73, lorsque la profondeur de sol est faible, alors que qu'il a un critère *RRMSE* de 40.6%. Si une faible précision d'estimation est liée à une forte amélioration de l'estimation (cas de *epc(2)*), cela signifie que l'amélioration s'est opérée sur une large gamme de variation, rendant la précision peu significative. L'amélioration traduit l'apport de la procédure d'estimation des paramètres par inversion sur ce que l'on sait a priori des paramètres.

	Condition	*argi*	*Norg*	*epc(2)*	*HCC(1)*	*HCC(2)*	*Hinit*	*NO3init*
RE	–	0.96	0.98	**0.73**	**0.86**	**0.89**	**0.58**	0.91
	+	0.93	1	0.91	**0.81**	**0.83**	**0.55**	0.92
	sec	0.99	1.02	**0.80**	**0.82**	**0.78**	**0.41**	**0.85**
	humide	0.90	0.96	**0.84**	**0.85**	0.94	**0.71**	0.98

Tableau 4-2. Amélioration moyenne de l'estimation des paramètres du sol (critère *RE*) avec des observations synthétiques de blé, sachant la condition agropédoclimatique : faible profondeur de sol (**–**), forte profondeur de sol (+), climat sec (sec) ou climat humide (humide). En gras les *RE* inférieurs à 0.90.

La configuration d'observation a un effet significatif sur l'amélioration de l'estimation. En effet, les paramètres liés à la capacité de rétention en eau du sol (*epc(2)*, *HCC(1)*, *HCC(2)* et *Hinit*) ont une amélioration plus importante lorsque le climat est sec. Aussi, l'amélioration du paramètre *epc(2)* est plus forte en faible profondeur de sol. Ces résultats peuvent être expliqués par la sensibilité aux paramètres estimés. En climat sec, le modèle est plus sensible aux paramètres liés à l'eau du sol car ils s'expriment plus qu'en climat humide : ces paramètres sont donc plus facilement estimables en climat sec. En faible profondeur, le modèle est plus sensible à l'épaisseur du sol car elle peut limiter l'avancée du front racinaire lorsqu'elle est faible : *epc(2)* est donc plus facilement estimable en faible profondeur. Dans la partie suivante, nous allons présenter le lien qui existe entre analyse de sensibilité et amélioration de l'estimation des paramètres.

Lien entre analyse de sensibilité globale et amélioration de l'estimation

En ce qui concerne l'étude du lien entre analyse de sensibilité et estimation des paramètres, les critères basés sur les indices de sensibilité globaux se sont révélés efficaces pour mesurer la quantité d'information contenue dans les observations et son lien avec l'amélioration de l'estimation des paramètres, appelée qualité d'estimation dans l'article. Le critère GMS_i, qui concerne le paramètre, est capable de distinguer les paramètres qui peuvent être améliorés de ceux qui ne le peuvent pas (et qui peuvent être fixés à une valeur nominale). Plus précisément, il permet de classer les paramètres entre eux en fonction de leur qualité d'estimation, notée RE_i. Quant au critère *TGMS*, qui concerne l'ensemble des paramètres, il permet de classer les climats et les jeux d'observations entre eux en fonction de leur capacité à estimer l'ensemble des paramètres par inversion. Il est donc lié à la qualité d'estimation de l'ensemble des paramètres, notée *TRE*.

L'article montre que les critères proposés permettent de diagnostiquer et de pronostiquer la qualité d'estimation des paramètres en fonction du jeu d'observations utilisé, ainsi que de classer les paramètres, les climats et les jeux d'observations entre eux en fonction de la quantité d'information contenue dans les observations et de la qualité d'estimation des paramètres du sol. Ces résultats peuvent être utilisés à des fins de compréhension des performances d'estimation des paramètres. Par exemple, lorsque le critère (celui défini au niveau du paramètre) est négatif pour un paramètre donné, la performance d'estimation est mauvaise car il agit sur les variables observées essentiellement à travers ses interactions. Lorsque le critère est nul, la performance est également mauvaise mais parce qu'il agit de manière globalement insignifiante sur les variables observées. Ces résultats peuvent aussi être utilisés à des fins d'optimisation du jeu d'observations pour maximiser les performances d'estimation des paramètres et minimiser le coût des observations. Par exemple, si l'on désire estimer un paramètre en particulier, il est possible de trouver un jeu d'observations hypothétique qui maximiserait le critère associé à ce paramètre, avant de procéder à un véritable recueil de ces observations.

L'estimation des paramètres peut être une fin en soi, à savoir qu'il est possible de n'utiliser STICS que par inversion, ou bien être le moyen par lequel les prédictions du modèle peuvent être améliorées. Pour cela, il est nécessaire de comprendre comment les performances de prédiction du modèle réagissent en fonction des performances d'estimation des paramètres du sol. Cette démarche de compréhension sera traitée dans l'article présenté au chapitre suivant.

4.4. Article 2 : "Global sensitivity analysis measures the quality of parameter estimation: The case of soil parameters and a crop model"

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Global sensitivity analysis measures the quality of parameter estimation: The case of soil parameters and a crop model

Hubert Varella*, Martine Guérif, Samuel Buis

INRA, UMR 1114 INRA-UAPV EMMAH, Domaine Saint Paul, Site Agroparc, F84914 Avignon Cedex 9, France

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ABSTRACT

One common limitation of the use of crop models for decision making in precise crop management is the need for accurate values of soil parameters for a whole field. Estimating these parameters from data observed on the crop, using a crop model, is an interesting possibility. Nevertheless, the quality of the estimation depends on the sensitivity of model output variables to the parameters. The goal of this study is to explain the results for the quality of parameter estimation based on global sensitivity analysis (GSA). The case study consists of estimating the soil parameters by using the STICS-wheat crop model and various synthetic observations on wheat crops (*LAI*, absorbed nitrogen and grain yield). Suitable criteria summarizing the sensitivity indices of the observed variables were created in order to link GSA indices with the quality of parameter estimation. We illustrate this link on 16 different configurations of different soil, climatic and crop conditions. The GSA indices were computed by the Extended FAST method and a function of RMSE was computed with an importance sampling method based on Bayes theory (GLUE). The proposed GSA-based criteria are able to rank the parameters with respect to their quality of estimation and the different configurations (especially climate and observation set) with respect to their ability to estimate the whole parameter set. They may be used as a tool for predicting the performance of different observation datasets with regard to parameter estimation.

1. Introduction

Dynamic crop models are very useful to predict the behavior 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 (Launay and Guérif, 2003; Irmak et al., 2001; Ferreyra et al., 2006). However, knowledge on soil properties and therefore model soil parameters is scarcely available at an appropriate scale. Direct measurements would be highly costly and time consuming. Detailed soil maps adapted to the field scale are scarcely available, while the use of more automated techniques like remote sensing or electrical resistivity is still hampered by a lack of robust interpretation of the signal (Samouelian et al., 2005; 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, observations on crops provided by remote sensing (Weiss and Baret, 1999; Houborg and Boegh, 2008) or yield monitoring (Blackmore and Moore, 1999; Pierce et al., 1999) are widely available and allow soil parameters being estimated through the inversion of crop models. Thus Timlin et al. (2001) explored the possibility of finding the Water Holding Capacity of three soil layers by using maize yield maps and a very simple model; Braga and Jones (2004) compared the performances of two kinds of data (maize yield and soil water content) for estimating five soil parameters in nine soil layers, using the CERES crop model; Guérif et al. (2006) estimated 12 soil parameters from the assimilation of leaf area indices and absorbed nitrogen estimated from remote sensing.

* Corresponding author. Tel.: +33 432 72 24 07; fax: +33 432 72 23 62.
E-mail address: hvvarella@avignon.inra.fr (H. Varella).

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Although the estimation process is quite efficient when a small number of parameters have a clearly identifiable influence on the observed output variables, estimating parameters of complex models such as crop models may be not so easy (Tremblay and Wallach, 2004; Launay and Guérif, 2005). It is clearly a difficult problem, as a lot of parameters have similar effects and observations are generally scarce. The use of Bayesian methods, including prior information on parameters, is a way of improving the estimation process, but the results can be deceptive (Guérif et al., 2006). 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., 2000b). The problem of parameter identifiability is commonly studied using local sensitivity analysis (Brun et al., 2002; Rodriguez-Fernandez et al., 2006). However, these techniques are only well suited for linear or near-linear models. For complex non-linear models, only 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. In recent years, many studies have focused on this subject, namely, how to choose the main parameters to be estimated (Campolongo and Saltelli, 1997; Gomez-Delgado and Tarantola, 2006; Manache and Melching, 2008; Post et al., 2008). Some of them have used crop models (Ruget et al., 2002; Makowski et al., 2006; Jongschaap, 2007; Pathak et al., 2007) 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, to evaluate the feasibility of characterizing soil properties of agricultural fields by the inversion of a dynamic crop model, using the many observations collected on those fields either from remote sensing or by yield monitoring. In particular, we will investigate which parameters are the most accessible in the configurations of observations available. Secondly, 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. 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 data 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. This choice also allows eliminating the impact of model errors, which may complicate the interpretation of the results.

2. Methods

2.1. The crop model STICS, its parameters and output variables

2.1.1. The STICS model

The STICS model (Brisson et al., 2002) is a non-linear 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 (Flenet et al., 2003). 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. The soil parameters

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, after checking that the model was valid for the conditions explored in our application. 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, the thickness of the first layer was set at 0.30 m. Based on the measurements made on this precision agriculture experimental site in Chambry (49.35°N, 3.37°E) (Guérif et al., 2001), we added relations, specific to our conditions, linking the initial contents of water *Hinit* and mineral nitrogen *NO3init* of the two soil layers. 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 seven parameters.

The seven 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.

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

Parameter	Definition	Range	Unit
argi	Clay content of the 1st layer	14–37	%
Norg	Organic nitrogen content of the 1st layer	0.049–0.131	%
epc(2)	Thickness of the 2nd layer	0–70 or 50–130[a]	cm
HCC(1)	Water content at field capacity (1st 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 (1st layer)	4–21.5 or 25–86[b]	$kgN\,ha^{-1}$

[a] The first range is for a shallow soil and the second for a deep soil.
[b] The first range is for a wheat cultivated after sugar beet and the second for a wheat cultivated after pea.

2.1.3. Observable output variables

In this study, we focus on output variables of the STICS-wheat model which correspond to possible observations on the canopy. They consist of:

- the leaf area index (LAI_t) and the nitrogen absorbed by the plant (QN_t) at various dates t, $t = 1, \ldots, T$, during the crop season – possibly derived from a set of remote sensing images (Weiss and Baret, 1999; Houborg and Boegh, 2008),
- the yield at harvest (Yld), possibly provided by yield monitoring systems.

2.2. Global sensitivity analysis

Methods of global sensitivity analysis are particularly interesting because they allow the full uncertainty range of the parameters to be explored and analyzed through a complex model, and their interactions to be estimated by varying them concurrently (Saltelli et al., 2000a). Among these methods, variance-based methods use model output variance as an indicator of importance for parameters. When the number of parameters is not too large, as it is the case in this study, a variance-based method can be applied directly on the complex model. When this number is very large, it is possible to apply this method on a metamodel (polynomial approximation of the model) to calculate sensitivity indices very efficiently (Ziehn and Tomlin, 2009). A variance-based method generally needs a lot of model simulations but its application does not rely on special assumptions about the behavior of the model (such as linearity, monotonicity and additivity of the relationship between input factors and model output). Because of the non-linear structure of the STICS model and the acceptable computational cost of one run of the model (about 1s), we chose this type of method.

2.2.1. Variance decomposition method 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):

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

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

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

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

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 ith 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 ith 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 ith 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 ith 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

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. 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. The uncertainties considered for the soil parameters are assumed independent and follow uniform distributions. These distributions are given in Section 2.5. 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 $7 \times 2000 = 14\,000$ 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 4 h.

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 ones in order to account for the redundancy between observable output variables:

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

where k is a given observed output variable in a subset composed of K variables among $\{LAI_t, QN_t, t = 1, \ldots, T; Yld\}$, $R_i^k = ST_i^k - S_i^k$ 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): $\alpha_k = \frac{1}{K-1}\sum_{k' \ne k}|r_{kk'}|$, $K > 1$.

The GMS_i criterion is based on the following rules:

- if ST_i^k is low (and thus S_i^k), observation k is assumed not to contain enough information to estimate parameter $\theta_i (S_i^k - R_i^k)$ should be low,
- if S_i^k is high (and thus ST_i^k), observation k is assumed to contain sufficient information to estimate parameter $\theta_i (S_i^k - R_i^k)$ should be high,
- if S_i^k is low and ST_i^k is high, then the model is over-parameterized and difficulties in identifying parameter θ_i are expected (Ratto et al., 2007): $(S_i^k - R_i^k)$ should be low,
- high correlation between output variables indicates that the information content of these variables is redundant: $(1 - \alpha_k)$ should be reduced.

GMS_i varies within the range $[-1, 1]$. It tends to 1 when S_i^k 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^k 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:

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

It measures the information contained in a set of observations to estimate the all set of parameters considered. 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 allows existing information on the parameters to be taken into account in the estimation process and an estimate of the posterior probability distribution of parameter values to be computed.

2.3.1. The Bayesian approach and the GLUE method

The posterior parameter distribution is given by Bayes' theorem:

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

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

We chose an Importance Sampling method, GLUE (Beven and Binley, 1992; Beven and Freer, 2001; Makowski et al., 2002) which principle is to approximate the posterior parameter distribution $\pi(\theta/Z)$ given in (6) by a discrete probability distribution (θ_n, p_n), $n = 1, \ldots, N$, $\sum_{n=1}^{N} p_n = 1$, 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, $n = 1, \ldots, N$, from the prior parameter distribution $\pi(\theta)$.
(2) Calculate the likelihood values $\pi(Z/\theta_n)$ and the prior density $\pi(\theta_n)$, $n = 1, \ldots, N$, associated with the different generated parameter vectors.
(3) Calculate $p_n = \frac{\pi(Z/\theta_n)}{\sum_{m=1}^{N} \pi(Z/\theta_m)}$.

The pairs (θ_n, p_n), $n = 1, \ldots, N$, can be used to determine various characteristics of the posterior distribution, including:

- the mean of the posterior joint distribution of θ, $\bar{\theta}^{\text{post}} = \sum_{n=1}^{N} \theta_n p_n$
- the correlation between two parameters θ_i and θ_j, $\frac{\sum_{n=1}^{N} (\theta_{i,n} - \bar{\theta}_i^{\text{post}})(\theta_{j,n} - \bar{\theta}_j^{\text{post}}) p_n}{\delta_i \cdot \delta_j}$, where $\delta_i^2 = \sum_{n=1}^{N} \theta_{i,n}^2 p_n - (\bar{\theta}_i^{\text{post}})^2$ is the variance of the parameter θ_i.

This correlation coefficient permits to evaluate the pair-wise interaction structure between parameters. In particular, when a positive coefficient is detected, the pair of parameters acts in the model as a quotient or a difference, and when it is negative they act as a product or a sum (Ratto et al., 2001; Kanso et al., 2004). A high level of correlation between two parameters indicates that they may compensate each other to give the same values of model outputs. In this case, bringing new information on one of them (by incorporating new measurements or improving its prior information) may also reduce the uncertainty on the other one.

We assume that the sums of the errors of modeled 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:

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

A prior assumption is that parameters are independent and their distribution uniform. They correspond to the uncertainties used for GSA and are given in Section 2.5. We have implemented the GLUE 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. Criteria expressing the quality of parameter estimation

As in the previous section, we created criteria related to the quality of parameter estimation both for a given parameter and for the whole set of parameters. These criteria express the error of the estimate obtained by the mean of the posterior distribution of the parameter i, $i = 1, \ldots, 7$: $\bar{\theta}_i^{\text{post}}$, relative to that obtained from the mean of the prior distribution: $\bar{\theta}_i^{\text{prior}}$. This relative error can be considered as an indicator of the quality of the estimation process.

For one single parameter θ_i, the Relative Error RE_i is defined as follows:

$$RE_i = \frac{RMSE\left(\bar{\theta}_i^{\text{post}}\right)}{RMSE\left(\bar{\theta}_i^{\text{prior}}\right)} \tag{8}$$

where $RMSE(\bar{\theta}_i^{\text{post}}) = \sqrt{\frac{1}{P}\sum_{p=1}^{P} (\theta_{i,p}^{\text{true}} - \bar{\theta}_{i,p}^{\text{post}})^2}$ and similarly for $RMSE(\bar{\theta}_i^{\text{prior}})$, where $\theta_{i,p}^{\text{true}}$ is one of the true P values of soil parameter θ_i defined to generate the synthetic observations (see Section 2.5), and $\bar{\theta}_{i,p}^{\text{post}}$ is the corresponding estimation given by the GLUE method.

For all parameters, the second criterion, called Total Relative Error (TRE), is defined by the mean of the seven values of RE_i:

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

2.4. Quality of the link between GSA and parameter estimation

An important issue in this work concerns the quality of the relationship between the criteria based on GSA indices and the criteria expressing the quality of parameter estimation. If the link is strong, GSA can be used to predict which parameters may be estimated with some accuracy. We use Spearman's rank correlation analysis (Spearman, 1904) to assess the quality of the link. It allows quantifying the correlation between the parameter ranking list given by the criteria based on GSA indices and the one given by the criteria expressing the quality of parameter estimation. The Spearman's rank correlation coefficient ρ, between two lists x_1 and x_2, is calculated as:

$$\rho = 1 - \frac{6\sum_{s=1}^{S} (x_1^s - x_2^s)^2}{S\left(S^2 - 1\right)} \tag{10}$$

where S is the size of the vectors x_1 and x_2.

2.5. Numerical experimentation

2.5.1. Configurations

The STICS model output variables depend on the soil, climate and agronomic conditions for which the crop is simulated. In view of this, we use different configurations in our study, as presented in Table 2: four contrasting climates, two different soil depths (shallow and deep), and two agronomic conditions (preceding crop 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 bounds of soil parameters' distributions were deduced from experimental data acquired on a precision agriculture site in northern France (Chambry, 49.35°N, 3.37°E) (Guérif et al., 2001). They are given in Table 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. Therefore 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*.

2.5.2. Generation of observations

We consider observations on wheat crops obtained for the different configurations described before. They consist of LAI_t and QN_t available at ten 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* at harvest. Three possible sets of observations (see Table 3) were considered for the parameter estimation experiments. In order to compute the synthetic observations, 50 vectors of true values θ^{true}, corresponding to 50 soils, were randomly generated from the distributions defined above. Corresponding values of STICS-wheat model output variables were simulated for each configuration leading to 50 × 16 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:

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

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 $\epsilon_{q,t}$ is the observation error term. Following the assumptions made in Section 2.3 to compute the likelihood function of the GLUE method, the vector of observation error is given by: $\varepsilon_{q,t} \sim N(0, \sigma_{q,t}^2)$ where $\sigma_{q,t} = \sigma_q^0 f_{q,t}(\theta^{\text{true}}, x)$, $\sigma_{Yld}^0 = 9\%$, $\sigma_{LAI}^0 = 17\%$ and $\sigma_{QN}^0 = 30\%$ according to results obtained in field measurements on wheat crops (Machet et al., 2007; Moulin et al., 2007).

2.5.3. Total number of experiments

To sum up, GSA was applied to 16 configurations involving 21 output variables, GSA-based criteria were computed for 16 configurations × 3 sets of observations, GLUE was applied and RE_i and *TRE* criteria were computed for 16 configurations × 3 sets of observations × 50 soils defined by 50 different θ^{true}.

3. Results

3.1. Global sensitivity analysis

Fig. 1a shows the results for one configuration (dry climatic conditions, shallow soil, cultivated after sugar beet) labeled *dry−beet*. The sensitivity indices for all the output variables and each

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

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 3
Description of the 3 sets of observations.

Set number	Variables used	Size K
1	LAI_t on dates $t = 1, \ldots, 10$[a]	$K = 10$
2	LAI_t and QN_t on dates $t = 1, \ldots, 10$	$K = 20$
3	LAI_t and QN_t on dates $t = 1, \ldots, 10$, and *Yld*	$K = 21$

[a] See dates in Section 2.5.

Table 4
Criteria GMS_i and *TGMS* calculated for the *dry − beet* configuration and for the 3 sets of observations.

	GMS_i							*TGMS*
	argi	*Norg*	*epc(2)*	*HCC(1)*	*HCC(2)*	*Hinit*	*NO3init*	Parameter set
Set 1	−0.01	−0.009	0.063	−0.008	−0.008	0.155	−0.009	0.174
Set 2	−0.006	−0.003	0.071	0.004	−0.005	0.147	−0.001	0.207
Set 3	−0.006	−0.003	0.073	0.005	−0.004	0.145	−0.001	0.209

parameter are presented both for first-order indices S_i (area in black) and for interaction indices $R_i = ST_i - S_i$ (area in gray). The corresponding GMS_i criterion computed for the 3 sets of output variables is given in Table 4. Only two parameters (*Hinit* and *epc(2)*) have strong first-order indices and little interaction with the other parameters. The others have moderate (*HCC(1)* and *HCC(2)*) to low (*argi*, *Norg* and *NO3init*) first-order and interaction indices. The parameters *Hinit* and *epc(2)* are involved in soil water content and are determinant for the crop in dry conditions. Parameters *argi* and *Norg* which are mainly involved in organic matter mineralization induce little sensitivity because this process is blocked in dry conditions. Accordingly, the GMS_i values computed for the set #3 are high for *Hinit* and *epc(2)* (0.145 and 0.073), and close to 0 or even negative for the other parameters. These nil values correspond to two situations: either both first-order indices and interaction are low (*argi* and *Norg*), or both first-order indices and interaction are moderate but equal (*HCC(1)*, *HCC(2)* and *NO3init*). For parameter *epc(2)*, *LAI* and *QN* have similar sensitivity profiles and their indices for the last date are close to those of *Yld*. Thus, the information contained in these output variables may be quite redundant for this parameter. It is confirmed by the fact that *TGMS* increases only by 18% from set #1 to set #2 and that the average correlation coefficient between *LAI* and *QN* is about 59% for this configuration.

Table 5 summarizes the results of the two criteria, for the 8 configurations with sugar beet as preceding crop and for the set #3 of output variables. Concerning these results, it can be said that:

- Only the parameters *Hinit* and *epc(2)* have significant values of GMS_i, as in the configuration examined previously.
- The effect of climate is significant for *Hinit*: the drier the climate the higher the criterion for *Hinit* (GMS_i decreases 0.145–0.052 from dry to wet climates for shallow soils and 0.136–0.063 for deep soils). It is also the case for *epc(2)* for shallow soils.
- The type of soil depth has a big effect on GMS_i for parameter *epc(2)*. This parameter is not linearly related to water stress on the entire range of values (the relationship is more of

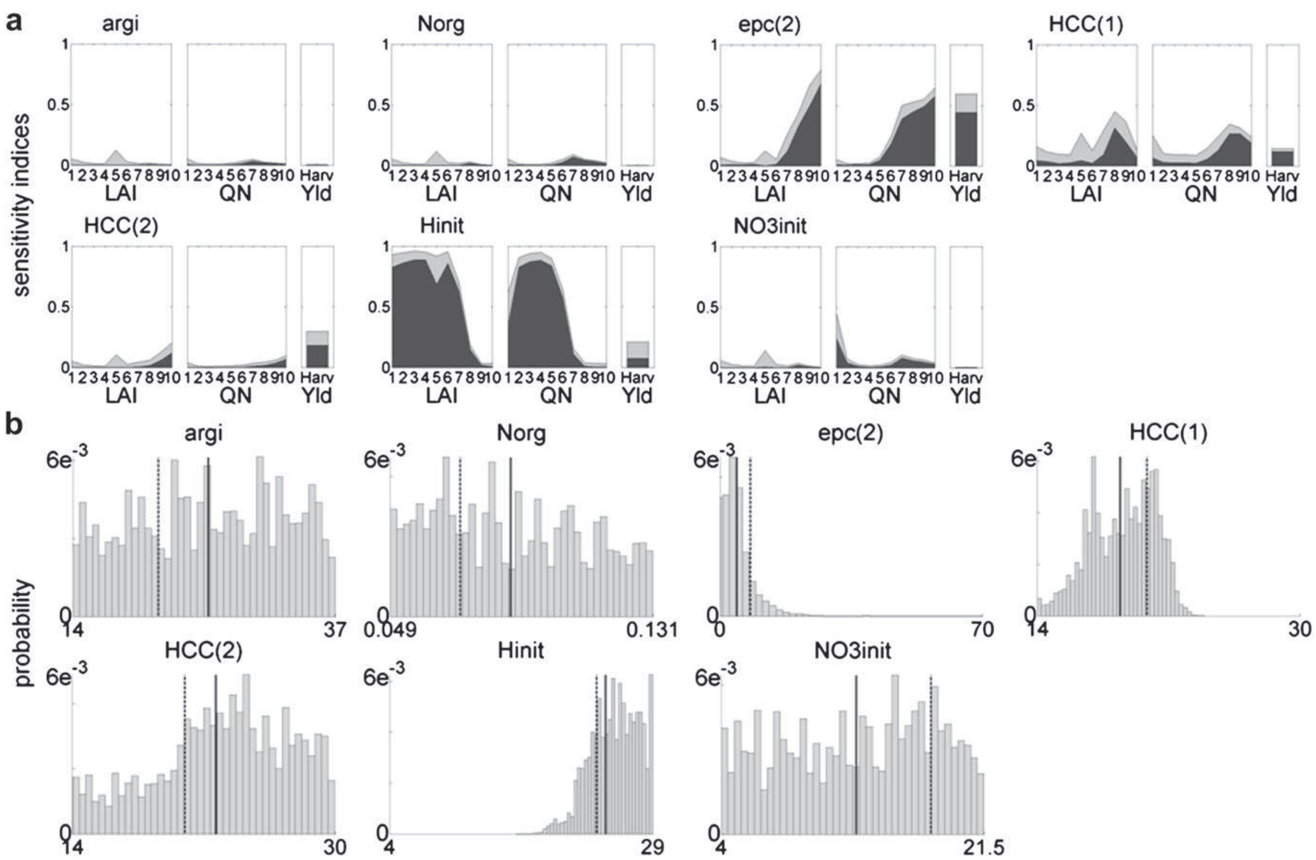

Fig. 1. GSA results and parameter estimation results for the configuration *dry − beet*. a) Sensitivity profiles (first order: area in black and interaction: area in gray) of the output variables to the 7 parameters. On the *x*-axis, numbers 1–10 correspond to the 10 dates for LAI_t and QN_t, and *Harv* corresponds to harvest. b) Posterior distributions calculated for the 7 parameters with the set #3 of observations: one of the 50 replicates is represented. The dashed line corresponds to the true value of the parameter and the solid line corresponds to the mean of the distribution.

Table 5
Criteria GMS_i and *TGMS* for the 8 configurations having sugar beet as preceding crop and for the set #3 of output variables. GMS_i values higher than 0.03 are in bold.

	Climate	Soil depth	GMS_i							TGMS
			argi	*Norg*	*epc(2)*	*HCC(1)*	*HCC(2)*	*Hinit*	*NO3init*	Parameter set
(1)	*dry*	–	−0.006	−0.003	**0.073**	0.005	−0.004	**0.145**	−0.001	0.209
(2)	*mdry*	–	0.002	0.011	**0.066**	−0.012	−0.003	**0.148**	−0.004	0.208
(3)	*mwet*	–	−0.001	0.012	**0.037**	−0.016	−0.012	**0.118**	−0.001	0.138
(4)	*wet*	–	−0.021	−0.005	**0.033**	−0.048	−0.029	**0.052**	−0.035	−0.054
(5)	*dry*	+	−0.005	−0.001	−0.008	0.019	−0.001	**0.136**	0.007	0.148
(6)	*mdry*	+	0.011	0.028	−0.004	−0.010	0.011	**0.128**	0.002	0.166
(7)	*mwet*	+	0.008	0.027	−0.015	0.017	−0.002	**0.118**	0.022	0.175
(8)	*wet*	+	−0.011	0.018	−0.034	−0.023	−0.035	**0.063**	−0.009	−0.030

a linear-plus-plateau type): *LAI*, *QN* and *Yld* are sensitive to *epc(2)* for shallow soil (involving GMS_i between 0.033 and 0.073) whereas they are not for deeper soils (involving GMS_i close to 0 or negative).

- *TGMS* mainly exhibits the same behavior as *Hinit* which is the most sensitive parameter. It increases from wet to dry climates for shallow soils: from −0.054 to 0.209; and for deeper soils: from −0.03 to 0.148.

3.2. Parameter estimation (GLUE)

Fig. 1b illustrates the results of the parameter estimation process described in Section 2.3 for the seven soil parameters, for the *dry – beet* configuration and the third observation set, applied to one of the 50 true soils defined in the synthetic experiments (see Section 2.5). The posterior distributions of the parameters exhibit different patterns: some are similar to the uniform prior distribution (*argi*, *Norg*, *NO3init*), some have a profoundly modified distribution with a marked mode (*Hinit* and *epc(2)*) and some have an intermediate pattern (*HCC(1)* and *HCC(2)*). These patterns will be referred to in the following as: "unmodified", "modified" and "intermediate". The parameter estimates (given by the mean of the posterior distributions) are close to the true values for the "modified" patterns, less close for the "intermediate" and quite dissimilar for the "unmodified". The "modified" distributions indicate that the uncertainty of the corresponding parameters has been reduced with respect to the uncertainty associated with the prior information: observations have brought enough information to provide certainty on the estimates. On the contrary, the uncertainty of the "unmodified" parameters has only been slightly reduced. It is striking that these patterns and goodness of parameter estimates are closely related to the patterns of the GSA presented above (Fig. 1a): the higher the GMS_i, the more informative is the distribution ("modified" pattern) and the closer is the estimate to the true value. The "modified" patterns correspond to parameters whose variations induce large variance in the output variables, allowing a good maximization of the likelihood in the GLUE process, unlike the "unmodified" ones.

The results of the parameter estimation process in terms of RE_i and *TRE* are reported in Table 6 for the set #3 and the 8 configurations considered in the previous section (Table 5):

- *Hinit* has the lowest value of the RE_i criteria for each configuration, meaning a large reduction of the error of estimate when using observations as compared to the error of the prior information.
- Conversely, *argi*, *Norg* and *NO3init* have generally high values of RE_i, which correspond to no reduction or even an increase of the error of estimate. The quality of estimation of *epc(2)*, *HCC(1)* and *HCC(2)* varies from medium to poor, depending on the configurations.
- The drier the climate, the better the estimation of *Hinit*. For example, the *dry – beet* configuration allows a greater reduction in the error on *Hinit* ($RE_i = 0.428$) than the *wet – beet* configuration ($RE_i = 0.727$). This is also the case for deep soils. Conversely, the estimation of the parameters involved in organic matter mineralization (*argi* and *Norg*) is poor but slightly improved in wet climates as compared to dry climates. However, the type of climate has little effect on the reduction of *epc(2)* estimate error.
- The type of soil depth has a big effect on the estimation of *epc(2)*: its estimate is better for shallow soils (RE_i from 0.749 to 0.694) than for deep soils (RE_i from 0.966 to 0.871). This is still in accordance with the sensitivity analysis results that show higher indices for shallow soils than for deep ones.
- The *TRE* criteria exhibit similar, but less pronounced, behavior to the RE_i of the best estimated parameter *Hinit*: they decrease slightly from wet to dry climates. The effect of soil depth on *TRE* is not significant.

Fig. 2 shows the correlations calculated on the posterior parameter values for each pair of parameters, for the *dry – beet* configuration and the observation set #3. High correlations are observed only between *HCC(1)* and *Hinit* (about 0.331 in average), between *HCC(2)* and *epc(2)* (about −0.516 in average) and between *HCC(1)* and *epc(2)* (about −0.368 in average). These results reveal that the pair (*HCC(1)*, *Hinit)* acts in the STICS model as a quotient or a difference, whereas (*HCC(2)*, *epc(2)*) as (*HCC(1)*, *epc(2)*) acts as a product or a sum (see Section 2.3). Such significant correlations have been noted for configurations having a climate rather dry and only concern pairs of parameters which have good estimates: *epc(2)*, *HCC(1)*, *HCC(2)* and *Hinit*. These results suggest that these parameters can compensate to produce similar good simulation results with respect to observations. This can be due to model structure as well as to model error, data error and sparsity (Rodriguez-Fernandez et al., 2006). As a consequence, part of the uncertainty of the estimated parameters is due to these interactions.

The effect of the observation set on the *TRE* criterion is finally examined. Considering all the configurations, set #2 allows decreasing the value of *TRE* only about 3% compared to set #1 (0.898–0.873) while set #3 allows decreasing *TRE* about the same amount compared to set #2 (0.873–0.844). This is to relate with the average correlation coefficient between set #1 and set #2 which is about 61% while it is about 37% between set #2 and set #3.

3.3. The link between GSA and quality of parameter estimation

3.3.1. At a single parameter level

In the previous sections we highlighted the analogy between the behavior of criteria based on GSA indices and the criteria expressing the quality of parameter estimation for some configurations and some sets of output variables or observations. We

Table 6
Criteria RE_i and *TRE* for the 8 configurations having sugar beet as preceding crop and for the set #3 of output variables. RE_i values lower than 0.7 are in bold.

	Climate	Soil depth	RE_i							*TRE*
			argi	*Norg*	*epc(2)*	*HCC(1)*	*HCC(2)*	*Hinit*	*NO3init*	Parameter set
(1)	*dry*	−	1.003	1.018	0.724	0.854	0.844	**0.428**	0.85	0.817
(2)	*mdry*	−	1.007	0.887	0.749	0.824	0.79	**0.49**	0.946	0.812
(3)	*mwet*	−	1.003	0.921	**0.694**	0.743	0.922	**0.694**	0.876	0.836
(4)	*wet*	−	0.916	0.949	0.728	0.866	0.929	0.727	0.967	0.869
(5)	*dry*	+	0.979	1.014	0.871	0.779	0.708	**0.399**	0.856	0.801
(6)	*mdry*	+	0.958	0.917	0.966	0.906	0.913	**0.486**	0.982	0.875
(7)	*mwet*	+	0.931	0.915	0.962	0.811	0.886	**0.593**	0.899	0.857
(8)	*wet*	+	0.882	0.980	0.960	0.839	0.943	**0.697**	0.986	0.898

present here the results for the three sets of observations and the 16 soil, climatic and agronomic conditions.

Fig. 3 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 *ith* 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.

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 (see Fig. 1a for *LAI*), *Hinit* has a big main effect ($S_i = 0.582$ 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 considerable improvement of its uncertainty through the parameter estimation process. 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 a large improvement in 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, for the *wet* − *beet* configuration and the first observation set, *HCC(1)* has a small main effect ($S_i = 0.089$ on average) and a large interaction (equal to 0.251 on average), leading to a negative value of GMS_i ($GMS_i = -0.099$). In this case, its RE_i value is high ($RE_i = 0.921$), meaning a poor improvement in parameter estimation. 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.

Spearman's rank correlation analysis between GMS_i and RE_i allows us to quantify the quality of the relationship illustrated in Fig. 3. It is performed after discarding the parameters having a negative GMS_i (from two to five) which have always a poor quality of estimation and whose rank would still be high. The averaged Spearman's correlation coefficient is about 75.4%, which is a satisfactory value, means that the GMS_i criterion is effective for ranking the accessible parameters (for which the criterion is positive) with respect to their quality of estimates.

3.3.2. At the whole parameter set level

When considering the whole parameter set (Fig. 4a), there is a slight relationship between the *TGMS* criterion created with the GSA indices of the parameter set and the *TRE* criterion computed

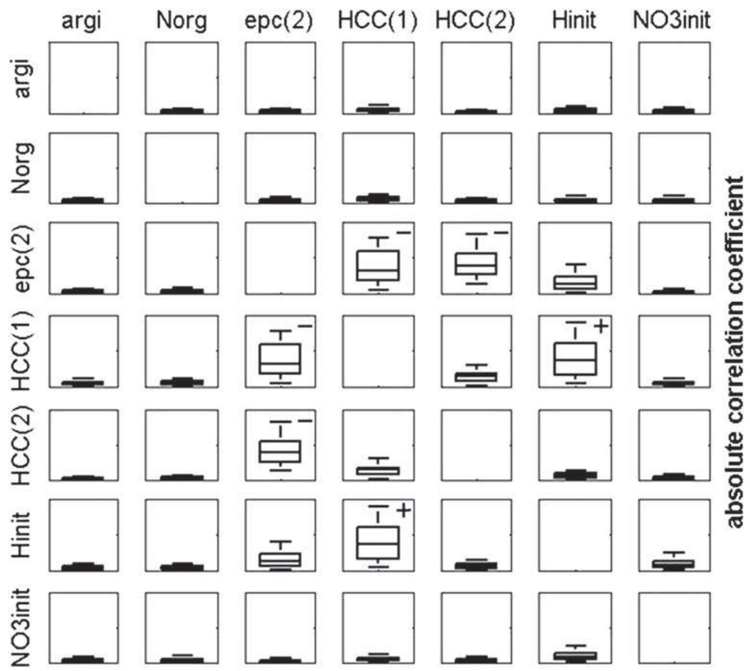

Fig. 2. Boxplot of the absolute values of the correlation coefficients calculated on the posterior distributions of the 50 replicates, for the *dry* − *beet* configuration and the set #3. The sign of the 3 most correlated pairs of parameters is given in the symmetrical corresponding square.

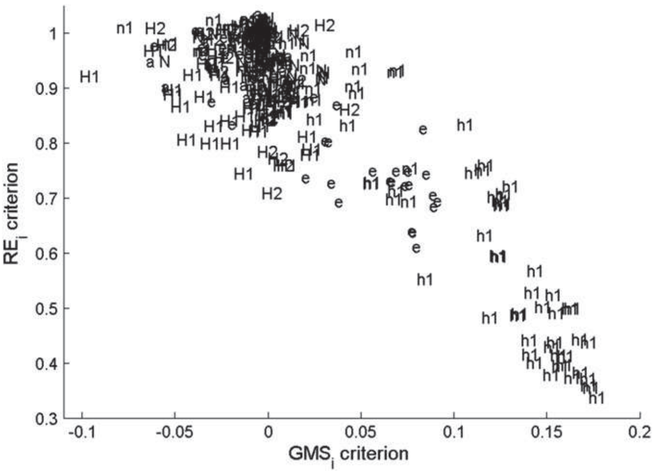

Fig. 3. Scatter diagram of the criteria RE_i and GMS_i of the 7 soil parameters for the 3 sets of observations and the 16 configurations. Label *a* corresponds to *argi*, *N* to *Norg*, *e* to *epc(2)*, *H1* to *HCC(1)*, *H2* to *HCC(2)*, *h* to *Hinit* and *n* to *NO3init*.

from errors of estimate for this parameter set. 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 global relationship is no longer linear and two clusters of configurations appear: one corresponds to shallow soils (in white symbols) and still exhibits a quite linear relationship between *TGMS* and *TRE,* the other corresponds to deep soils (in black symbols), for which the relationship is non-linear. According to the results presented Section 3.2, the first cluster leads to a slightly better estimate of the whole parameter set than the second cluster, because the estimation of parameter *epc(2)* is better for shallow soils than for deeper ones.

In Fig. 4b the values of *TRE* and *TGMS* have been averaged over the two soil depths and the two preceding crops. The relationship between *TRE* and *TGMS* appears stronger. The effect of climate is striking, according to results presented in the Sections 3.1 and 3.2. 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). As it was seen before, the greater the number of observations considered in the estimation process, the lower is the *TRE.* As expected and as it was seen in Fig. 4b, *TGMS* often decreases when the number of observations increases. Although some of the observed variables are mutually correlated, 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 four climates given by both *TGMS* and *TRE*. The averaged value is about 72%. The Spearman correlations were therefore 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 about 91%. Both values are very satisfactory and indicate that *TGMS* is effective to rank the climates and the observation sets with respect to their ability to estimate the soil parameters.

4. Discussion

4.1. Retrieval of soil parameters from observations on crops

The results of parameter estimation vary greatly according to the soil/climate/preceding crop configuration, the parameters, and the set of observed variables. However, some general trends can be drawn. *Hinit* is the best estimated parameter because the observed variables are in general sensitive to this parameter (high first-order indices and poor interaction) and the drier the climate of the configuration the better is the estimate of *Hinit*. The parameters *argi* and *Norg* are the worst estimated parameters because the observed variables are in general less sensitive to those parameters (poor first-order indices and poor interaction) than to the others. The quality of *epc(2)* estimation depends on soil depth: for shallow soils its estimation is good because the observed variables are in general quite sensitive to this parameter, whereas for deep soils the estimate is poor because the observed variables in this case are not very sensitive to it. Considering the quality of estimation of the whole parameter set, the drier the climate the better is the quality of estimation, because the first-order indices are generally higher for dry climates than for wet ones. It was also observed that the greater the number of observations the better is the quality of parameter estimation. This improvement is quite small due to the correlations existing between the observed output variables *LAI*, *QN* and *Yld*. However, it must be noted that a single observation of *Yld* provides as much information for estimating the parameters as ten observations of *QN*. This can be explained by lower correlations between *Yld* and *LAI* + *QN* than between *LAI* and *QN*.

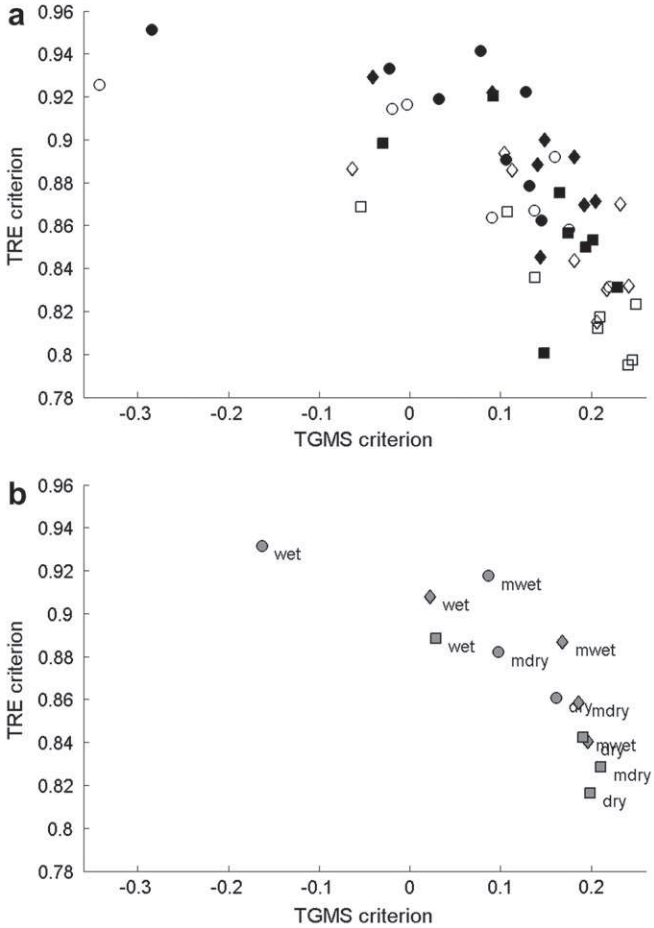

Fig. 4. a) Scatter diagram of the criteria *TRE* and *TGMS* at the whole parameter set level. a) For the 3 sets of observations and the 16 configurations. The symbol "○" corresponds to the set #1, "◆" to set #2 and "□" to set #3. A white symbol corresponds to a shallow soil and a black one to a deeper soil. b) For the 3 sets of observations and 4 types of climate (each of the 12 points is averaged over the 2 soil depth and 2 preceding crop configurations). The labels of the climate types are described in Table 2.

Concerning the parameters which are to be estimated, the question of interaction between them is essential. GSA and GLUE are complementary for explaining this point. Although GSA supplies information on the basic features of interaction structure, it does not allow a complete representation of such a structure (Ratto et al., 2001): the EFAST method does not allow computing each interaction term and computing these terms with the Sobol' method would require an enormous amount of simulations. The GLUE method completes the knowledge of the general interaction structure, allowing pair-wise interactions to be quantified through the computation of correlation coefficients between parameters. In particular, a high level of correlation between two parameters indicates possible compensation between them. This means that bringing new information on one of the two parameters may reduce the posterior uncertainty of the other. This may be done by measuring it and fixing it at the measured value, or improving its prior information, or adding new observations related to this parameter in the estimation process (observations on soil water content for example, as did Braga and Jones (2004)). In our case, if the parameter *HCC(1)* could be measured, the parameters *Hinit* and *epc(2)* would be better estimated than when estimated together with *HCC(1)*. Thus, interactions between these parameters would no longer exist and this may improve the use of the STICS crop model for appropriate management decision support. Some promising possibilities are offered by using electrical geophysical measurements (Samouelian et al., 2005).

4.2. Link between GSA and quality of parameter estimates

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. 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 accounting for both the sensitivity indices and the correlation between variables, and showed its good relationship with the criterion RE_i which measures the quality of estimation of parameter *i*. The criterion GMS_i proved to be effective for ranking the accessible parameters with respect to their quality of estimation. Particularly, GMS_i is able to provide information on which parameters can be estimated and which can be fixed as they do not deserve an accurate determination. 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 may be 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.

5. Conclusion

This study shows on various synthetic experiments that a few soil parameters are accessible by inversion of the STICS crop model from observations of yield at harvest, leaf area index and nitrogen absorbed by the plant at various dates. However, the quality of their estimation largely depends on several factors, in particular the climate of the observed year and the type of soil depth. In view of this, it would be useful to explore the potential of accumulating several years of observations, possibly on different crops, to maximize the effectiveness of soil parameters retrieval. Using additional observations on soil variables should also help in increasing the quality of parameter estimates that sometimes shows strong correlations between them or even retrieving parameters that are not accessible from the observations used in this study. One should also think about using other models giving access to the same or to other soil parameters from the same or from new observed variables. Nevertheless, if the value of estimating some key soil parameters lies in the information produced *per se*, it also lies in the consequent reduction in the uncertainty of the predictions by the STICS model of agro-environmental variables which are used in decision making. Further studies should focus on this aspect.

This study also shows that the quality of parameter estimation can be explained by the results of global sensitivity analysis (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. Other criteria could be proposed and other applicative studies could be useful to explore the link between GSA and parameter estimation in other cases. 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.

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Chapitre 5. Amélioration de la qualité de prédiction des variables d'intérêt à partir de l'estimation des paramètres du sol

Article 3 : "The estimation of soil properties using observations on crop biophysical variables and the crop model STICS improves the predictions of agro-environmental variables". Soumis à European Journal of Agronomy..

5.1. Objectif

Nous avons vu dans le chapitre précédent que la quantité d'information apportée par le jeu d'observations, telle qu'on peut la mesurer par analyse de sensibilité détermine la qualité d'estimation des paramètres sol. Nous proposons ici d'étudier comment elle détermine également la qualité des prédictions des variables d'intérêt agroenvironnemental. Les paramètres considérés sont ceux étudiés au chapitre précédent. Les variables retenues, parmi celles étudiées au Chapitre 3, sont les variables agroenvironnementales déterminées à la récolte : rendement *Yld*, qualité de la production *Prot* (teneur en protéine pour le blé) et quantité d'azote minéral dans le sol *Nit*. La bonne prédiction de ces variables permet en effet de raisonner de manière efficace les choix de l'agriculteur vis à vis de son travail technique, en conciliant intérêts agronomique et environnemental. Par exemple, Houlès et al. (2004) ont montré que des cartes de préconisation de doses d'engrais azoté pouvaient être élaborées à partir de prédictions spatialisées de ces variables et de l'optimisation d'un critère agroenvironnemental. Nous étendrons dans cette étude la diversité des jeux d'observations en considérant, comme dans le Chapitre 3, des observations réalisées non seulement sur blé d'hiver mais aussi sur betterave sucrière, culture qui permet d'exprimer davantage les propriétés des sols.

5.2. Méthodes

Nous avons vu au Chapitre 1.3.2, à travers des résultats bibliographiques, que l'amélioration des prédictions à partir de l'estimation repose sur le fait que les variables à prédire et les variables observables ont des sensibilités similaires aux paramètres estimés. Nous essaierons donc d'expliquer l'amélioration des prédictions en fonction de leurs sensibilités aux paramètres du sol et de déterminer les jeux d'observations qui, grâce à leur quantité d'information efficace, permettent de réduire les incertitudes sur les prédictions. Nous avons défini cette réduction comme l'amélioration de la qualité des prédictions issues des valeurs estimées des paramètres relativement à celle des prédictions issues de l'information a priori (sa valeur moyenne). Comme pour le chapitre précédent, l'estimation des paramètres du sol par inversion sera effectuée par la méthode Importance Sampling et la même information a priori sur les paramètres sera considérée (déduite de mesures expérimentales sur le site de Chambry). Dans une première partie, ce travail est réalisé avec des observations synthétiques du couvert végétal, afin d'explorer toutes les configurations d'observations éventuelles. Ces différentes configurations seront ici composées de :

- deux cultures annuelles différentes (blé d'hiver et betterave à sucre),
- quatre climats contrastés caractérisés comme sec, moyen sec, moyen humide et humide (les même que ceux du Chapitre 4),
- deux gammes de profondeurs de sol (de 30 à 100 cm pour les sols peu profonds et de 80 à 160 cm pour les sols profonds),
- trois types/tailles de jeux d'observations : des observations composées de *LAI* seulement, de *LAI*+*QN*, et de *LAI*+*QN*+rendement.

Dans une seconde partie, de vraies observations réalisées sur le bassin versant de Bruyères (voir Chapitre 2.4) seront utilisées afin de valider, de manière réaliste, les résultats obtenus avec les observations synthétiques. Sachant que les sites de Chambry et de Bruyères sont proches et qu'on y retrouve des formations pédologiques voisines (voir Chapitre 2.4), l'information a priori considérée dans l'application aux observations de Bruyères est la même que celle utilisée pour les observations synthétiques (déduite de Chambry).

5.3. Résultats

Précision et amélioration de l’estimation des paramètres

Nous avons vu dans le Chapitre 4.3 les résultats de l’estimation des paramètres, en termes de précision et d’amélioration, lorsque des observations synthétiques sur couvert végétal de blé étaient considérées. Nous allons à présent présenter ces deux quantités dans le cas où des observations synthétiques sur couvert végétal de betterave sont considérées (résultats non présentés dans l’article). Que ce soit en termes de précision (voir le Tableau 5-1) ou en termes d’amélioration (voir le Tableau 5-2), nous voyons que les observations synthétiques de betterave permettent de diminuer significativement le critère, par rapport à ceux obtenus dans le Chapitre 4.3. Les observations de betterave sont donc plus efficaces pour estimer les paramètres du sol. Pour preuve, les paramètres *HCC(1)*, *HCC(2)* et *epc(2)* ont un critère qui diminue énormément grâce à ces observations (sensibilité à ces paramètres plus importante). Par exemple, en forte profondeur de sol, le critère *RE* du paramètre *HCC(1)* passe de 0.81 (observations de blé) à 0.22 (observations de betterave). Nous noterons que la condition initiale *Hinit* est le seul paramètre moins bien estimé qu’avec des observations de blé (sensibilité à ce paramètre moins importante).

	Condition	*argi*	*Norg*	*epc(2)*	*HCC(1)*	*HCC(2)*	*Hinit*	*NO3init*
RRMSE (%)	–	24.3	25	30.5	**7.8**	**15.1**	39	33.7
	+	24.7	25.2	**18.8**	**4.5**	**12.6**	35.1	32.1
	sec	24.2	26.1	25	**6.2**	**13.6**	33.3	31.4
	humide (humide +)	24.8 (24.9)	24.1 (24.6)	24.3 (**18.5**)	6.1 (**4.5**)	14.1 (**11.6**)	40.8 (39.2)	34.4 (32.4)

Tableau 5-1. Précision moyenne d’estimation des paramètres du sol (*RRMSE*) avec des observations synthétiques de betterave, sachant la condition agropédoclimatique : faible profondeur de sol (**–**), forte profondeur de sol (+), climat sec (sec), climat humide (humide) ou climat humide en forte profondeur de sol (humide +). En gras les *RRMSE* inférieurs à 20%.

	Condition	*argi*	*Norg*	*epc(2)*	*HCC(1)*	*HCC(2)*	*Hinit*	*NO3init*
RE	–	0.96	0.86	**0.49**	**0.31**	**0.63**	0.89	0.98
	+	0.90	0.86	0.86	**0.22**	**0.65**	0.83	0.96
	sec	0.96	0.97	**0.68**	**0.24**	**0.66**	**0.74**	0.94
	humide (humide +)	0.90 (0.88)	**0.75** (**0.72**)	**0.68** (0.85)	**0.29** (**0.26**)	**0.62** (**0.57**)	0.98 (0.95)	1 (1)

Tableau 5-2. Amélioration moyenne d'estimation des paramètres du sol (critère *RE*) avec des observations synthétiques de betterave, sachant la condition agropédoclimatique : faible profondeur de sol (**–**), forte profondeur de sol (+), climat sec (sec), climat humide (humide) ou climat humide en forte profondeur de sol (humide +). En gras les *RE* inférieurs à 80%.

La dernière ligne de chacun des deux tableaux précédents, concernant des conditions climatiques humides et une forte profondeur de sol, permet de comparer les résultats de l'estimation des paramètres issus d'observations synthétiques avec ceux issus d'observations réelles sur le bassin de Bruyères. Ces résultats, présentés dans le Tableau 5-3, montrent que les paramètres *HCC(1)* et *epc(2)* sont effectivement estimables avec une bonne précision lorsque des observations sur couvert de betterave sont considérées (*RRMSE* respectivement égal à 7.6 et 18.6%). Nous voyons également que l'estimation de *HCC(1)* est fortement améliorée par l'inversion avec des observations réelles de betterave (*RE* égal à 0.54).

	argi	*Norg*	*epc(2)*	*HCC(1)*	*HCC(2)*	*Hinit*	*NO3init*
RRMSE %	**17.9**	22.5	**18.6**	**7.6**	26.9	55	87.6
RE	0.8	**0.78**	**0.62**	**0.54**	0.95	1.37	1.41

Tableau 5-3. Précision (*RRMSE*) et amélioration (critère *RE*) moyenne d'estimation des paramètres du sol avec des observations réelles de betterave, pour la condition agropédoclimatique : climat humide en forte profondeur de sol (humide +). En gras les *RRMSE* inférieurs à 20% et les *RE* inférieurs à 80%.

Dans le Chapitre 4, nous avons vu que la configuration d'observation avait un effet significatif sur l'amélioration de l'estimation des paramètres : un climat sec et une faible profondeur de sol permettent d'obtenir les meilleures améliorations des paramètres liés à l'état hydrique du sol (*epc(2)*, *HCC(1)*, *HCC(2)* et *Hinit*), les autres étant difficilement estimables. Nous voyons à présent, avec ces nouveaux résultats, que les observations sur couvert végétal de betterave permettent d'améliorer encore plus l'estimation de ces paramètres, mis à part pour la condition initiale *Hinit*. Dans la partie suivante, nous allons montrer comment l'estimation des paramètres, sous différentes configurations d'observations, peut améliorer les prédictions.

Amélioration des prédictions

Les résultats de l'article montrent qu'il est possible d'améliorer la prédiction des variables agronomiques, telles que le rendement et la qualité du rendement, mais qu'il est malheureusement plus difficile d'améliorer celle des variables environnementales, telles que la quantité d'azote encore présent dans le sol à la récolte. Dans le cas des observations synthétiques, les prédictions issues des valeurs moyennes de l'information a priori peuvent être améliorées par l'estimation jusqu'à 61.4% pour le rendement et jusqu'à 58.9% pour la qualité, alors que la teneur en azote du sol ne peut être améliorée que jusqu'à 19.6%. Lorsqu'une amélioration est possible, les résultats montrent que cela vient principalement du fait que les variables à prédire sont sensibles aux mêmes paramètres que le sont les variables observables. De plus, l'article montre qu'il existe un certain degré dans les améliorations possibles, dans le sens où les jeux d'observations acquis dans différentes configurations contiennent des quantités d'information variables permettant d'améliorer l'estimation, et par conséquent la prédiction, de manière plus ou moins significative. Par exemple, nous avons vu que les conditions climatiques dans lesquelles les observations ont été recueillies ont un effet significatif sur l'estimation et par conséquent sur la prédiction, dans le sens où les conditions sèches sont plus efficaces que les conditions humides. Dans le cas des observations synthétiques, les conditions sèches améliorent les prédictions – relativement aux conditions humides – d'environ 25% pour le rendement et la qualité et d'environ 5% seulement pour la teneur en azote du sol. Le type de profondeur de sol a lui aussi un effet important dans le sens où les résultats d'estimation et de prédiction sont de meilleure qualité sur un sol peu profond que sur un sol profond. Toujours dans le cas des observations synthétiques, la prédiction du rendement est d'environ 0.4 fois meilleure pour le rendement, 0.5 fois meilleure pour qualité et 0.1 fois meilleur pour la teneur en azote du sol, lorsqu'un sol peu profond est considéré au lieu d'un sol profond. Pour finir, l'utilisation de jeux d'observations recueillis sur deux différentes