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A method to assess the impact of soil available water capacity uncertainty on crop models with tipping-bucket approach

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Running title: *Critical Uncertainty of AWC in Crop Models*

Summary

Most agronomic crop models use a reservoir tipping-bucket approach to model the water budget in the soil. Soil available water capacity (AWC) is the main soil property considered in this approach. Because AWC is difficult to measure, uncertainty in AWC may be high. We developed a method using a specific kriging technique to determine the effects of uncertainty in AWC on crop model predictions. The AqYield crop model was used as an example to assess the effects of uncertainty in AWC on two agronomic output variables (grain yield and drainage). The factors considered were the climatic region, crop type and soil depth. We assessed the results using the coefficient of variation (*CV*) and sets of critical values for which *CV* exceeded 5%, 10% and 15%. The experiment provided insight into the criticality of AWC uncertainty over a wide range of agropedoclimatic situations according to crop, model and output of interest. The method revealed the greater effect of AWC uncertainty on both outputs for the spring crop than for the winter crop and to identify cases where AWC uncertainty was critical. There was a stronger effect of AWC uncertainty on yield for shallow soil and climatic water deficit conditions. For each situation, the AWC uncertainty levels were determined above or below which the impact becomes significant on a given output since the sensitivity was very dependent on climate-crop-soil combinations. It was also observed that uncertainty in AWC had little effect in AqYield for a wide range of situations. The method developed uses a small number of model simulations to produce accurate results to better understand the impact of this major soil input data according to the target model and specific objectives. It could help to determine the level of accuracy needed in AWC measurement depending on the objectives.

Keywords: sampling, kriging, uncertainty quantification, drainage, yield

Highlights

- The method quantifies the effects of AWC uncertainty on crop models with a tipping-bucket approach.
- This method can assess the impact of uncertainty with only a few runs using a kriging approach.
- The method identifies critical situations for a wide range of agropedoclimatic conditions.
- Critical region graphs give critical thresholds for accuracy needed in AWC.

Introduction

Many studies use modelling and simulation to analyze the effect of climate on agricultural production or to determine the most suitable irrigation management practices (e.g. Teegavarapu, 2010; Nendel et al., 2014; Ma et al., 2017). Most are based on the description of a biophysical system that includes a crop and a soil component and daily carbon, water and nitrogen fluxes in the soil-plant-atmosphere system influenced by climate and cropping practices. Crop growth and development in such crop models are simulated for a homogeneously managed plot at the one-dimension scale. Effects of climate, soil properties, crop management and ecophysiological crop characteristics are analyzed for different crops and environmental outputs (e.g. phenology, biomass accumulation, grain yield, evapotranspiration, drainage, nitrate leaching, soil carbon storage). Most agronomic crop models use a tipping-bucket approach to model the water budget in the soil (Ritchie, 1981; Ranatunga et al., 2008). In this approach, the soil is considered as a reservoir that provides a given amount of water. Precipitation and irrigation (minus runoff) fill the reservoir, and losses are due to evapotranspiration and, when the reservoir is full (i.e. at field capacity), drainage. Several representations, with differing degrees of abstraction, exist, mainly dividing the soil into different layers subject to different biological and physical processes (e.g. evaporation, transpiration, water uptake, drainage). Available water capacity (AWC) is the main water-related property in these layers.

Available water capacity is the maximum amount of water the soil can store that is available for plant growth. It is an integrative value, determined throughout the entire soil profile, from water content at field capacity to water content at the permanent wilting point, below which a plant is unable to recover the remaining water (Behrman *et al.*, 2015). These two water content limits, whose physical definition remains under discussion (Czyz and Dexter, 2012), are empirical concepts and can have different meanings for soil scientists, agronomists and ecophysiologists. However, AWC is a widespread concept used in many crop models. Different approaches are used to estimate AWC: (i) measurements (e.g. field experiments with different crops to analyze effects of several irrigation regimes by proxy sensor measurements, in-situ water content monitoring, and laboratory measurements of soil cores in pressure chambers) (e.g. Veihmeyer and Hendrikson, 1949); (ii) pedotransfer functions, which are statistical relationships (e.g. with texture, bulk density and organic matter) that are more easily determined (e.g. Bruand et al., 2004); and (iii) optimization processes that use inverse modeling of crop models to compare model outputs and real observations of the soil-plant-atmosphere system, such as soil moisture, crop leaf area index or evapotranspiration (e.g. Guerif et al., 2006).

Whether measured or statistically estimated, uncertainty in the AWC may be considerable, which might influence the quality of crop model predictions. Sensitivity analyses of crop models have demonstrated the sometimes strong but not systematic influence of uncertainty in AWC or its components (e.g. field capacity or wilting point) on predictions of yield, soil water content or annual drainage for instance (Aggarwal, 1995; Lawless *et al.*, 2008; Varella *et al.*, 2012). The uncertainty here is as defined by Spielgelhalter and Riesch (2011) as the uncertainty essentially due to limitations in information, in particular, a lack of quality or accurate data. It concerns input data uncertainty, which is one of the three main sources of uncertainty in modelling, along with parameter data and model structure (Walker et al., 2003). Information about AWC may be limited for several reasons. In soil considered as homogeneous, there is still some spatial variability in its properties, and there are some uncertainties in the methods used to measure AWC directly. In the case of pedotransfer functions, applied to a national database, for instance, there is uncertainty in soil parameters such as clay content, soil depth and soil organic matter, as well as on the function chosen that uses this information to estimate field capacity and permanent wilting points. Usually, the distribution for these parameters is unknown, and the uncertainty can be large.

Consequently, the main research question is: “How important is accuracy in estimating the AWC and to what extent does the level of accuracy depend on soil properties, climate and crop species?” Depending on the weather, crop and management practices, the accuracy in AWC may influence the accuracy of simulation model predictions. The objective of our study was to develop a modelling approach to quantify the effects of uncertainty in AWC on agronomic model predictions according to the crop type, climate and soil depth and to identify critical thresholds for accuracy. This differs from a classic sensitivity analysis, since we aim to define critical sets of input variables that provide a given accuracy in output variables.

Materials and Methods

AqYield crop model overview

AqYield is a simple and generic crop model that simulates crop production and water balance at a daily time-step (Fig. 1). A complete description of the model and its quality of prediction for different crops and soil and climate conditions can be found in Constantin et al. (2015). The model was designed to be generic, i.e. simulating several crops using one single approach and changing only crop parameters. Crop phenology is defined by three stages as a function of thermal time corrected with photoperiodic effects for winter crops: emergence, flowering and physiological maturity. Crop development is simulated using a crop coefficient to calculate water requirements, and root elongation is used to estimate the available water in the soil. The model does not simulate biomass growth; it calculates yield at harvest using a production function based on the water stress during the crop development period and a maximum yield that is an input of the model. Soil is simulated using a tipping-bucket approach. The user inputs clay content, depth and AWC throughout the entire soil profile. Available water capacity in the model is the maximal water content available for the crop over the soil depth reachable by roots. It is usually defined as the water amount between the wilting point and field capacity. AqYield simulates water-balance components (e.g. evaporation, transpiration, drainage and runoff) and the daily soil water content above wilting point. AqYield is simpler than other crop models (Palosuo *et al.*, 2011; Rötter *et al.*, 2012) and is well suited to demonstrate our approach. It is important to highlight that AqYield was chosen to illustrate the method we developed, not to understand the model's internal behaviour better.

Figure 1

Identifying thresholds

AWC uncertainty and probability distribution law

In our approach, AWC was considered as an uncertain input in the AqYield model. A classic approach is to perform simulation-based uncertainty propagation. More formally, given X, a random input variable with known distribution $\mathcal{F}(X)$, the output of interest $Y=f(X)$ with f the AqYield model is also random, with (unknown) distribution $\mathcal{F}(Y)$. To quantify the uncertainty in the output variable (Y), we used the coefficient of variation (CV), according to Varella et al. (2012). The CV of output Y was defined as $CV(Y) = \frac{\sigma(Y)}{E(Y)}$, with σ the standard deviation and E the mathematical expectation. $CV(Y)$ can be considered a function of the input distribution $\mathcal{F}(X)$. Our objective was to find at what values of $\mathcal{F}(X)$ $CV(Y)$ reached a critical level (a maximum variation in the output chosen by the model user depending on the user's objectives). Here, we chose grain yield (t ha^{-1}) and water drainage (mm).

Without losing generality in the approach, we assumed that AWC followed a uniform distribution ($\mathcal{U}$) between a lower (X_L) and upper boundary (X_U), $\mathcal{F}(X)$=$\mathcal{U}(X_L,X_U)$, which we characterized by its mean and standard deviation ($\mu_X = \frac{X_L + X_U}{2}$ and $\sigma_X = \frac{X_L - X_U}{\sqrt{12}}$, respectively). Next, we defined the set of critical values $\mathcal{F}(X)$ as all pairs (μ_X,σ_X) for which the *CV* exceeded a given threshold: Ω_c = {(μ_X,σ_X) such that $CV(\mu_X,\sigma_X) > \alpha$}. We chose three values for α: 5%, 10% and 15%, which are common levels of *CV* for experimental results in agronomy (Bassu et al., 2014). Our objective was then to identify the critical region(s) Ω_c in the (μ_X,σ_X) plane.

Since the AqYield model is considered as a (non-linear) "black-box", the distribution $\mathcal{F}(Y)$ can be inferred (using parametric or non-parametric techniques) only by drawing random samples of *X* for a given pair (μ_X,σ_X), $\{X_1,\ldots,X_n\}$ and evaluating model outputs for these samples: $\{Y_1 = f(X_1),\ldots,Y_n = f(X_n)\}$. For *CV*, one may simply use the empirical estimator $\widehat{CV}(Y) = \frac{\sigma(Y_1,\ldots,Y_n)}{E(Y_1,\ldots,Y_n)}$.

Obtaining accurate estimates requires a sufficient sample size *n*; however, sample size is limited by computational resources because it directly determines the number of runs of AqYield.

Kriging

A typical way to obtain the set Ω_c is to discretize the $\{\mu_X,\sigma_X\}$ domain across a grid and calculate $\widehat{CV}(Y)$ for all value combinations. However, this approach would result in overly-intensive simulation experiments because even a coarse grid (10 μ_X values ×10 σ_X values) with n=100 replicates would require 10,000 runs of AqYield. Instead, we followed the strategy developed by Picheny et al. (2010) that relies on the kriging model, as follows:

1. *CV* is calculated for an initial set of nine pairs of (μ_X,σ_X) evenly distributed in the (μ_X, σ_X) space.
2. A kriging model is fitted to these data.
3. Nine additional pairs of (μ_X,σ_X) for which *CV* is calculated are chosen sequentially according to a criterion calculated using the kriging model (namely the *targeted IMSE criterion* of Picheny et al. (2010)), the model being updated after each new *CV* value is calculated.

In brief, after the initialization step, the kriging-based approach iteratively chooses new observations so that the boundary between critical and non-critical regions (i.e. where the *CV* exceeds or does not exceed the threshold, respectively) quickly becomes accurate. The numbers of initial and additional pairs required to obtain an accurate kriging model generally depends on the problem. We determined that nine initial observations followed by nine sequential observations provided a reasonable trade-off between kriging accuracy and computational cost. This number is in line with the classic kriging rule-of-thumb of setting the number of observations equal to 5-10 times the dimension (here, two).

The sequential strategy was conducted using the R package KrigInv (see Chevalier et al., 2014 for more details about its theoretical elements and implementation). The kriging equations and relevant technical details are provided in the Supporting Information, along with an illustration of the method.

Experimental design

We analyzed two crop model outputs to evaluate effects of uncertainty in AWC: (i) yield, for the influence on crop production, and (ii) cumulative water drainage during crop development, for the influence on an environmental variable (Table 1). We selected two major crops: winter wheat (winter crop) and sunflower (spring rainfed crop). Winter wheat was simulated from 1 October to 10 July and sunflower from 1 May to 1 October, both starting with maximum AWC at sowing. Both crops were assumed to be limited only by water (well fertilized and well protected against pests and diseases). Crop variety remained the same for each crop regardless of the soil, site or climate. Sunflower reached physiological maturity at 1720°C-days (base 4.8°C) and wheat at 2015°C-days (base 0°C). For both sites, based on statistics from both regions (https://stats.agriculture.gouv.fr/disar-web/accueil.disar), maximum yield was defined as 7.3 and 4.2 t ha^{-1} for winter wheat and for sunflower, respectively, using the highest values found in the statistical data since it is a potential yield.

Table 1

To test our method, two 15% clay soils were selected: a 0.8 m shallow soil and a 1.5 m deep soil. We chose soils with contrasting depth, hypothesizing that a user would have some prior knowledge about the soil and that the impact of AWC uncertainty may vary with the amount of total available water in the soil and its availability for the crop during its development. For each soil, we assumed that the volumetric AWC ranged from 0.10-0.16 mm_{water} mm_{soil}^{-1}. This range was chosen from field experiment measurements obtained during the RUEdesSOLS project (unpublished data). Multiplying soil depth by the volumetric AWC yielded AWCs of 80-140 mm for the shallow soil and 140-240 mm for the deep soil. As a result, μ_X varied from 80-140 mm and σ_X from 0-50 mm for shallow soil. For deep soil, μ_X varied from 140-240 mm and σ_X from 0-50 mm.

We chose two contrasting sites for climate data, one in southwestern France (Toulouse, 43° 33' N, 1° 26' E) and one in western France (Poitiers, 46° 33' N, 0° 17' E), in regions where both crops are cultivated. Our initial climate data consisted of daily measurements of mean temperature, potential evapotranspiration (PET) and precipitation from 1975-2012. Because the effect of uncertainty in AWC may depend greatly on weather conditions, due to the large difference in water inputs that can occur, we performed the analysis using a representative set of climates. To simplify the approach (see next section), we classified the 38 years of records into four types of climates for each site (Warm&Dry, Warm&Wet, Cold&Dry, Cold&Wet). For each crop development period, we first calculated the thermal time (TT, in °C-days) to split the dataset into warm and cold years for each crop according to its base temperature (0°C and 4.8°C for wheat and sunflower, respectively). Then, each subset was split in half again according to a water deficit indicator (WD_c, in mm), and calculated as the cumulative difference between precipitation and PET, to distinguish dry and wet years. The division was based on median values to obtain four subsets of equal size. Finally, the year closest to the centre of each subset (Euclidian distance) was selected as that subset's representative year.

Modelling and simulation

AqYield was used in the modelling and simulation platform RECORD (Bergez et al., 2013), which creates and connects models with a graphical user interface (using a "box and arrow" approach) and performs multiple simulations. All simulations were performed using R (R Core Team, 2014) and the "rvle" package (http://www.vle-project.org/vle-11/rvle/) to run models in RECORD directly under R. Our experiments required 115,200 runs of AqYield to generate for one output all the graphs for the 32 conditions (2 sites × 4 climate types × 2 soil depths × 2 crops); the model also required 3600 runs for the three α levels.

Results

Presenting kriging results in "critical region" maps

Using the kriging approach, we are able to represent, for a given soil depth, climate region and crop type, a threshold value and intervals of variation for both AWC mean and standard deviation, the corresponding map of the critical region in the (μ_X,σ_X) space. Since the critical region corresponding to a given threshold is a subset of the region corresponding to a smaller threshold, we represent the three critical regions (for α= 5%, 10% and 15%) in a single graph (Fig. 2). With this approach, unfavourable combinations of AWC mean and standard deviation as a function of the targeted level of uncertainty can be directly identified.

Figure 2

In the example (Fig. 2), *CV* exceeds 15% at small μ_X values and large σ_X values. Conversely, at large μ_X values, even high uncertainty has little effect on the output; for example, an AWC of 125 ± 50 mm leads to a stable prediction of yield (variation below 15%). If the acceptable variability is smaller, 10% for instance, for an expected value of 125 mm AWC, the uncertainty should not exceed ± 35 mm.

In addition to the graphical representation, we calculated the average critical region as a summary measure (Fig. 2, approximately 0.18 for α=15%). In this example, this critical region of 0.18 means that 18% of the set of distributions considered for AWC (the (μ_X, σ_X) space) leads to variability in yield prediction above the chosen threshold.

Climate selection

As expected, the climate in Toulouse was warmer and drier than that in Poitiers during the periods of sunflower and wheat crop development (Fig. 3). During sunflower development, WD_c ranged from -572 mm to -238 mm in Toulouse and -388 to -167 mm in Poitiers, while TT ranged from 2010-2336°C-days in Toulouse and 1752-1999°C-days in Poitiers. During winter wheat development, WD_c ranged from -249 to +114 mm in Toulouse and +7 to +271 mm in Poitiers, while TT ranged from 2599-3011°C-days in Toulouse and 2282-2643°C-days in Poitiers.

Figure 3

Regardless of the crop, the same type of climate always had higher TT and lower WD_c in Toulouse than in Poitiers (Table 2). As expected, the spring crop had a greater WD_c than the winter crop. Dry years were drier in hot years than in cold years, and wet years were wetter in cold years than in hot years.

Table 2

Agronomic results

The model slightly overestimated grain yield compared to those in regional statistics, which is not surprising since AqYield cannot represent all limiting factors. As expected, yield was lower, by 0.71 and 0.58 t_{DM} ha^{-1} on average for sunflower and wheat, respectively, and drainage was slightly higher, by 8 and 4 mm on average under sunflower and wheat, respectively, in shallow soils than in deep soils regardless of the climate, site and crop (Fig. 4). No general trend was observed regarding the site, but yields tended to be lower when the climate was drier, because of greater water stress due to greater WD_c. On average, the water stress index was 0.50 and 0.64 (1 = no stress) in dry years and 0.67 and 0.73 in wet years for sunflower and wheat, respectively. The standard deviation of yield was always higher for shallow soils than for deep soils due to the greater variation in yields from 30 to 190 mm AWC, which implies different levels of water stress (from 0.42 to 0.73, respectively, on average). Yields were much more stable in deep soil, where the AWC ranged from 90-290 mm, due to the absence of impact of AWC on water stress, which remained stable on average.

The amount of drainage depended greatly on the length and timing of crop development with, on average, 42 mm under sunflower compared to 265 mm under wheat. Since sunflower grew for five months in spring and summer, precipitation and then drainage during its development were lower than those during winter wheat development, which lasted nine months and included winter precipitation. In fact, mean precipitation was 277 mm under sunflower vs. 539 mm under wheat. Significant site effects were predicted for drainage under wheat, which was twice as high in Poitiers (353 mm) as in Toulouse (176 mm).

Figure 4

Effects of uncertainty in AWC on yield and drainage

We present here the main results in the form of an average critical region (Table 3) and probability of critical region (Fig. 5) for the 32 agropedoclimates. The critical region of the thresholds always followed this order: 5% threshold ≥ 10% threshold ≥ 15% threshold (Table 3). This was due simply to the smaller degree of tolerance for variation in output at 5% than at 15%.

Table 3

The effect of uncertainty in AWC ranged from never critical (area=0.00) to highly critical (area=0.99), with many intermediate situations. Unexpectedly, for approximately two-thirds of the simulated cases, AWC uncertainty was not critical for either model output. Uncertainty in AWC had greater effects on the two outputs when simulating sunflower (spring crop) than when simulating winter wheat (winter crop), which could be due to different crop sensitivity to water stress. For example, the critical region at the 15% threshold reached a maximum of 0.81 for sunflower yield but was always 0.00 for wheat yield (i.e. for the set of distributions considered for AWC, 81% and 0% led to excessive variability in yield prediction for sunflower and wheat, respectively). The crop also had a strong influence on drainage, with one-third of cases having 0.35 critical region at the 10% threshold for sunflower, while no case exceeded 0.01 critical region for wheat. In some cases for sunflower, the critical region reached 0.99, meaning that even a small uncertainty had a large impact on drainage. Conversely, the critical region for wheat was almost always 0.00 for yield and drainage at 10% and 15% thresholds.

The critical region for yields was higher for shallow soil than for deep soil. For sunflower, the critical region at the 5% threshold ranged from 0.00-0.20 for deep soil and from 0.13-0.95 for shallow soil. It was lower at the 15% threshold but still reached 0.81 in the

Hot&Dry climate. Certain situations remained sensitive to uncertainty in AWC when the threshold was changed to 15%, such as the Hot&Dry climate in Poitiers in shallow soil, which had a critical region of 0.81. The critical regions for wheat yield were lower than those for sunflower, with 0.00-0.01 for deep soil and 0.00-0.44 for shallow soil at the 5% threshold. Areas tended to be larger in a Hot&Dry climate than in a Wet&Cold climate for both crops on yield.

For drainage, the influence of climate was less clear, especially for sunflower. The period of crop development (spring vs. winter) seemed to be the main factor. Drainage under sunflower was more sensitive to uncertainty in AWC than that under wheat, for which uncertainty in AWC had no influence except for two cases in Toulouse. In Dry&Hot years in Toulouse for both soil depths and in Poitiers for deep soil, drainage was null under sunflower; so, uncertainty in AWC had no influence, regardless of its value. The Hot&Dry climate in Toulouse had no critical region due to the lack of drainage. Soil depth also influenced drainage sensitivity to uncertainty in AWC, with more sensitivity in shallow soil than in deep soil. However, effects of uncertainty could be substantial in deep soil, such in the Cold&Wet climate in Toulouse or the Hot&Wet climate in Poitiers, which had critical regions greater than 0.45 at the 15% threshold. Fig. 5 shows all simulation results and graphs of the critical regions reported in Table 3. The main differences occurred in yield and drainage between sunflower and winter wheat, followed by differences in sunflower yield between shallow and deep soils. Depending on the graph, the critical region did not occur for the same AWC mean and standard deviation combination and three main patterns can be distinguished.

Figure 5

In the first pattern, AWC mean and standard deviation do not influence the output of interest greatly in a specific context (Fig. 5, dark grey only). In the second pattern, critical

AWC uncertainty occurred for small mean and large standard deviation (Fig. 5, top left of graphs). The second pattern was found mostly on yield response to AWC but on some drainage response as well (e.g. {Cold&Dry, Toulouse, Shallow soil, Winter wheat}). This pattern allows, for each condition and threshold, two interesting values to be determined: the mean AWC above which uncertainty has no impact on the output of interest and the uncertainty below which the output does not vary more than the threshold, regardless of the mean AWC. In the third pattern, critical AWC uncertainty occurred when both standard deviation and mean AWC were large, as on drainage (Fig 5, top right of graphs) (e.g. {Cold&Dry, Poitiers, Shallow soil, Sunflower}). This pattern also shows some interesting thresholds, such as the mean AWC below which uncertainty matters little or not at all. These graphs complement quantitative critical regions (Table 3) since they can be used to define such thresholds and identify combinations of mean and standard deviation of AWC for which uncertainty matters or does not.

Discussion

The method developed

Our experiments enabled the identification of critical situations of AWC uncertainty for a given output and variation threshold (Fig. 4 & 5). Transferring this method to more computationally demanding and sophisticated models potentially raises two challenges. First, the maximum feasible number of runs may decrease greatly. Second, the shape of critical AWC uncertainty areas might become more complex, which requires more model runs to provide an estimate. Our approach accommodates such a framework because the combined use of kriging models and adaptive sampling has been shown to be an efficient alternative when data are scarce, even for multimodal functions (Picheny et al., 2010). The number of runs required to estimate a single *CV* value (n, see section 2.2) can be drastically reduced (e.g. to a dozen) as long as the kriging model accounts for the loss of accuracy (Ankenman et al., 2009). A more complex but more efficient solution could be to fit a single kriging model to all conditions by considering conditions as qualitative factors (Qian et al., 2012).

The uniform distribution to model uncertainty in AWC was chosen since we did not have information about the actual distribution. A different distribution (e.g. triangular, truncated normal) can be used without changing our method; however, in a preliminary study, we found that it had little influence on *CV* areas of exceedance (data not shown). This method, applied to AWC in this study, can also be used to determine the degree of accuracy needed for other input parameters in a particular context and for a given crop model. It may be relevant to apply it to important input data that are uncertain, such as soil properties, like AWC in this study.

Data sampling and accuracy

This method can determine several key values, such as the AWC value above which uncertainty does not influence the output of interest above a chosen threshold. It can also assess the uncertainty in AWC below which, regardless of the AWC, this uncertainty does not influence the output above the threshold. These types of quantification are not easily accessible information and likely depend on the model chosen, as well as the agropedoclimatic conditions considered. If one has prior knowledge of the type of climate, the crop and desired outputs, the method can determine the degree of accuracy required to estimate soil AWC used as input for a specific model. Therefore, our method could identify situations in which accuracy in AWC is not important and situations in which it is essential for the chosen model. This could save time and resources to focus on more important inputs under specific conditions. It could also help to choose the most suitable methods to estimate or measure AWC, with differing degrees of accuracy according to the research objective. For example, if uncertainty in AWC has little influence on the model output of interest, one can choose a small number of soil measurement replicates to sample. In contrast, it could be important to have as little uncertainty as possible and increase the number of samples to obtain an accurate AWC. Thus, the influence of uncertainty in AWC can be analyzed prior to measurements to provide recommendations for measuring it.

Effects of uncertainty in AWC for the AqYield model

This analysis shows that, for yield, uncertainty in AWC influenced spring crop predictions more than winter crop predictions due to less precipitation during sunflower development and the absence of irrigation, especially in dry climates. We expected this result according to previous knowledge on water availability and crop production (e.g. Zhang & Oweis, 1999; Pandey *et al.*, 2000). Since potential yield was lower for sunflower (4.2 t_{DM} ha^{-1}) than for wheat (7.5 t_{DM} ha^{-1}), a smaller absolute variation in sunflower yield was required to exceed a given threshold. If the potential yield were higher than the ones we chose here, larger absolute variation would have been required to reach the critical thresholds and conversely if they were lower. In fact, using the CV induces higher sensitivity to small mean values, which may not be relevant for all outputs.

Notably, our study highlights that the accuracy in AWC measurements or estimates is not important in two-thirds of the cases in our simulation experiment, for both outputs. This result is consistent with that of Vanuytrecht et al. (2014), indicating that model sensitivity to parameter uncertainty depends on agropedoclimatic conditions. Like these authors, we found that uncertainty in soil water properties has more influence on yield when environmental conditions induce water stress. In deep soil, our analysis shows that ±40 mm of uncertainty in AWC has no significant effects on simulated wheat yield regardless of the climate or sunflower yield in several climates because it did not change the degree of water stress significantly. Consistent with other studies on yield and AWC (Lawless *et al.*, 2008), greater accuracy in AWC is needed for shallow soil due to the greater water stress induced by low AWC. In our method, the minimum level of accuracy needed can be determined using graphical analysis (Fig. 5). For instance, uncertainty in AWC measurement less than ±20 mm has no influence on winter wheat yield.

For drainage, unlike with yield, in several cases uncertainty in AWC had great influence in both shallow and deep soils. Interestingly, for a given AWC, the critical level of uncertainty changed with soil depth (e.g. for sunflower, at AWC = 140 mm, the critical uncertainty was sometimes lower in shallow soil than in deep soil (Fig. 5)). In this case, drainage was higher in the deep soil than in the shallow one, as opposed to the general tendency presented in figure 4. This trend is due to a difference in evaporation from the soil. Available water capacity of the layer where evaporation can occur is reduced in the deep soil, with less water available at the surface. As a result, drainage is higher in deep soil than in shallow soil for the same AWC. It takes a larger change in drainage due to AWC uncertainty to reach the critical threshold since the coefficient of variation depends on the mean value. Given the formula for calculating the coefficient of variation (division by the average value), to reach the same percentage requires a larger change in absolute value if the average value is higher.

The size of the critical region depended greatly on the crop, due mainly to the period of development. Drainage under sunflower was low (usually < 100 mm), and small changes in its value due to uncertainty in AWC caused it to cross the critical threshold, while larger changes were required for winter wheat drainage. The choice of the threshold (here, 5%, 10% and 15%) should consider this fact in combination with the purpose of the study. Comparing the two outputs reveals that they do not respond in the same way, and critical cases in which accuracy in AWC is needed are not necessarily the same. This is due to differences in mechanisms driving these outputs, which indicates that, for other outputs, the method needs to be applied to determine their sensitivities to uncertainty in AWC.

Application to other soils, climates and sites

Two soils of contrasting depth were studied to show the potential interaction between crop development, soil depth and AWC uncertainty. As hypothesized, soil depth can change the critical conditions for AWC uncertainty and should be considered in future studies if it is known. If not, the method can be applied to a continuum from low to high AWC and even with increased uncertainty in AWC if relevant (e.g. for some soil types). The study simulated four climate years at each of two contrasting sites, which represents non-exhaustive diversity in climate; however, it does identify several trends according to the type of climate. Based on our results for the two sites, we can extrapolate that in wetter climates than those tested, uncertainty in AWC would have less influence on yield due to less water stress and little or no influence on winter drainage due to the increase in drainage with more precipitation. We also expect AWC to have less influence in summer due to the increase in drainage, which then requires more absolute variation to exceed the critical threshold.

In climates drier than those studied, summer drainage under sunflower, for instance, would tend to be null, and uncertainty in AWC would no longer have an influence, while winter drainage would decrease and probably become more sensitive to uncertainty in AWC than that in dry years in Toulouse. For yield, a drier climate might have a stronger influence with less AWC, especially spring crops. When irrigation is introduced, the importance of uncertainty in AWC for yield predictions decreases greatly because more water is available to the crop, becoming more similar to the results of the wet climate simulated.

For a given site, selecting four contrasting years in a 38-year time series allowed us to explore a good part of the climatic variability while limiting the number of simulations, even though it did not represent the more extreme years. Since we classified and selected the "representative" years for each crop according to important climatic variables (temperature and precipitation minus potential evapotranspiration), we obtained good representation of climate variability for spring and winter crops at these sites. Statistical analysis of the 38 years of climate could be useful for extrapolating our results and calculating the probability of AWC uncertainty having a high influence and the need for accurate measurements. Nevertheless, if one is interested in extreme years, these years should be analyzed using the method developed. As mentioned, while some extrapolation is possible, it is interesting to apply this method to specific conditions to assess the pattern of response to and useful threshold of AWC uncertainty.

Use of other models

The method we developed and applied to the AqYield model as an example is applicable to other crop models. AqYield used AWC throughout the soil profile as a direct input, but crop models using field capacity and wilting points as inputs to calculate AWC would need to have consistent variations in these two soil parameters generated first. Since all models do not necessarily have the same response to water stress and availability, predictions and sensitivity to AWC uncertainty can differ. A trend similar to that observed for AqYield would probably occur since crop models simulate the same phenomenon, but with different degrees of uncertainty above which outputs would change significantly. Another potential extension is to apply our method to other input parameters, such as soil clay content, initial biomass of a perennial crop, and initial nitrogen or carbon content of the soil.

Consequences for water management

We simulated crops without irrigation because rainfed systems are expected to be the most sensitive to uncertainty in AWC. Regarding irrigation and the influence of uncertainty in AWC on water management, uncertainty in AWC may have an influence on beginning and ending dates for irrigation and also change the frequency and amount of irrigation (Bergez et al., 2001). However, for uncertainty in AWC to have an influence on irrigation, indicators used to trigger irrigation should be related to the AWC. Typical indicators such as dates, precipitation and phenological stages are not directly related to AWC; in contrast, tensiometer indicators, closely related to AWC, are most often used. In the latter case, the influence of AWC uncertainty on irrigation management could be quantified.

Conclusion

This study developed a method to identify critical thresholds for uncertainty in AWC, according to specific conditions of climate, soil, crop and outputs of interest. It allows, with a limited number of simulations, to assess the critical conditions for which a given output is influenced by uncertainty in this major input variable in a crop model using a tipping-bucket approach. In this case study, it has highlighted in which cases AWC has a significant impact and identified the numerous situations where the outputs were not sensitive to AWC uncertainty due to the climatic conditions. The method is not specific to AWC and can be applied to other model parameters that are uncertain and assumed to influence outputs of interest, such as AWC, that are major inputs, difficult to measure accurately and that can influence crucial water resources. This method can be applied to other models, with some adaptation of wilting point and field capacity input instead of AWC, and conditions depending on the objectives of future studies. It can give some indications to choose the effort needed to measure model input parameters as a function of the influence of their uncertainty on the outputs of interest.

Acknowledgments

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Data aavailability statement

Data available on request from the authors

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TABLES

Table 1. Factors simulated and outputs analyzed in the simulation experiment. Each crop was simulated in all soils and sites. A given climate type differs according to the site (i.e. the Hot&Dry climate is hotter and drier in Toulouse than it is in Poitiers).

Crops	Species	Sunflower	Winter wheat
	Sowing & harvest dates	1 May - 1 Oct	1 Oct - 10 Jul
	Flowering & maturity	1120-1720°C-days	1300-2015°C-days
Soils	Depth	Shallow - 0.8 m, Deep - 1.5 m	
	Available water capacity	Shallow - 80-140 mm, Deep - 140-240 mm	
Climate	Site (coordinates)	Toulouse (43° 33'N, 1° 26'E), Poitiers (46° 33'N, 0° 17'E)	
	Climate types by site	Cold&Dry, Hot&Dry, Cold&Wet, Hot&Wet	
Outputs		Crop yield, Water drainage	

Table 2. Characteristics of the four years selected for each site during crop development. Thermal time (TT) is the sum of temperatures between sowing and harvest calculated with a base temperature of 0°C for wheat and 4.8°C for sunflower. WD_c is the water deficit, calculated as the difference between precipitation and potential evapotranspiration during the crop development period.

		Sunflower		Winter wheat	
Characteristic	Climate	Toulouse	Poitiers	Toulouse	Poitiers
TT (°C-days)	Cold&Wet	2010	1752	2669	2282
	Cold&Dry	2113	1823	2599	2348
	Hot&Wet	2281	1966	2897	2545
	Hot&Dry	2336	1999	3011	2643
WD_c (mm)	Cold&Wet	-238	-167	114	271
	Cold&Dry	-402	-321	-18	7
	Hot&Wet	-403	-227	-90	249
	Hot&Dry	-572	-388	-249	58

Table 3. Critical region at 5%, 10% or 15% thresholds of variation for each output according to uncertainty in available water capacity (AWC). Darker shading indicates higher values. On average, AWC ranged from 80-140 mm and 140-240 mm for shallow and deep soil, respectively. *NA: drainage under the crop is null regardless of the AWC.

			Critical region graphs for yield				Critical region graphs for drainage			
			Sunflower		Winter wheat		Sunflower		Winter wheat	
Climate	Site	α	Shallow soil	Deep soil	Shallow soil	Deep soil	Shallow soil	Deep soil	Shallow soil	Deep soil
Hot&Dry	Toulouse	0.05	0.72	0.02	0.44	0.01			0.31	
		0.10	0.40	0.00	0.06	0.00	NA*	NA	0.01	0.00
		0.15	0.06	0.00	0.00	0.00			0.00	
	Poitiers	0.05	0.95	0.20	0.36		0.99			
		0.10	0.88	0.09	0.01	0.00	0.97	NA	0.00	0.00
		0.15	0.81	0.03	0.00		0.96			
Cold&Dry	Toulouse	0.05	0.73	0.02	0.24		0.53	0.07	0.22	
		0.10	0.43	0.00	0.05	0.00	0.23	0.00	0.00	0.00
		0.15	0.16	0.00	0.00		0.08	0.00	0.00	
	Poitiers	0.05	0.83	0.08			0.71	0.39		
		0.10	0.63	0.00	0.00	0.00	0.42	0.03	0.00	0.00
		0.15	0.43	0.00			0.13	0.00		
Hot&Wet	Toulouse	0.05	0.68	0.02	0.10		0.42	0.01		
		0.10	0.34	0.00	0.00	0.00	0.01	0.00	0.00	0.00
		0.15	0.10	0.00	0.00		0.00	0.00		
	Poitiers	0.05	0.13		0.12		0.99	0.95		
		0.10	0.01	0.00	0.00	0.00	0.97	0.90	0.00	0.00
		0.15	0.00		0.00		0.95	0.84		
Cold&Wet	Toulouse	0.05	0.35				0.92	0.82		
		0.10	0.06	0.00	0.00	0.00	0.83	0.63	0.00	0.00
		0.15	0.00				0.75	0.45		
	Poitiers	0.05	0.52				0.20			
		0.10	0.21	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		0.15	0.06				0.00			

FIGURE CAPTIONS

Figure 1. Conceptual diagram of the AqYield model. PET is potential evapotranspiration, P+I is precipitation plus irrigation, T is temperature and AWC is available water capacity for crops.

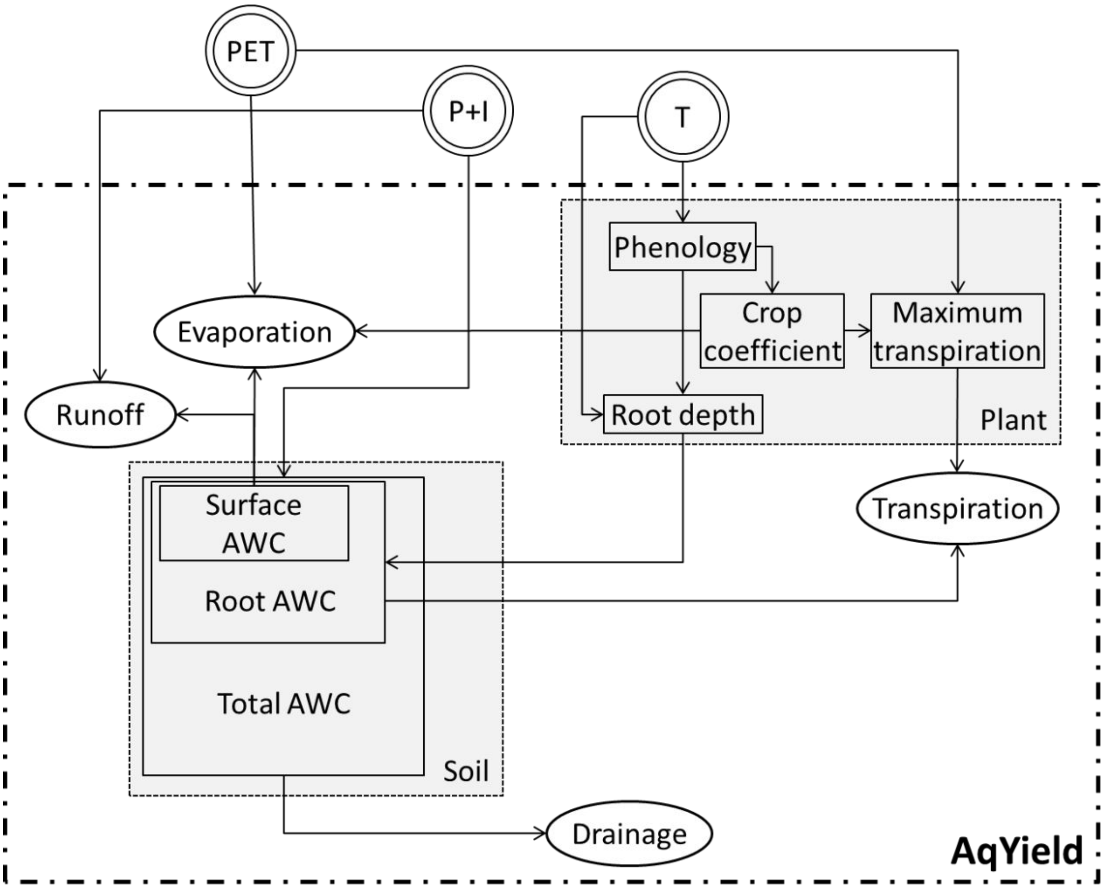
Figure 2. Sample illustration of the threshold graph. The x-axis shows mean available water capacity (AWC), ranging from 80-140 mm for shallow soils and, not shown, 140-240 mm for deep soils. The y-axis shows the standard deviation of AWC, ranging from 0-50 mm. A: areas in which the coefficient of variation (*CV*) exceeds all three thresholds (5%, 10% and 15%); B: area in which the *CV* does not exceed either 5%, 10% or 15% threshold; C: thresholds between A and B (depending on the threshold chosen). X*: average AWC above which the *CV* is always non-critical (for $\alpha<15\%$), regardless of the standard deviation (up to 50 mm), Y*: standard deviation below which the *CV* is always non-critical (for $\alpha<15\%$), regardless of the average AWC.

Figure 3. Representation of the climates (cumulative precipitation minus potential evapotranspiration (P-PET) as a function of thermal time) of (a and c) Poitiers and (b and d) Toulouse for 1975-2012 (circles) during the development periods of (a and b) sunflower (1 May – 1 October) and (c and d) winter wheat (1 October – 10 July). Each graph is divided into four types of climates: warm and wet (green), warm and dry (red), cold and wet (blue) and cold and dry (purple).Triangles indicate means of all climate years.

Figure 4. Predicted mean yield of (a) sunflower and (c) wheat and mean drainage under (b) sunflower and (d) wheat according to crop, type of climate and soil depth when AWC varies uniformly from 30-190 mm and 90-290 mm for shallow and deep soil, respectively.

Error bars represent the standard deviation due to the variation in AWC (30-190 and 90-290 mm according to the soil type).

Figure 5. Threshold graphs for yield and drainage according to type of climate, site, soil depth and crop (described in Fig. 2). The x-axis shows mean available water capacity (AWC), ranging from 80-140 mm for shallow soil and 140-240 mm for deep soil. The y-axis shows the standard deviation of AWC, ranging from 0-50 mm (as in Fig. 2). The three thresholds of 5%, 10% and 15% are represented on the graphs if relevant (dark gray <5%, gray > 5%, light gray > 10% and very light gray > 15%). NA: drainage under the crop is null regardless of the AWC.



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703 Figure 1

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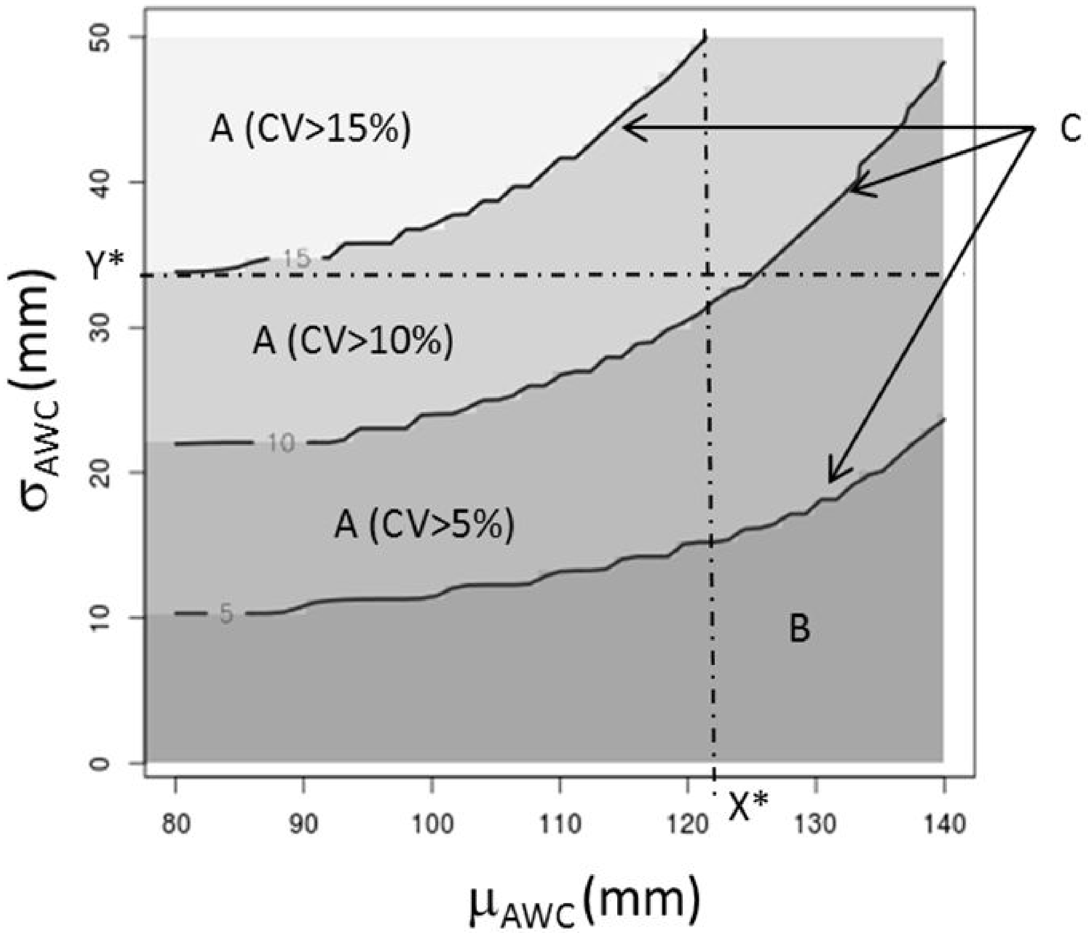

A (CV>15%)
A (CV>10%)
A (CV>5%)
B
C
Y*
X*
15
10
5
σ_{AWC} (mm)
μ_{AWC} (mm)
0
10
20
30
40
50
80
90
100
110
120
130
140

Figure 2

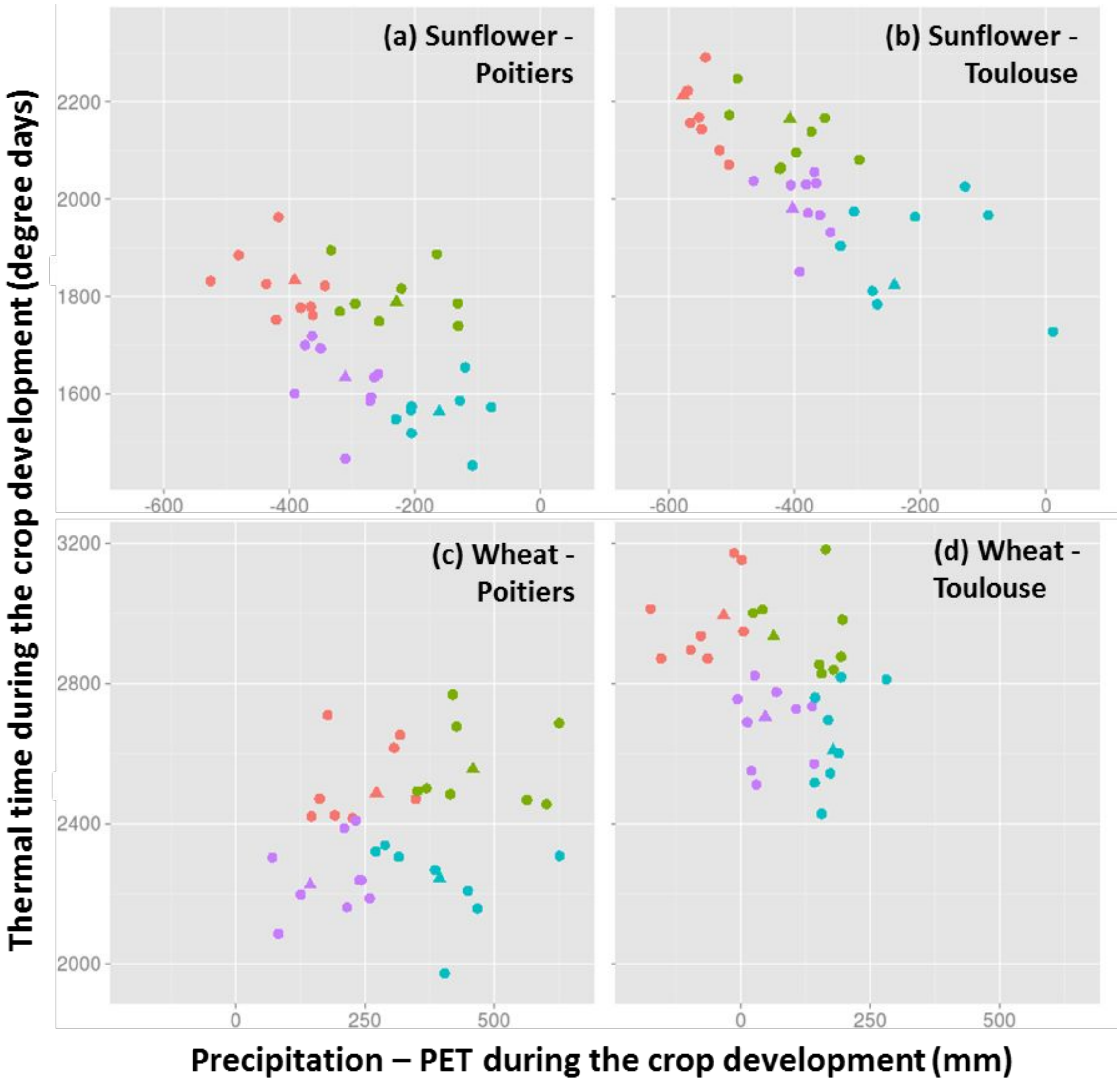

(a) Sunflower - Poitiers
(b) Sunflower - Toulouse
(c) Wheat - Poitiers
(d) Wheat - Toulouse
Thermal time during the crop development (degree days)
Precipitation – PET during the crop development (mm)
2200
2000
1800
1600
-600
-400
-200
0
3200
2800
2400
2000
0
250
500

Figure 3

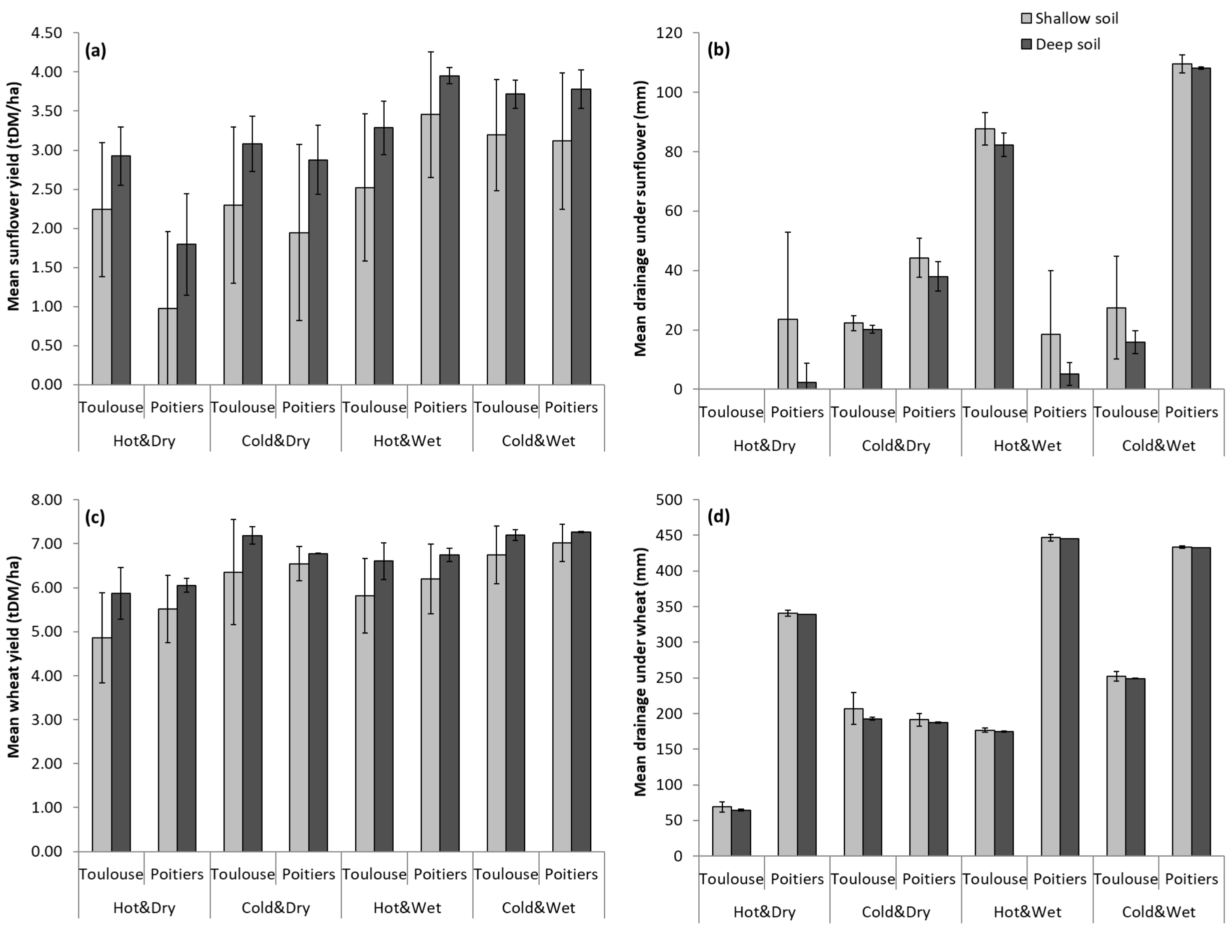

(a)
Mean sunflower yield (tDM/ha)
(b)
Mean drainage under sunflower (mm)
Shallow soil
Deep soil
(c)
Mean wheat yield (tDM/ha)
(d)
Mean drainage under wheat (mm)
Toulouse
Poitiers
Hot&Dry
Cold&Dry
Hot&Wet
Cold&Wet

Figure 4

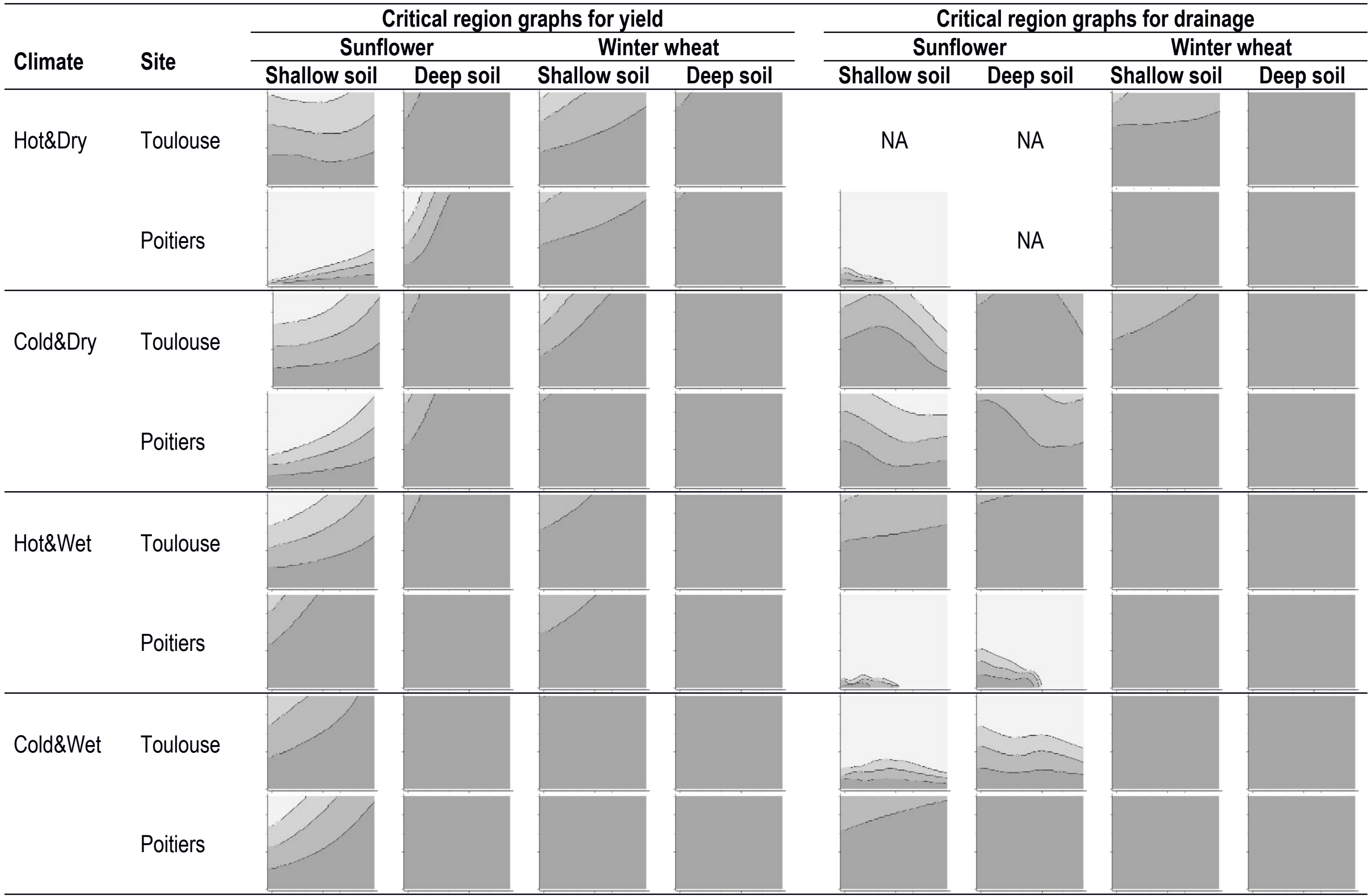

Critical region graphs for yield
Critical region graphs for drainage
Sunflower
Winter wheat
Sunflower
Winter wheat
Climate
Site
Shallow soil
Deep soil
Shallow soil
Deep soil
Shallow soil
Deep soil
Shallow soil
Deep soil
Hot&Dry
Toulouse
NA
NA
Poitiers
NA
Cold&Dry
Toulouse
Poitiers
Hot&Wet
Toulouse
Poitiers
Cold&Wet
Toulouse
Poitiers

Figure 5

Supporting Information

In our simulation experiment, kriging models were fitted using the R package DiceKriging (Roustant et al., 2012) with the default options, in particular a constant trend (i.e. *ordinary kriging*) and Matérn covariance, as described below. Provided a set of n observations $(x_1,f_1),\dots,(x_n,f_n)$ and given a covariance function *c*, the kriging predictor for any **x** is equal to:

$$m(x) = \hat{m} + c_n(x)C_n^{-1}(F_n - \hat{m}1_n)$$

with:

- $F_n = (f_1,\dots,f_n)^T$ the vector of observed values,
- $C_n = (c(x_i,x_j))_{1\leqslant i,j\leqslant n}$ a n x n covariance matrix,
- $c_n(x) = (c(x_1,x),\dots c(x_n,x))^T$ a covariance vector,
- 1_n is a n x 1 vector of ones, and
- $\hat{m} = \frac{1_n^T C_n^{-1} F_n}{1_n^T C_n^{-1} 1_n}$ is a constant.

Here, **x** corresponds to a pair $(\mu_{X,}\ \sigma_X)$ and f to the corresponding *CV.*

In general, kriging models depend largely on the covariance function *c,* for which a large catalogue is available in the literature. We used the default value of the DiceKriging package, which is the Matérn kernel with shape parameter 3/2, defined as:

$$c(x,x') = \sigma^2\left(1 + \sqrt{3}\sum_1^2 \frac{|x_i - x'_i|}{\theta_j}\right)\exp\left(-\sum_1^2 \frac{|x_i - x'_i|}{\theta_j}\right)$$

which depends on parameters σ^2,$\theta_{1,}\theta_2$, which are estimated by maximum likelihood within DiceKriging.

One advantage of the kriging model is its probabilistic interpretation (Cressie, 2015), since it also provides a local error estimate, often referred to as *prediction variance*, equal to:

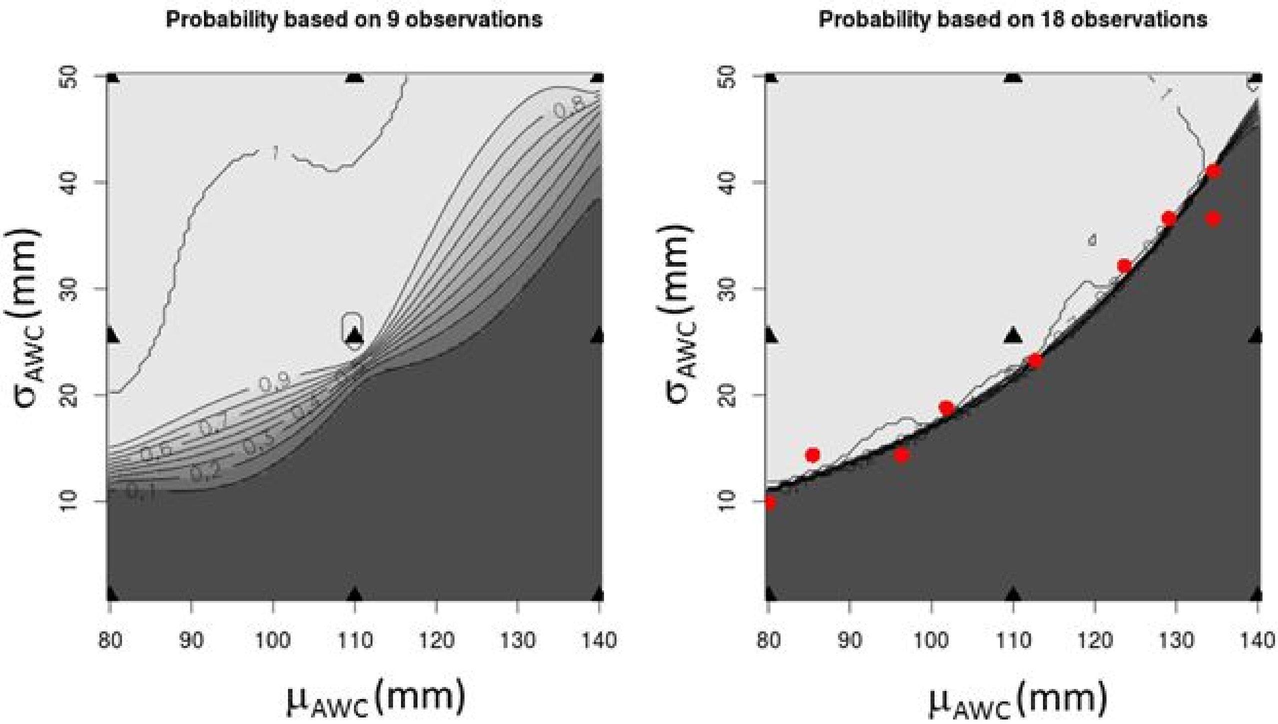
$$s(x)^2 = \sigma^2 - c_n(x)^T C_n^{-1} c_n(x) + \frac{\left(1 - 1_n^T C_n^{-1} c_n(x)\right)^2}{1_n^T C_n^{-1} 1_n}$$

In our context, we used this information to compute the probability, given a set of observations $(x_1,f_1),\ldots,(x_n,f_n)$, that the *CV* at a point x exceeds α. This probability is equal to

$$P(x) = \Phi(\frac{\alpha - m(x)}{s(x)})$$

with Φ the cumulative distribution function of the standard normal law. Probabilities close to 0.5 indicate that the kriging prediction is inaccurate (large s), while probabilities close to 0 or 1 show accurate prediction with respect to the classification objective (below or over the threshold, respectively).

In an illustration of the kriging strategy (Fig. S1), the soil, climate and crop are fixed, while the AWC mean and standard deviation vary between lower and upper bounds (μ_X = 80-140 mm and σ_X = 0-50 mm). We consider the yield for Y and the threshold α = 10%. We represent the probability of exceeding α at the initial stage (based on 9 observations) and after the sequential procedure (based on 18 observations).



After the initial observation stage (Fig. A1, left), the critical set Ω_c is identified only roughly (large region with values close to 0.5), while after the sequential procedure (Fig. A1, right), the probability is either close to 0 or 1 everywhere, indicating that the critical region (Fig. A1, white) was accurately determined, due to the additional observations next to its boundary.