# Multi-model ensemble simulations to assess the impact of climate change on agro-ecosystems

## Towards robust soil-crop models for better projections

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**Global climate change will alter the water, nitrogen and carbon cycles of agroecosystems. To predict future agricultural production under climate change, numerical soil-crop models are used. These soil-crop models can represent the complex and coupled processes of agroecosystems in a deterministic manner for a given environment. The projections made by soil-crop models suffer from two kinds of uncertainty: (1) epistemic uncertainty and (2) parameter uncertainty. Additionally, it is assumed that the parameterization is applicable to other environments. Therefore, this study has two major aims. The first aim is to quantify the above-mentioned uncertainties simultaneously by combining two methods: multi-model ensemble modeling and Bayesian statistics. The multi-model ensemble allows to quantify epistemic uncertainty by comparing individual model outputs. This has been demonstrated in many studies. Bayesian methods are common to assess credible parameter intervals for highly nonlinear process models. The second aim of this study is to provide a framework for assessing the robustness of the parametrization of soil-crop models. Therefore, a preliminary numerical study was conducted to test different calibration schemes and to investigate parameters sensitivities in dependence of the environment. The soil-crop modelling software ExpertN 3.0 will be used to set up a multi-model ensemble with eight soil-crop models. The model output will be analyzed by comparison with data from two sites, five soil types and two crops gathered by the DFG Research Unit 1695 since 2010. To achieve the second aim a global sensitivity analyses was conducted to rank the input factors for each soil-crop model. The result of the global sensitivity analyses will clarify the impact of model input on model output in regard to environment, model combinations, and extent. Additionally, different calibration schemes will be tested to identify the method yielding the most robust parametrization. We used a Latin Hypercube sampling scheme. In total, the whole study requires 1,000,000 CPU hours. We expect that the results will enable us to develop a generally applicable and feasible strategy of how soil-crop models have to be set up to produce reliable predictions of agroecosystem behavior under climate change.**

***Keywords — soil-crop modelling; global sensitivity analysis; uncertainty quanitfication;multi-model ensemble;***

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## I. Introduction

Soil-Crop models have been designed to coherently simulate crop growth, water and nitrogen dynamics in a given environment. The typical model outputs are soil water content, yield, evapotranspiration, groundwater recharge and nitrogen leaching. However, the state-of-the-art soil-crop models differ in complexity and representations of the various processes of plant growth and water regime as well as solute turnover and transport. Furthermore, these processes depend on environmental conditions such as climate, crop management and soil properties.

Soil-crop models represent the complex, coupled processes in agroecosystems in a deterministic manner. While they have been traditionally used to forecast yields and, later, nitrogen concentrations in seepage and ground water, they are now often used to predict the impact of environmental changes on agroecosystems. In the context of food security for a growing world population the Agricultural Model Intercomparison Project (AgMIP) set itself the goal to predict how global agricultural production will be affected by climate change [1]; [15]. Among others, [4]; [3] used a set of 30 crop models to predict how the grain yield of wheat - one of the world population’s staple crops - will change with rising temperature in the future.

Taking a different approach, the DFG Research Unit 1695 has incorporated a soil-crop model into a land surface model [9]. The aim is to improve the accuracy of regional climate projections by capturing the dynamic feedbacks between the soil-crop system and the atmosphere. This is not possible with current climate models. It can be expected that the new approach will also lead to improved yield predictions.

In practice, soil-crop models are often used to assess the impacts of agricultural management in regard to fertilization or irrigation. This is especially important in regions where water is scarce or where the groundwater gets polluted by nitrate and pesticides - which is the case in some regions in Germany [7].

Because, as in the application areas listed above, soil-crop modeling serves as a building block for decision making, it is of utmost importance to achieve highest levels of confidence regarding both kinds of model uncertainty, i.e., (1) epistemic uncertainty and (2) parameter uncertainty [18].

Epistemic uncertainty emerges from differences in the representation of the underlying processes in different models. Parameter uncertainty provides information about credible parameter intervals. This is especially important when true parameter values are non-existent due to spatial and temporal natural heterogeneity and measurement inaccuracy. To quantify these uncertainties simultaneously it is planned to combine two methods: multi-model ensemble and Bayesian methods as suitable tools demonstrated by recent studies [11]; [3]; [20].

Equally important to the uncertainty quantification is the robustness of the models' parametrization. Put simply, robustness means that simulation results for environments the model was not trained in, are still in good agreement with additional measurements. As a first step in the quantification of the parameter uncertainty and the parameterizations' robustness, a global sensitivity analysis will be conducted. This will identify the influential model parameters for a set of different environments. Afterwards we plan to test different calibration schemes differing in the size of the training data sets (i.e., different sites and climate conditions) and in the targeted output variables being trained on. The drawback of all these methods is their computational cost. Soil-crop models easily depend on 50 parameters. To sample the parameter space representatively up to 1,000,000 model runs per method and environment are necessary.

In the next sections preliminary results are presented for the global sensitivity on a subset of the available data and for one model combination.

## II. Material and Methods

### A. Study Site and measurements

The data used in this study were measured in two agricultural fields - one located on Swabian Alb (EC6, 13 ha), the other one in Kraichgau (EC1, 15 ha). The sites are contrasting in climate and soils. The Swabian Alb (48.5°N 9.8°E, 690 m a.s.l.) has a cold, harsh climate with average temperature of 6.5 °C and annual precipitation of 962 mm. Mean temperature in Kraichgau (48.9°N 8.7°E, 319 m a.s.l.) is 9.3°C and annual precipitation 777 mm. At the EC1 site the soil is deeply developed and fertile (depth >165 cm) with a high storage capacity of plant available water. In contrast, at the EC6 site the soil profile is very shallow and clay rich (depth < 30 cm) why the storage capacity of plant available water is very low.

All measurements have been carried out within the DFG Research Unit 1695 since 2009. The fields are managed and cropped by local farmers (best practice). In this study we only used years when winter wheat was grown. Winter wheat is usually sown in October and harvested between the end of July and mid-August, depending on weather. At EC1 this was the case in the vegetation periods 2010/11, 2012/13 and 2014/15 and at EC6 in 2010/11 and 2013/14. At each site the energy and water fluxes are measured with the eddy-covariance technique. Volumetric soil water content is measured using FDR probes in 5, 15, 30, 45 and 75 cm depth at EC1 and in 5 and 15 cm depth at EC6. Nitrate and ammonium concentration in the soils are measured 2-4 times during the vegetation period, depending on the year under consideration, in 0-30 cm depth at both sites and in Kraichgau additionally in 30-60 cm and 60-90 cm. Leaf Area Index (LAI), vegetative and generative biomass, nitrogen content of the plant and development stage (BBCH) are measured as common plant characteristics in regular intervals. Weather stations record net radiation, rainfall, temperature, relative humidity and wind speed. For a detailed description of the measurement instruments and data processing see [8] and [19].

### B. Model

Models were set up and run in the framework of the soil-crop modeling software ExpertN 3.1. As a first model combination we tested the CERES crop model [14], the SOILN [10] carbon and nitrogen turnover model and the Hydrus1D [17] model for the soil water regime. The FAO-Penman-Monteith [2] approach is used to estimate potential crop-specific evapotranspiration.

The CERES - SOILN model combination uses a diverse set of ordinary differential equations to simulate the crop e.g. growth, development stage and yield and the carbon and nitrogen turnover in the soil, e.g., nitrification and mineralisation. The soil water regime is described by the Richards equation (partial differential equation, PDE). Soil nitrogen dynamics are described by the Advection-Dispersion Equation (also a PDE). ExpertN 3.1 solves the set of coupled ordinary and partial differential equations using a fully implicit finite difference scheme with time step control. The CERES model has eight parameters which are typically adjusted (PD, PV, P1, P4, P5, PHINT, G1, and G2). The van Genuchten parameterization for the hydraulic functions was used to simulate the water regime. Since the hydraulic properties vary over the profile depth several sets of van Genuchten parameters are needed (n1, n2, a1, a2, KS1, KS2, l1 and l2). For assessing potential evapotranspiration we consider the crop factors (ki ($kc_{ini}$), km ($kc_{mid}$), ke ($kc_{end}$)). Nitrification and denitrification rates in the topsoil (Ni, Dn) are parameters of the SOILN model. Additionally, the maximum root water uptake rate and the maximum root nitrogen uptake as parameters for the interrelations of the different submodels are considered.

### C. Global Sensitivity Analyses

A global sensitivity analysis answers the question of what model input - if fixed - reduces the variance of the model output most [16]. The first-order sensitivity indices (S1) quantify how much of the total model output variance can be directly related to a specific parameter.

To calculate the S1 values for each parameter we conducted Latin Hypercube samples [12] with sizes ranging from 100,000 to 1,000,000 and followed the approach of [13]; [5]

as implemented in the python package SALib [7]. The approach has the advantage of not depending on a certain sampling design. Therefore, S1 can be estimated also in cases when the model sometimes crashes. Since this method needs a scalar as input and model outputs are time series we used the sum of squares (ssq) as a summarizing criteria. The ssq was calculated for each measurement point individually and then summed up separately for the four target model outputs (target variable): soil water content, nitrogen content in the soil and crop characteristics, and evapotranspiration. Based on ssq, we calculated S1 for each parameter, site, year and target variable. Replacing the model output through the ssq in the sensitivity analysis yields S1 values that give information on how the model performance changes with respect to one parameter. Notice that this is different from the traditional sensitivity analysis which quantifies how changes in the model output depend on changes in parameters.

All simulations and calculations are performed on the bwUniCluster. The big Latin Hypercube samples (1,000,000 model runs) are distributed among 560 cores and take 10-12 hours to finish. The resulting 150 GB of model output per sample are also analyzed in parallel on the bwUniCluster.

## III. Results &Discussion

Figure 1 shows the S1 values for the different years and study sites for each target variable calculated for a sample size of 100,000. Depending on the site and year, 30 % to 80 % of the original sample can be used for the analysis. The other samples lead to crashes of ExpertN for numerical reasons.

The parameters shown in figure 1 have an S1 greater than 0.05. Hence, each parameter explains > 5 % of the variance in the output variable. Note that, across target variables, the van Genuchten parameters *a1*, *a2*, and *l1*, the interaction parameter *mW*, *P1* as a crop parameter and the *km* parameter, related to evapotranspiration explain most of the models output variance.

The sum of first-order sensitivities (S1 values) of all parameters shown ranges between 0.65 and 0.81 for the different output variables. This means that 65% - 81% of the variance can be explained by first-order effects. Only in 2014 at EC6 for the output variable N the sum is only 0.45.

Upon comparison of the two sites, one can see that at EC6 the simulated soil nitrogen content and the evapotranspiration also depend on a crop model specific parameter. In 2011 and 2015 the crop model performance is

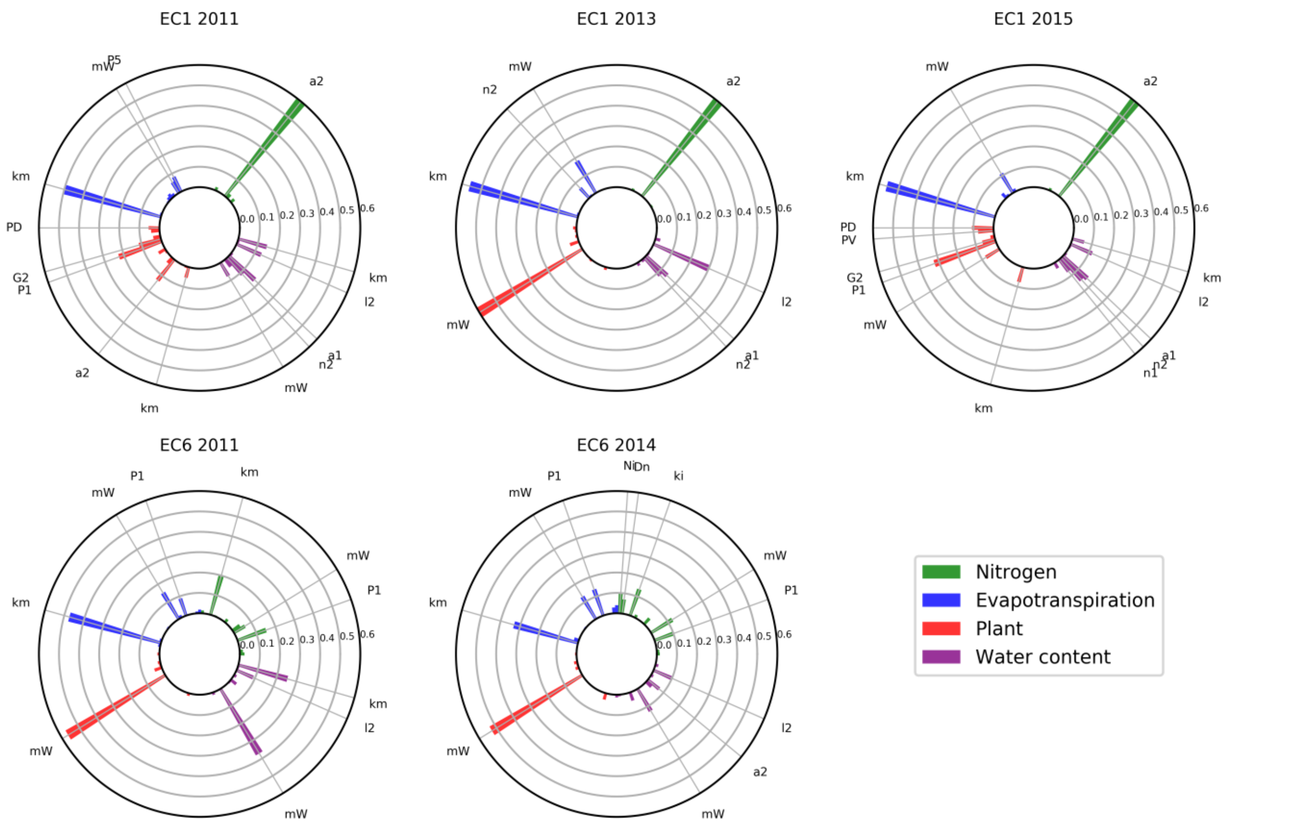


*Figure 1. First order sensitivity indices (S1) for the two sites (EC1 and EC6) and the four years (2011, 2013, 2014 and 2015). Each circle plots the S1 for one year x site combination and the four target variables Nitrogen, Evapotranspiration, Plant and Water Content. The labels refer to parameters which have a S1 of higher than 0.05.*

also related to crop specific parameters at EC1.
Rainfall during the vegetation period in these two years was 20-30% lower than in 2013 indicating that the amount of water entering the system affects the parameter sensitivities. In 2014 and 2015, vegetation periods were warmer than in 2011 and 2013, (+15% at EC1, 2015; +20% at EC6, 2014). Especially the winters were mild with mean temperatures over 0°C. However, this is apparently not affecting the parameter sensitivities. The shallower soil profile of EC6 results in an insensitivity to the van Genuchten parameter n as well as an insensitivity to the van Genuchten parameters in the first soil layers.

## IV. Conclusions & Outlook

We identified 6 parameters that explain most of the variance in soil-crop model performance. This result is independent from the targeted model output. However, the target variable affected the most by these six parameters is different between the two sites. Specific crop and carbon-nitrogen model parameters play a minor role although this result seems to be site- and year-specific. We conclude that the parameters belonging to the soil water regime are the most important for the overall model performance. Our planned next step is to calculate S1 independently from the measurements. S1 will be calculated for each simulation point and afterwards averaged in accordance with [6]. Besides, we will investigate if the S1s are affected by within-sample dependencies originating from the crashed simulations. Further, S1 values will be calculated for more sites and years to evaluate inasmuch the differences in the S1 values depend on year and site. We will also evaluate if our findings hold true with other popular crop models. We think that it is important to test to what extent parameters that control overall model performance affect also single target variables. The underlying hypothesis is that training soil-crop models with more comprehensive sets of target and non-target variables makes them more robust.

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