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Monte Carlo based calibration and uncertainty analysis of a coupled plant growth and hydrological model

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Abstract

Computer simulations are widely used to support decision making and planning in the agriculture sector. On the one hand, many plant growth models use simplified hydrological processes and structures, e.g. by the use of a small number of soil layers or by the application of simple water flow approaches. On the other hand, in many hydrological models plant growth processes are poorly represented. Hence, fully coupled models with a high degree of process representation would allow a more detailed analysis of the dynamic behaviour of the soil–plant interface.

We used the Python programming language to couple two of such high process oriented independent models and to calibrate both models simultaneously. The Catchment Modelling Framework (CMF) simulated soil hydrology based on the Richards equation and the van-Genuchten–Mualem retention curve. CMF was coupled with the Plant growth Modelling Framework (PMF), which predicts plant growth on the basis of radiation use efficiency, degree days, water shortage and dynamic root biomass allocation.

The Monte Carlo based Generalised Likelihood Uncertainty Estimation (GLUE) method was applied to parameterize the coupled model and to investigate the related uncertainty of model predictions to it. Overall, 19 model parameters (4 for CMF and 15 for PMF) were analysed through 2×10^6 model runs randomly drawn from an equally distributed parameter space. Three objective functions were used to evaluate the model performance, i.e. coefficient of determination (R^2), bias and model efficiency according to Nash Sutcliffe (NSE).

The model was applied to three sites with different management in Muencheberg (Germany) for the simulation of winter wheat (*Triticum aestivum L.*) in a cross-validation experiment. Field observations for model evaluation included soil water content and the dry matters of roots, storages, stems and leaves. Best parameter sets resulted in NSE of 0.57 for the simulation of soil moisture across all three sites. The shape parameter of the retention curve n was highly constrained whilst other parameters

of the retention curve showed a large equifinality. The root and storage dry matter observations were predicted with a NSE of 0.94, a low bias of $-58.2\,\mathrm{kg\,ha^{-1}}$ and a high R^2 of 0.98. Dry matters of stem and leaves were predicted with less, but still high accuracy (NSE = 0.79, bias = $221.7\,\mathrm{kg\,ha^{-1}}$, $R^2 = 0.87$). We attribute this slightly poorer model performance to missing leaf senescence which is currently not implemented in PMF. The most constrained parameters for the plant growth model were the radiation-use-efficiency and the base temperature. Cross validation helped to identify deficits in the model structure, pointing out the need of including agricultural management options in the coupled model.

1 Introduction

Plant growth and hydrological models are widely used to evaluate strategies such as climate adaption, risk management of pesticide or fertilizer application in agricultural sciences and politics. However modelling comes along with limitations. Different models can lead to deviating results although they are driven by the same input and forcing data. Such effects are represented by model uncertainty. Furthermore, the selection of input parameter can change the results and also increase uncertainty. This effect is commonly known as parameter uncertainty. Hence, a good knowledge about these uncertainties is crucial, especially when plant growth models are used to project food supply and hydrological models are applied to develop strategies for water resource management. The importance of a comprehensive knowledge about the capabilities and limitations of such models applied in the field of decision making has also been highlighted by Kersebaum (2007).

Most current plant growth models integrate plant growth and hydrological processes tightly, leading to very complex models. Therefore, the calibration of such models is often done step by step. In a number of studies (e.g. Pathak et al., 2012; Wang et al., 2005; Iizumi et al., 2009) the hydrological model has been calibrated in a first step and the plant growth model in a second step to reduce the number of parameters varied in one calibration step. However, in such a setup feedbacks between biomass production and hydrology are not considered (Pauwels et al., 2007). Alternatively, the past years have seen modular model developments and the promotion of comprehensive model coupling strategies (Priesack et al., 2006). Kraft et al. (2011) coupled the Catchment Modelling Framework (CMF) (Kraft et al., 2011) with the Plant growth Modelling Framework (PMF) (Multsch et al., 2011) to simulate the direct feedbacks of soil hydrological conditions on plant development. However, their coupled version of CMF and PMF has only been used for virtual modelling experiments so far (Multsch et al., 2011; Kraft et al., 2011), but not yet for real observed data.

Instead of calibrating single models step by step, we favour the use of a Monte Carlo algorithm to iterate many parameter combinations of the entire coupled model and apply the GLUE (Generalized Likelihood Uncertainty Estimation) method, a widespread Bayesian technique to investigate model performance and parameter uncertainty (Beven and Binley, 1992). The GLUE results in a range of parameter sets, which all lead to acceptable model runs, rather than only one "optimal" calibrated parameter set (Candela et al., 2005). This behaviour is known as "equifinality". Model realisations are grouped into behavioural and non-behavioural model runs and associated parameter sets. The former describes an acceptable model application, allowing some degree of error in simulating a target value (defined in an a priori threshold criteria). The latter describes parameter sets which return unacceptable model outputs and can be deleted (Beven, 2006). A further distinction is made between constrained and unconstrained parameters (Christiaens and Feyen, 2002). The more sensitive a model parameter for predicting a given target value is, the more does it get constrained in the remaining behavioural parameter sets.

The level of improvement of the model by the GLUE approach depends on the used likelihood function threshold criterion and the number of sampled parameters. However, the choice of the likelihood function itself has also a strong influence on the results, which has also been reported by He et al. (2010), who additionally highlight the importance of the likelihood-function to ensure statistical validity. A number of likeli-

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hood functions have been applied, e.g. the inverse error variance with a shaping factor (Beven and Binley, 1992), the Nash and Sutcliffe model efficiency (Freer et al., 1996), scaled maximum absolute residuals (Keesman and van Straten, 1990) as well as the index of agreement (Wilmott, 1981), model bias and coefficient of determination.

A number of studies applied the GLUE method to achieve a better understanding of plant growth models and their parameters. For example, Wang et al. (2005) utilized the GLUE method for evaluation of the EPIC model with the mean squared error as a likelihood function. He et al. (2010) tested the influence of different likelihood functions with the crop-environmental-resource-synthesis (CERES)-Maize model. They used modifications of the variance of model errors and mean squared error as likelihood functions. Mo and Beven (2004) applied the method with the index of agreement as a likelihood function for calibration of a soil-vegetation-atmosphere-transfer model. Pathak et al. (2012) considered bias, root mean squared error and the index of agreement as likelihood functions in the uncertainty assessment of the CSM-CROPGRO-cotton model.

In this study, the combined set of model parameters from a fully coupled plant growth model (PMF) and a hydrological model (CMF) was calibrated parallelly. Hence, the objectives of this study were as follows:

- In-depth analysis of the coupled model setup through a GLUE analysis to investigate the sensitivity of plant growth and hydrological model parameters and to derive a range of behavioural model runs.

- Cross validation of parameter transferability on three different sites against observed soil moisture and biomass data for storages, roots as well as stems and leaves (further summarized as plant dry matters) of winter-wheat.

To describe the "goodness-of-fit" of our model prediction, we used a set of three likelihood-functions (model efficiency, bias and coefficient of determination). Subsequently, we will distinguish between (i) forcing data (e.g. meteorological observations), (ii) input data (e.g. soil information) and (iii) model parameters (e.g. plant coefficients).

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2 Materials and methods

2.1 Model set up

2.1.1 Catchment Modelling Framework (CMF)

A plot scale hydrological model for the unsaturated zone was built by using the Catchment Modelling Framework (CMF) (Kraft, 2011). CMF is a computer software to set up individual hydrological models. A programming library facilitates the design of water transport models between soil layers in up to three dimensions. It allows the development of detailed mechanistic models as well as lumped large scale linear storage based models. A model in CMF works as a network of storages and boundary conditions, connected by flux calculating sub models. It works as an extension to Python and can easily be coupled with other models.

The specific realisation of CMF was done with a one dimensional setup. Water fluxes were simulated with the Richard's equation. We simulated the soil moisture with a van-Genuchten–Mualem retention curve (van Genuchten, 1980) for 50 soil layers. The k_{sat} parameter was used to simulate the saturated conductivity. The porosity parameter is defined by pore volume per soil volume, while alpha and n as known van-Genuchten parameters. The interaction of the lowest soil layer with the groundwater is modelled as a Neumann boundary condition. To initiate the water content of CMF we used existing climate data for the year 1992 and calibrated it for the years 1993–1994.

2.1.2 Plant growth Modelling Framework (PMF)

As a plant growth model, we used the Plant growth Modelling Framework (PMF), developed by Multsch et al. (2011). PMF is a dynamic and integrative tool for setting up individual plant models. In general, PMF consists of four core elements: (i) *Plant Model*, (ii) *Process Library*, (iii) *Plant Building Set* and (iv) *Crop Database*. The basic idea of PMF is to divide the plant into its physical components root, shoot, stem, leaf and storage organs, which interact on a numerical level during the growth process. This structure builds up the *Plant Model*. A process library contains mathematical formulations of biophysical processes, such as biomass accumulation, water uptake and development. The user can connect the *Plant Model* with a set of biophysical processes by using the *Plant Building Set*. The plant parameters are taken from the *Crop Database*.

The biomass accumulation is affected by the radiation use efficiency (RUE). The higher the RUE, the higher is the biomass accumulation. RUE is used to calculate the biomass growth with the biomass radiation-use-efficiency concept (Monteith and Moss, 1977). The mathematical solution of the radiation-use-efficiency in PMF is based on Acevedo et al. (2002). The photosynthetically active absorbed radiation is calculated by solar radiation and its intercepted fraction. The simulation of biomass accumulation from photosynthetic active radiation is performed with the canopy extinction coefficient (k). The minimum temperature for plant development is defined by the base temperature (t_{base}). It acts as a threshold temperature above which development occurs. Each plant development step is defined by a temperature sum. If the temperature sum is reached, the developing process begins. If this parameter is too high, the plant starts its growing process too late, and vice versa. For simplicity, the parameter t_{base} is independent from further environmental influences. Development stages are used to control biomass allocation between plant organs. The plant development is divided into the eight stages by a thermal time threshold: emergence, leaf development, tillering, stem elongation, anthesis, seed fill, dough stage and maturity. Root elongation determines the daily root growth rate. The last group of parameters (kcb_{ini}, kcb_{mid}, kcb_{end}) is used to assess plant transpiration from potential evapotranspiration. The simulation of the evapotranspiration in PMF is based on the FAO Penman–Monteith approach (Allen et al., 1998). All PMF parameters are chosen on the basis of their influence on roots, stems and leaves or storages dry matter outputs, based on one-parameter-at-a-time sensitivity analyses and expert-knowledge.

2.1.3 Coupling CMF-PMF

Both model frameworks provide interfaces for the communication with other models. In case of PMF, an atmosphere and a soil interface from counterpart models are needed. The interfaces define functions from the plant growth model which are used to obtain data, e.g. temperature, rainfall or soil water content. Furthermore, PMF exposes properties such as evapotranspiration or biomass which can be described by other models. In case of CMF, a set of predefined functions can be used to obtain information on the current status of the soil water balance such as matrix potential or soil water content.

A Python script was used to run and synchronize both models in a daily step and to store output data. This synchronization in terms of evapotranspiration and available water for the plant was part of the run time loop. The models provided a wide range of output results for plant information such as root carbon content, potential growth or development stages (PMF) and hydrology such as deep percolation, flux and porosity (CMF). Here, we used the outputs of soil moisture (CMF), root, stem and leaves as well as storage dry matters (PMF). These output values were saved in an array for every daytime step.

2.2 GLUE set up

2.2.1 Likelihood functions

The performance of a parameter set to predict observations was evaluated by way of a "goodness-of-fit" value, represented by the likelihood function. The choice of the likelihood function depends on the situation and is often ambiguous, if no accurate information about the probability distribution of the measurement errors is available (Beven and Binley, 1992). But the choice of only one objective function for the calibration is in most cases inaccurate (Vrugt et al., 2003). We therefore used a combination of three likelihood functions:

(1) The bias function was used as a central statistical measurement to summarize overall model performance:

$$L_1(\theta|Y) = \text{Bias} = \frac{1}{N} - \sum_{i}^{N} Y_i - \hat{Y}_i \tag{1}$$

where $L(\theta_j|Y)$ is the likelihood measure for each model run with parameter set θ, N is the total number of measurements, Y_i is the measured value for the ith measurement and $\hat{Y}_i$ is the corresponding output of the model. The bias measures the differences between measurements and model outputs. For under-predictions of the model, the bias is positive, for over-predictions the bias is negative. Thus, it is a useful measure for assessing whether structural changes of the model equations are necessary for reducing the overall bias of the prediction (Wallach, 2006). However, bias alone is not sufficient to evaluate model errors, as a bias of zero could also be due to cancelation of large errors with different signs (Wallach, 2006).

(2) In order to measure the deviation of model prediction and measurement data we used the coefficient of determination, which is defined as:

$$L_2(\theta|Y) = R^2 = \left(\frac{\sum_{i=1}^{N} \left[\left(Y_i - \bar{Y}\right) \left(\hat{Y}_i - \bar{\hat{Y}}\right) \right]}{\left(\sum_{i=1}^{N} \left(\hat{Y}_i - \overline{Y}\right)^2 \sum_{i=1}^{N} \left(\hat{Y}_i - \bar{\hat{Y}}\right)^2 \right)^{0.5}} \right)^2 \tag{2}$$

where $\bar{Y}$ is the average of the measured and $\bar{\hat{Y}}$ is the average of the simulated data. A maximum value of $R^2 = 1$ indicates that a perfect linear relationship between measured and calculated values exists, while the minimum value of $R^2 = 0$ indicates a low performance of the model. R^2 alone is also not a good measure of the model agreement with the observations, as R^2 could also be equal to 1 if the model systematically over- or under predicts.

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(3) Finally, we employed the Nash–Sutcliff index (Nash and Sutcliffe, 1970) for measuring the model's sensitivity to outliers. This widely used function (e.g. Garnier et al., 2001; Beven and Binley, 1992) is calculated as follows:

$$L_3(\theta|Y) = NSE = 1 - \frac{\sum_{i=1}^{N}\left(Y_i - \hat{Y}_i\right)^2}{\sum_{i=1}^{N}\left(Y_i - \bar{Y}\right)^2} \quad (3)$$

If the model predicts the measurements perfectly, we have $Y_i = \hat{Y}_i$ implying NSE = 1. If $\hat{Y}_i = \bar{Y}$ for all i, then NSE = 0. Thus, a model which gives NSE = 0 has the same "goodness-of-fit" as using the average of the measured data for every situation (Wallach, 2006).

The three proposed likelihood functions cover most aspects in an adequate manner. They are widely used in hydrology (e.g. Li et al., 2010; Besalatpour et al., 2012; Pathak et al., 2012) with high explanatory power. It has to be noted that other choices for the likelihood function would certainly be imaginable (Beven and Freer, 2001).

2.2.2 GLUE sequence

The general GLUE method proceeds in several consecutive steps (Beven and Binley, 1992), which were adapted to this specific study:

1. *Selection of sensitive parameters*: A full list of all parameters considered in GLUE from CMF and PMF are given in Table 1. Fifteen plant specific parameters from PMF which influence plant development, transpiration and biomass production were altered in the analysis. The hydrological parameters were given by the van-Genuchten–Mualem parameters. These parameters were selected on the basis of a "one-parameter-at-a-time" sensitivity analysis, which is not presented in this study.

2. *Creation of a priori distribution*: A random function from the Python package Numpy (Oliphant, 2006) was used to create 2×10^6 parameter sets, whereby each parameter set consisted of nineteen parameters. Since their a priori distribution was unknown, a uniform distribution was assumed. The parameter ranges were selected on the basis of expert-knowledge and other publications.

3. *Execution of model runs*: The 2×10^6 realisations of the coupled CMF-PMF model were forced with same climate data on three different sites by using a high performance computing cluster.

4. *Creation of posteriori distribution*: The simulated variables of both models were compared with observed data by using the three likelihood functions NSE, R^2 and bias. The variables of PMF are root, stem and leaves as well as storage dry matter and soil moisture in case of CMF, respectively. Three threshold criteria were used to obtain parameter settings which fit the measured data equally well. All parameter sets that resulted in a bias $> \pm 500\,\mathrm{kg\,ha^{-1}}$ for the plant dry matters and $> \pm 10\,\%$ soil moisture respectively, a NSE < 0 and a $R^2 < 0.3$, were discarded.

These four steps resulted in behavioural parameter sets for the coupled model for each study site. In order to test the limitations of the behavioural parameter sets a full cross-validation on all three sites was conducted.

2.3 Study site and data

Study site: The coupled CMF-PMF model was parameterized and evaluated using data from three agricultural field sites. They are located at the Muencheberg experimental stations, 50 km to the east of Berlin, Germany, where the ZALF (Leibniz Centre for Agricultural Landscape Research) recorded a comprehensive experimental data set (Mirschel, 2007). This extensive data set was used in several previous modelling studies (e.g. Wegehenkel, 2000; Palosuo et al., 2011; Kersebaum et al., 2007). The three sites are characterized by a primarily sandy *Eutric Cambisol*, with volumetric sand content between 80 to 90 % and silt/clay content around 5 to 10 %. The bulk density was found to be around 1.5 $g\,cm^{-1}$ and the organic matter in the first 0.3 m around 0.6 % (Mirschel, 2007).

Forcing data: The climate data comprise daily sum of precipitation, minimum and maximum temperature, mean relative humidity, early morning vapour pressure, global radiation and mean wind speed. During 1994 (the year for which winter wheat was cultivated), the conditions were relatively humid, with an annual precipitation of 714 mm and an annual average temperature of 9.1 °C. During the growing season (May–October), precipitation of 588 mm and average temperature of 15.8 °C were measured. The day of sowing and the day of harvest were set to observed dates (15 October 1993 and 29 July 1994).

Evaluation data: Soil moisture was measured on each site in three soil depths at 0.15 m, 0.45 m and 0.75 m on 33 days during the observation period from 1992–1998. The average soil moisture ranged from 12.1 to 12.9 % on site 1–3, with a minimum of 3 % and a maximum of 21.2 %. Soil moisture was very similar across all three sites. The sites differed in their management strategies, with high level intensive (site 1), organic (site 2) and extensive management (site 3) and in their winter wheat cultivar, namely *Busard*, *Ramiro,* and *Greif*. Crop growth data for winter wheat are available for five different days in 1994. Data on root dry matter [$kg\,ha^{-1}$], stem and leaves dry matter [$kg\,ha^{-1}$] and storage dry matter [$kg\,ha^{-1}$] are given for all three sites.

3 Results and discussion

3.1 Parameter uncertainty

To assess the range of each parameter in the behavioural parameter sets, we need to take a closer look at the parameter distributions for the different likelihood functions. Table 1 summarizes the results of the GLUE approach, providing the a priori and posteriori parameter ranges for the 19 model parameters as well as the reduction of the parameter uncertainty. For five parameters we were able to substantially reduce their uncertainty bounds by 30 to 70 %, while 11 parameters were rather unconstrained with uncertainty reduction of less than 10 %. Out of the eight parameters that define the growing stage through the thermal time requirement (°days) only the parameter tillering showed a large uncertainty reduction potential. This indicates that many of the parameters identifying plant growth stages lead to a high grade of equifinality.

A selection of 8 model input parameters in terms of behavioural model runs is shown in Fig. 1, where 4 CMF and 4 PMF parameters are given as interaction scatter plots. It depicts the mean NSE (calculated of the single, equally weighted NSE for soil moisture, roots, stems and storages, as well as storage dry matter) on site 1 as an example for constrained as well as non-constrained parameters of Table 1. On the interaction scatter plots, no correlations between parameters of PMF and CMF can be detected (Fig. 1). As the GLUE method cannot deal with such correlations, this is an important precondition of the GLUE method (Jin et al., 2010). The interaction scatter plots also show a clear prediction boundary for the parameter *n* at 1.3 [–] and for RUE at 6 $\mathrm{g\,MJ^{-1}}$ PAR. A setting of RUE above 6 $\mathrm{g\,MJ^{-1}}$ PAR and *n* below 1.3 [–] can never lead to an adequate model prediction for winter wheat and soil moisture in 1994 on site 1 in Muencheberg, no matter which values are selected for other model input parameters.

The most constrained parameter of PMF is RUE (Table 1, Fig. 1), which influences biomass accumulation. Good settings for RUE were found from 1.5 to 4.9 $\mathrm{g\,MJ^{-1}}$ PAR (Table 1). This range is in line with most other applications. Acevedo et al. (2002) suggested a RUE of 3.0 $\mathrm{g\,MJ^{-1}}$ PAR for wheat, which was used in the setup of Multsch et al. (2011). Calderini et al. (1997) found RUE across their investigated wheat cultivars between 1.08 and 1.16 g Mj-1 PAR. Lindquist et al. (2005) suggested a RUE of 3.8 $\mathrm{g\,MJ^{-1}}$ PAR. The DSSAT version 4.0 uses RUE with a setting of 4.2 $\mathrm{g\,MJ^{-1}}$ PAR (Jones et al., 1998). Due to high influence of weather variability to the RUE response, CERES-Maize developers do not recommend using RUE as a calibration pa-

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rameter (Ma et al., 2011). We therefore suggest fixing RUE at our found optimum of 2.02 g MJ^{-1} PAR for further applications of PMF.

The second most constrained parameter (Table 1, Fig. 1) is the CMF shape parameter of the retention curve n with a strict optimum at 1.45 [–] and a range reduction of 60 % through the threshold criteria. Christiaens and Feyen (2002) found n being not much constrained from 1.2 to 1.6 for the MIKE SHE model. In contrast, Vogel et al. (2000) reported the parameter to be quite sensitive. Ippisch et al. (2006) demonstrated that the van-Genuchten–Mualem model caused convergence problems with n close to 1.0 for the numerical solver, which we can confirm. They found a similar optimal setting with $n = 1.47 \pm 0.04$ for the A-Horizon in a *haplic Calcisol*.

When looking at the density distribution of the behavioural model runs in Fig. 1, we can locate an optimal parameter range with 0.015–0.025 [–] for alpha. But even within this range there is no guarantee for a good model response. Several parameter values in the considered range of alpha yield poor prediction with NSE < 0, depending on the settings of other model parameters. The parameter t_{base} provides best results within the range of 1.5 to 2.5 °C (Table 1). These settings are higher than the value given for PMF by Multsch et al. (2011) with 0 °C which was based on a study by McMaster and Wilhelm (1997). A wide range from 0 and 10 °C for t_{base} can be found in literature, strongly depending on cultivars (Porter and Gawith, 1999). The root growth shows a local optimum at 0.6 and a global optimum at 2.4 cm day^{-1}. Following our GLUE results the k parameter could not be confined, nevertheless, Pathak et al. (2012) found the k parameter constrained to around 0.64 [–] for the CROPGRO-Cotton model. All other investigated parameters are unconstrained within their boundaries to the outputs of various plant dry matters and soil moisture (Table 1, Fig. 1).

Finding mainly insensitive parameters corresponds well to prior studies using the GLUE procedure for models with a similar large number of model parameters (e.g. Viola et al., 2009; Rankinen et al., 2006). Part of the problem is that parameter rich models allow for equifinality, levelling out the impact of certain parameters.

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3.2 Model performance

3.2.1 Soil water balance

Figure 2 summarizes the capability of the coupled CMF-PMF model for predicting the soil moisture output in three depths. Along with the median of the GLUE derived behavioural model runs, we showed the 50 % and 95 % uncertainty bounds. Overall, approximately 90 % of the observed data were within the predicted uncertainty bounds. The distribution differs between all soil depths and remaining behavioural parameter sets were found to be around 10 % with respect to the measured value. The uncertainty of the prediction was higher during dry and wet days and lower during moderate moisture conditions. But the GLUE method per se has the tendency to overestimate uncertainty during low and high simulation events (Vrugt et al., 2008). In the soil depth from 0.3 to 0.6, as well as in the soil depth from 0.6 to 0.9 m, we have a constant uncertainty in the prediction of around 5 %. The median of the behavioural model run in the upper soil layer has a NSE of 0.57, bias of 2 % soil moisture and R^2 of 0.84. Model performance criteria in the soil depths below are of similar quality, with less good performance for R^2 values but improved biases (Fig. 2).

Compared with other studies, the median output for soil moisture after calibration was on the same quality level as previously reported findings. For example, Christiaens and Feyen (2002) published results of the GLUE method used for the MIKE SHE model with an NSE close to zero. Jiménez-Martínez et al. (2009) found a van-Genuchten parameter-set for Hydrus-1-D model resulting in a high R^2 of 0.9 and 0.029 % RMSE for soil moisture. They simulated the soil moisture under melons growing in southeast Spain. Scharnagl et al. (2011) found a RMSE of 0.009 % water content and NSE of 0.87 for their Hydrus-1-D modelling a site at Selhausen, near Jülich, Germany. Their uncertainty bounds for soil moisture varied around 3 %, with higher uncertainty during dry and wet situations, which is consistent with our findings. We obtained similar model efficiencies as the best performing model CERES (NSE = 0.66) in predicting the soil water content over all soil depths as a study of Kersebaum et al. (2007) on the same study site 1 in Muencheberg.

Despite the already good results, the prediction uncertainty could be further reduced by using more model runs and a stricter setting of threshold likelihood function. However, single model run time and the number of model runs had already pushed the overall computer run time of the uncertainty estimation provided here to three months. An efficient way might be the use of the DREAM-algorithm that is able to solve complex posteriori probability density functions for a large number of parameters. This algorithm could reduce model runs and the uncertainty of the posteriori distribution, but involving the risk of finding local optima of some parameter (Vrugt et al., 2008).

Nevertheless, the simulated parameter uncertainty can also depend on the chosen likelihood function and is not independent of errors in measured data (Mo and Beven, 2004). Thus, instead of attributing remaining model predictive uncertainty to the coupled CMF-PMF model structure itself, we should be aware that there are other sources of global uncertainty impact on the overall model performance.

3.2.2 Plant growth

Results for the root, stem and leaves as well as storage dry matters are given in Fig. 3. This distribution shows very good results for the root dry matter simulation. All observed values fall within the 50 % probability range. A high NSE of 0.94 and R^2 of 0.98 along with a very low bias of $-58.2\,\mathrm{kg\,ha^{-1}}$ indicate a very good model performance. The median of the stem and leaves dry matter simulation quality is lower (but still very good) than for the other simulated outputs with NSE of 0.79, bias of $221.7\,\mathrm{kg\,ha^{-1}}$ and R^2 of 0.87. Looking at the uncertainty boundaries, we can locate a relatively large uncertainty starting especially from July onwards and a somewhat lower uncertainty during the first half of June, without matching the observed value on 14 June. The observed value on this day is even higher than the next observation on 26 July, which may however occur in reality owing to decaying leaves (senescence). In the current model version PMF the model cannot represent a reduction of biomass during the growing season due to

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leave senescence. GLUE in this sense even facilitates the investigation of the model structure and identification of clear model limitations. The uncertainty of the prediction is constant around 500 $kg\,ha^{-1}$ for the root dry matter, while the stem and leaves as well as the storage dry matter has a mean uncertainty of around 2000 $kg\,ha^{-1}$. The storage dry matter simulation fits the measured data within the 50 % probability boundary.

In comparison to previously reported studies, we obtained very good results for the prediction of plant dry matter. For example, Jégo et al. (2010) found a RMSE of 1000 $kg\,ha^{-1}$ for spring wheat biomass simulation using the STICS model. Results are also excellent when compared to the model intercomparison study of plant growth models that was realized for the same forcing and evaluation data set by Kersebaum et al. (2007). Eight models were applied, resulting in RMSE from 773 $kg\,ha^{-1}$ to 3329 $kg\,ha^{-1}$ and NSE spanning from 0.19 to 0.96 in simulation of above ground biomass on site 1. The best performing model was the AGROSIM (note that this was the worst model in the intercomparisons project by Kersebaum et al. (2007) who looked at soil moisture prediction), while the CANDY model returned the worst results.

3.3 Cross-comparison of sites and parameter sets

We obtained reliable soil moisture and plant dry matter outputs for three experimental sites in Muencheberg with our coupled CMF-PMF model. But the observed data set is relatively small, as mostly the case in measured plant data analyses. Therefore it is even more essential to evaluate model performance across different field sites. We therefore chose to apply a cross-validation method, where parameter settings for one site were tested on another site and vice versa, to investigate the general model and parameter transferability (Pathak et al., 2012). This procedure has become an established method in dealing with small datasets in the course of model parameterization, calibration and validation (Nassif et al., 2012).

A comparison of the range of the behavioural parameter sets of the three sites is shown in Fig. 4. We can see small and similar ranges for the most constrained parameters RUE, t_{base}, alpha and n over all sites. Site 1 shows in this case the widest range

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for the constrained parameters k_{sat}, alpha, t_{base} and root growth. Medians shown as red lines in the boxplots indicate optimal parameter settings for the constrained parameters. They are located more or less at the same position for the 4 constrained parameters, while this position varies throughout the sites for the other parameters. We conclude that in further applications of CMF-PMF ranges for the constrained parameters as given in Table 1 can substantially be reduced to obtain improved model runs. One could also consider fixing the parameter to the median and exclude them from further calibration.

We deployed a cross-validation with each of the behavioural parameter sets we obtained for one site on the other remaining two sites. As examples we show results of the cross-validation for soil moisture 0.3–0.6 m (%) (Fig. 5) as well as for stem and leaf (Fig. 6). Transferability of model parameter sets worked well for soil moisture. In comparison to the other sites, we found the smallest uncertainty ranges on site 3. While site 1 has a mean uncertainty around 10 %, site 3 has only 5 %. Nevertheless, parameter sets found for site 1 worked well for the other sites. The NSE dropped from a high level of 0.48 at site 1 to NSE = 0.31 on site 2 and a NSE of 0.37 on site 3. The same cross-validation on the other sites resulted in a small but constant range of NSE between 0.23 and 0.37. The bias remains the same across all sites ranging between very low −0.6 to −1.0 % soil moisture.

Cross-validation for stem and leaves output of the CMF-PMF model worked well for sites 1 and 3, but less well for site 2 (Fig. 6). This is most likely related to the similar observed values for the stem and leaves dry matter in intensively managed site 1 and the extensively managed site 3, while the stem and leaves dry matter on the organically managed site 2 is significantly lower. Uncertainty boundaries for the organic site growths during the simulation period up to 2000 $\mathrm{kg\,ha^{-1}}$, while the uncertainty on the other sites increases up to 3000 $\mathrm{kg\,ha^{-1}}$, with a very low uncertainty around the 14 June 1994. We found similar NSE's of 0.79 on site 1 and 0.74 on site 2 and 3. Validated on the other sites, parameter settings for site 1 resulted in an acceptable NSE of 0.35 for site 2 and a very good NSE of 0.88 on the extensive site 3. R^2 remains on the same level through all tested sites between 0.79 and 0.91 indicating that the general dynamics of crop growth were captured for all sites. The variation of performance criteria in the cross-validation experiment (i.e. stable R^2 across all sites vs. a drop of NSE and an increase of bias from one site to another) highlight the importance of using a set of different likelihood functions.

One source for uncertainty in the prediction quality of the coupled model with regard to dry matter production is to be seen in our disregarding of further field management strategies. Even though fertilization is considered in the simulation of crop growth in the current model set up of CMF-PMF, we neglected other agricultural management options that significantly influence biomass production, e.g. pesticide application in conventional field management or weeding in organic farming. Selection of cultivars also has a significant impact on yields, which is also not considered in PMF. The reason for this is simple: PMF does not have a management tool. Site 1 was managed with a high level intensive, site 2 an organic and site 3 an extensive strategy. The winter wheat cultivar was also adapted to these strategies with elite winter wheat *Bussard* on site 1, infrequently used *Ramiro* on site 2 and elite winter wheat *Greif* on site 3. While these differences in management and cultivar lead to a high variability of plant matter production across sites (Fig. 6), it does not impact soil moisture conditions to a similar degree substantially (Fig. 5). Consequently, to apply PMF in the sense of a full crop growth model for agricultural application, a management module is required that considers typical management strategies in agriculture. Instead of a full inclusion of this management tool in the PMF model itself, we promote following the idea of the framework strategy of PMF as well as CMF and apply an external farm management model (Aurbacher et al., 2013; Windhorst et al., 2012).

4 Conclusions

Staying in line with standards for the development and evaluation of environmental models, our implementation of iterative steps for the validation of our coupled model is consistent with the postulations of Jakeman et al. (2006). Through the investigation of the parameter uncertainty, the CMF-PMF model performance was found to depend crucially on the parameter values for *n* (CMF) and RUE (PMF). Their uncertainty boundaries could be reduced by 60 and 77 %, respectively, through the GLUE analyses. Other parameters, including *k*, emergence, stem elongation and anthesis showed only a minor influence on the model outputs. The performance of our CMF-PMF model setup was found to be better than some previously tested models, given that model performance was good for soil moisture and plant dry matters on the same site. Overall, approximately 90 % of the observed soil moisture data were within the predicted uncertainty bounds that were determined through the GLUE method. The model performances for simulating observed plant dry matters was found to be in an uncertainty range from 500 to 2000 $\mathrm{kg\,ha^{-1}}$, with just one missed measured value. The found posteriori parameter settings can be used for a more efficient calibration of the CMF-PMF model in future case studies.

The cross-validation at different sites showed only slight reductions of the likelihood functions. From this, we conclude that the model is transferable in space, at least under similar soil conditions. Next steps should include a model test over several growing periods for which other crops need to be covered by PMF to be able to simulate crop rotation patterns.

Structural model uncertainty was identified with regard to the need of including agricultural management options and the missing capability of representing senescence in PMF. While the latter should be improved by considering processes reflecting senescence within PMF, we promote to couple an agricultural management model to CMF-PMF, an essential step to use PMF as a full crop growth model as well.

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Table 1. Parameter ranges of the Monte Carlo simulation for the coupled CMF-PMF for site 1 in Muencheberg. PAR stands for photosynthetically active radiation. Minimal to maximal input is the range for the GLUE analysis, while the output is the constrained range of the observed behavioural parameter sets (cf. Figs. 2 and 3). Uncertainty reduction in the output over 30 % is reflected in bold type.

Parameter	Definition	Min. input	Max. input	Min. output	Max. output	Reduction [%]
CMF						
alpha	inverse of the air entry potential [cm^{-1}]	0.001	0.1	0.007	0.1	6
k_{sat}	saturated conductivity [$m\,day^{-1}$]	0.1	25	4.1	24.9	16
porosity	pore volume per soil volume in [$m^3\,m^{-3}$]	0.3	0.7	0.35	0.7	13
n	shape parameter of retention the curve [–]	1	2	1.3	1.7	**60**
PMF						
RUE	radiation use efficiency [$g\,MJ^{-1}$ PAR]	0	15	1.5	4.9	**77**
k	canopy extinction coefficient in [–]	0.2	0.8	0.2	0.79	2
t_{base}	min. temp. above growth can take place [°C]	−1	5	−0.2	3.8	**33**
root growth	root elongation factor in [$cm\,day^{-1}$]	0.1	3	0.15	2.9	5
emergence		144	176	144	174	6
leaf development		176	229	176	228	2
tillering		229	463	230	380	**36**
stem elongation	total thermal time requirement	463	725	466	724	2
anthesis	for each growing stage [°days]	725	991	748	989	9
seed fill		991	1291	994	1284	3
dough stage		1291	1672	1292	1669	1
maturity		1672	1832	1683	1831	8
kcb_{ini}		0.05	0.4	0.08	0.22	**60**
kcb_{mid}	basal crop coefficient [–]	0.5	1.5	0.58	1.4	18
kcb_{end}		0.075	0.225	0.077	0.223	3

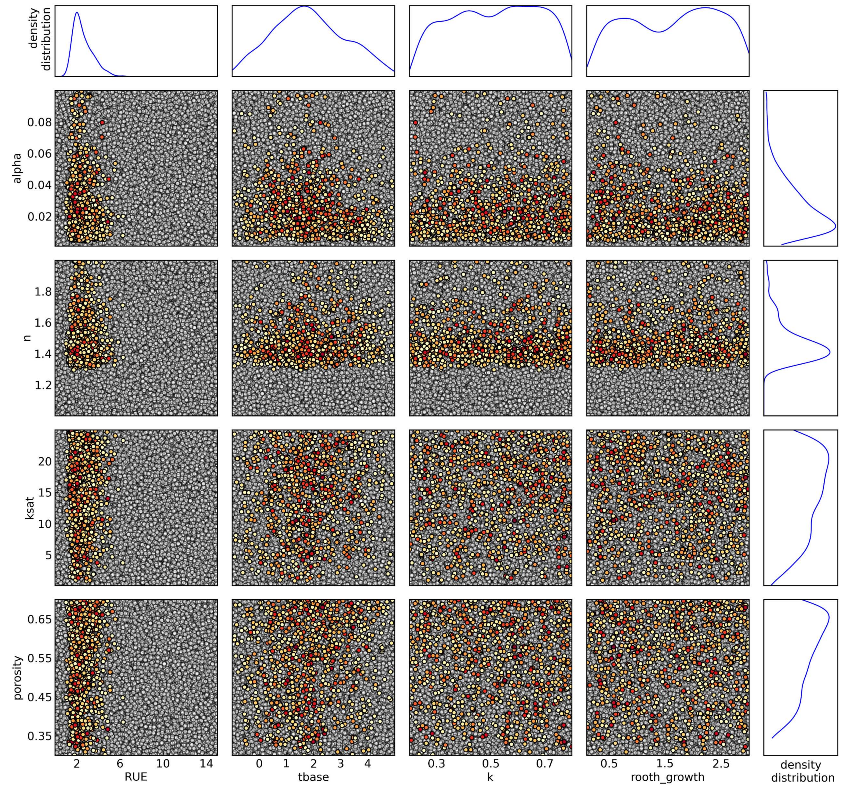

Fig. 1. Parameter uncertainty and interaction. The scatter plots show parameter interaction and correlations for behavioural model runs coloured from yellow to red for NSE > 0 and grey for NSE < 0 on site 1 in Muencheberg for the coupled CMF PMF model. PMF parameters are given on the x-axis while CMF parameters are plotted on the y-axis. The density distributions on top and to the right depict the parameter uncertainty. NSE are reported as mean, equally weighted NSE for soil moisture, roots, stems and storages, as well as storage dry matter.

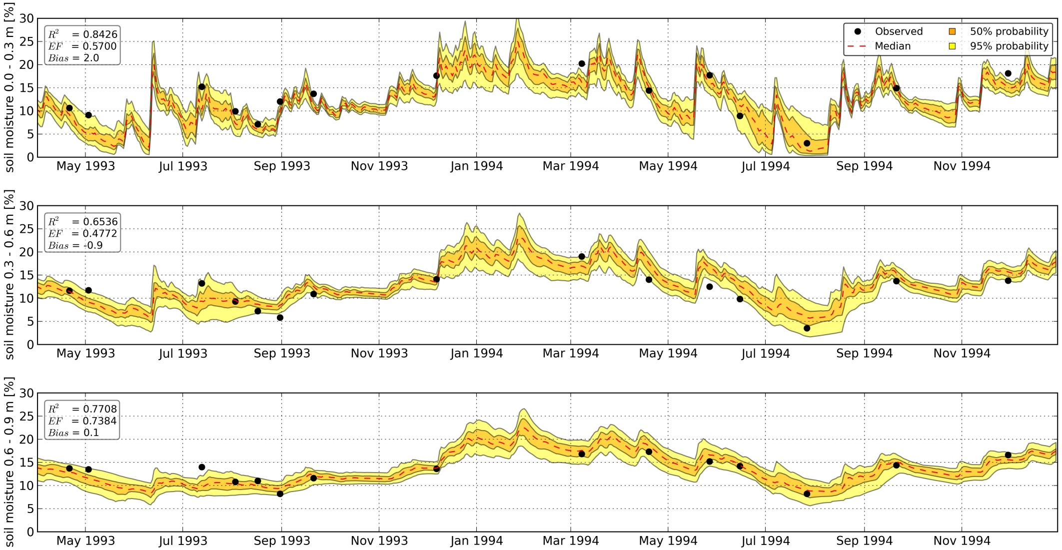

Fig. 2. Probabilistic time series for the simulation of soil moisture with behavioural (NSE > 0, bias < ±10 % soil moisture and $R^2 > 0.3$) CMF-PMF model runs on site 1 for three soil depths. Inserts: the likelihood functions quantify the median of the prediction range.

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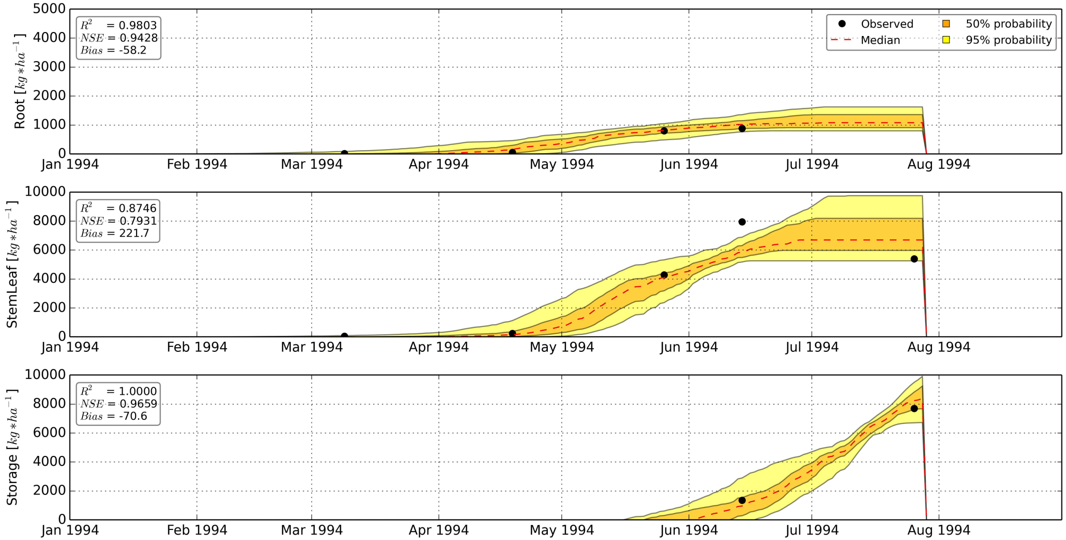

Fig. 3. Probabilistic time series for the simulation of plant dry matters with behavioural (NSE > 0, bias < ±500 kg ha^{-1} plant dry matter and $R^2 > 0.3$) CMF-PMF model runs on site 1. Inserts: The likelihood functions quantify the median of the prediction range. Note differences in scale of y-axis.

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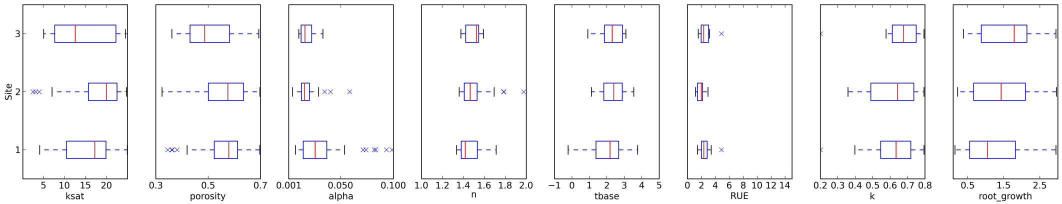

Fig. 4. Range of behavioural parameter sets considering all three threshold criteria of the CMF-PMF model for the three sites in Muencheberg. Results are shown for the same set of model input parameters as in Fig. 1.

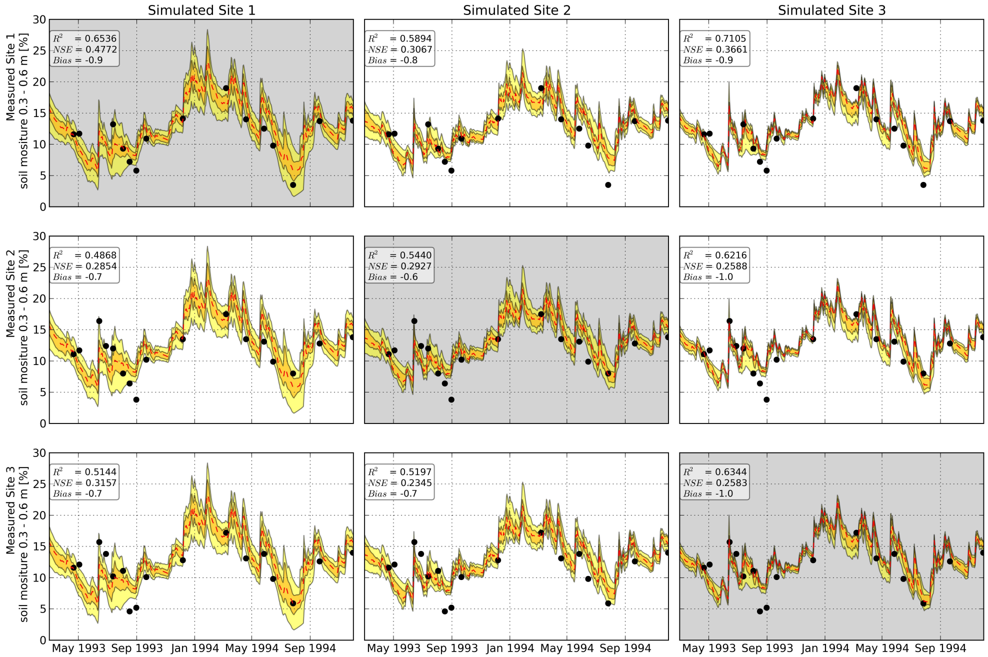

Fig. 5. Cross-validation of soil moisture prediction with uncertainty boundaries. Grey shaded sites are calibrated. Black dots are observed values, red dashed line is the median of the behavioural boundary condition (NSE > 0, bias < ±10 % soil moisture and R^2 > 0.3). The yellow area is the 95 % probability range of the simulation, the orange area the 50 % probability range.

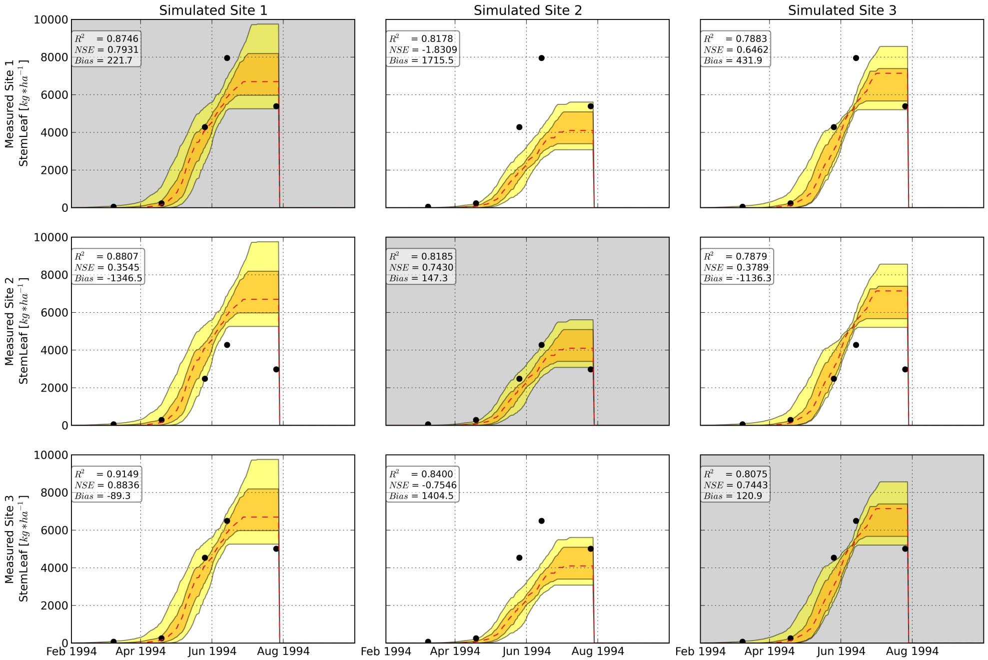

Fig. 6. Cross-validation of stem and leaves prediction with uncertainty boundaries. Grey shaded sites are calibrated. Black dots are observed values, red dashed line is the median of the behavioural boundary condition (NSE > 0, bias < ±500 kg ha^{-1} plant dry matter and $R^2 > 0.3$). The yellow area is the 95 % probability range of the simulation, the orange area the 50 % probability range.

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