

# 1 Crop rotation modelling – a European model intercomparison

2 Chris Kollas<sup>1\*</sup>, Kurt Christian Kersebaum<sup>1</sup>, Claas Nendel<sup>1</sup>, Kiril Manevski<sup>2</sup>, Christoph Müller<sup>3</sup>, Taru  
3 Palosuo<sup>4</sup>, Cecilia M. Armas-Herrera<sup>5</sup>, Nicolas Beaudoin<sup>5</sup>, Marco Bindi<sup>18</sup> Monia Charfeddine<sup>7</sup>, Tobias  
4 Conradt<sup>3</sup>, Julie Constantin<sup>8</sup>, Josef Eitzinger<sup>9</sup>, Frank Ewert<sup>11</sup>, Roberto Ferrise<sup>18</sup>, Thomas Gaiser<sup>11</sup>, Iñaki  
5 Garcia de Cortazar-Atauri<sup>12</sup>, Luisa Giglio<sup>7</sup>, Petr Hlavinka<sup>13</sup>, Holger Hoffmann<sup>11</sup>, Munir P. Hoffmann<sup>14</sup>,  
6 Marie Launay<sup>12</sup>, Remy Manderscheid<sup>15</sup>, Bruno Mary<sup>5</sup>, Wilfried Mirschel<sup>1</sup>, Marco Moriondo<sup>19</sup>, Jørgen E.  
7 Olesen<sup>2</sup>, Isik Öztürk<sup>2</sup>, Andreas Pacholski<sup>15,9</sup>, Dominique Ripoche-Wachter<sup>12</sup>, Pier Paolo Roggero<sup>6</sup>, Svenja  
8 Roncossek<sup>2</sup>, Reimund P. Rötter<sup>4</sup>, Françoise Ruget<sup>16</sup>, Behzad Sharif<sup>2</sup>, Mirek Trnka<sup>13</sup>, Domenico Ventrella<sup>7</sup>,  
9 Katharina Waha<sup>3,20</sup>, Martin Wegehenkel<sup>1</sup>, Hans-Joachim Weigel<sup>15</sup>, Lianhai Wu<sup>17</sup>

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11 \*Corresponding author: [chris.kollas@zalf.de](mailto:chris.kollas@zalf.de)

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13 1 Institute of Landscape Systems Analysis, Leibniz Centre for Agricultural Landscape Research (ZALF),  
14 Eberswalder Str. 84, 15374 Müncheberg, Germany

15 2 Department of Agroecology, Aarhus University, Blichers Alle 20, 8830 Tjele, Denmark

16 3 Potsdam Institute for Climate Impact Research, P.O. Box 601203, 14412 Potsdam, Germany

17 4 Natural Resources Institute Finland (Luke), Viikinkari 4, 00790 Helsinki, Finland

18 5 INRA UR1158 AgroImpact, 02000 Barenton-Bugny, France

19 6 Nucleo di Ricerca sulla Desertificazione e Dipartimento di Agraria, University of Sassari, 07100 Sassari, Italy

20 7 Consiglio per la Ricerca in Agricoltura e l'analisi dell'economia agraria, Unità di ricerca per i sistemi culturali  
21 degli ambienti caldo-aridi (CRA-SCA), Via Celso Ulpiani 5, 70125 Bari, Italy

22 8 INRA, UMR1248 AGIR, F-31326 Castanet-Tolosan, France

23 9 Institute of Meteorology, Department for Water, Atmosphere and Environment, University of Natural Resources  
24 and Applied Life Sciences, Peter Jordan Strasse 82, A-1190 Vienna, Austria

25 10 Graduate School/Inkubator, Leuphana University Lüneburg, Scharnhorststr. 1, 21335 Lüneburg, Germany

26 11 INRES, University of Bonn, Katzenburgweg 5, 53115 Bonn, Germany

27 12 INRA, US1116 AgroClim, F-84914 Avignon, France

28 13 Mendel University, Zemědělská 1665/1, 61300 Brno, Czech Republic

29 14 Crop Production Systems in the Tropics, Georg-August-Universität Göttingen, Grisebachstr. 6, 37077 Göttingen,  
30 Germany

31 15 Thünen Institute of Biodiversity, Bundesallee 50, 38116 Braunschweig, Germany

32 16 INRA, UMR1114 EMMAH, F-84914 Avignon, France

33 17 Rothamsted Research, North Wyke, Okehampton EX20 2SB, UK

34 18 Department of Agri-food Production and Environmental Sciences, University of Florence, P.le delle Cascine 18,  
35 50144 Firenze, Italy

36 19 Institute of Biometeorology of the National Research Council (CNR-IBIMET), via Caproni 8, 50145 Firenze,  
37 Italy

38 20 CSIRO Agriculture, 306 Carmody Road, 4067 St. Lucia QLD, Australia

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## 46 **Keywords**

47 Model ensemble, crop simulation models, catch crop, intermediate crop, treatment, multi-year

## 1 **Abstract**

2 Diversification of crop rotations is considered an option to increase the resilience of European  
3 crop production under climate change. So far, however, many crop simulation studies have  
4 focused on predicting single crops in separate one-year simulations. Here, we compared the  
5 capability of fifteen crop growth simulation models to predict yields in crop rotations at five sites  
6 across Europe under minimal calibration. Crop rotations encompassed 301 seasons of ten crop  
7 types common to European agriculture and a diverse set of treatments (irrigation, fertilisation,  
8 CO<sub>2</sub> concentration, soil types, tillage, residues, intermediate or catch crops).

9 We found that the continuous simulation of multi-year crop rotations yielded results of slightly  
10 higher quality compared to the simulation of single years and single crops. Intermediate crops  
11 (oilseed radish and grass vegetation) were simulated less accurately than main crops (cereals).  
12 The majority of models performed better for the treatments of increased CO<sub>2</sub> and nitrogen  
13 fertilisation than for irrigation and soil-related treatments. The yield simulation of the multi-  
14 model ensemble reduced the error compared to single-model simulations.

15 The low degree of superiority of continuous simulations over single year simulation was caused  
16 by a) insufficiently parameterised crops, which affect the performance of the following crop, and  
17 b) the lack of growth-limiting water and/or nitrogen in the crop rotations under investigation. In  
18 order to achieve a sound representation of crop rotations, further research is required to  
19 synthesise existing knowledge of the physiology of intermediate crops and of carry-over effects  
20 from the preceding to the following crop, and to implement/improve the modelling of processes  
21 that condition these effects.

22

# 1. Introduction

In many European countries, field crops are traditionally grown in rotation (a varying sequence of different crops, often including intermediate crops) for a number of economic and environmental reasons.

Firstly, most crops benefit from the nutrients released by mineralising residues of the preceding crop. This substitution of mineral fertiliser by the strategic use of nutrient-rich crop residues is especially important in low-fertilised cropping systems, where intermediate crops are grown for the purpose of catching and recycling nutrients, in particular nitrogen (N), from deeper soil layers (catch crops, see Askegaard and Eriksen, 2008). Furthermore, intermediate crops prevent rainfall from percolating through the soil and leaching nutrients out of the rooting zone of the main crops, also preventing erosion (cover crops, Boardman and Favis-Mortlock, 2014; Simoes et al., 2014).

In addition, intermediate crops are used as fertility-building crops or green manure to add further nutrients to the soil (Kirkegaard et al., 2008). Secondly, a well-designed crop rotation can contribute organic matter to the soil to compensate for decomposition under the prevailing environmental conditions (Kay, 1990), maintaining long-term soil fertility and habitat quality for soil organisms. Sufficient soil organic matter also reduces the risk of erosion and nutrient losses while increasing the potential water supply to the crop by increasing the soil water storage capacity. Thirdly, the risk of phyto-sanitary problems in the crop rotation can be minimised by accounting for the ability of different species to repel pests or diseases by interrupting the life cycle of host-specific pathogens via so-called break crops (Angus et al., 2011). The same applies to the control of weeds, the unwanted growth of which can be hampered effectively by selecting a suitable preceding crop, especially in cropping systems where resistance to herbicides has developed (Stevenson and Van Kessel, 1996).

1 In a wider context, crop rotations – and thus crop diversification – have been identified as  
2 prominent measures for increasing the resilience of the agricultural system (Reidsma et al., 2009;  
3 Lin, 2011, Smith et al. 2008), developing mitigative adaptation strategies to climate change  
4 (Olesen et al., 2011) and improving ecosystem services (Hauck et al. 2014). Consequently, the  
5 recent common agricultural policy (CAP) of the European Commission (2011) considers the  
6 diversification of crop rotations a key measure for more sustainable agriculture. While in organic  
7 farming the design of crop rotations is driven by the idea of reducing N losses by transferring it  
8 among crops and improving soil fertility, conventional crop rotations are driven by economic and  
9 political boundary conditions. Agricultural policies have a strong potential to modify cropping  
10 trends (European Commission 2010), such as the use of catch crops, which is promoted by policy  
11 incentives within agro-environmental action plans (e.g. European Water Framework directive,  
12 Uthes et al. 2010).

13 Crop models provide an explicit representation of fundamental bio-physical processes such as  
14 crop development and growth (photosynthesis, leaf area and canopy expansion, dry matter  
15 partitioning and root growth), and water/N cycles in a single crop season or within a crop rotation  
16 (Wallach et al., 2006). In the past, crop rotation modelling was regularly applied as a tool for  
17 investigating the soil water balance among certain crop sequences (Post et al., 2007; Salado-  
18 Navarro and Sinclair, 2009) and for estimating the amount of nitrate that leaches over long  
19 periods (Beaudoin et al., 2008; Kersebaum and Beblik, 2001; Kovács et al., 1995). In addition,  
20 growing interest in the carbon storage capacity of agricultural soils and crops has led to the  
21 application of crop rotation modelling studies focusing on long-term soil carbon dynamics (Li et  
22 al., 1994; Blombäck et al., 2003; Hlavinka et al., 2013). Last but not least, crop rotation models  
23 have also been used to study the development of above-/below-ground biomass and yields  
24 (Berntsen et al., 2006) as well as nitrogen uptake (Nendel et al., 2013). These examples show that

1 the precise simulation of crop rotations will help us to better address a wide range of challenges  
2 facing society, e.g. soil and water conservation, carbon sequestration, mitigation of greenhouse  
3 gas emissions, sustainable intensification of cropping practice, and food security.

4 One drawback of such models is that they do not deal specifically with uncertainty in explaining  
5 data, measurements or conditions in agro-climatic regions; instead, they inherently evoke  
6 uncertainty in the model predictions (Asseng et al., 2013). For this reason, emphasis has recently  
7 been placed on the multi-model ensemble methodology, which was recommended as a valuable  
8 tool for assessing and reducing uncertainties in crop simulations (Rosenzweig and Wilbanks,  
9 2010; Rötter et al., 2011; Challinor et al., 2014). In fact, previous studies demonstrated the  
10 strength of model intercomparisons (Palosuo et al., 2011; Rötter et al., 2012; Asseng et al., 2013;  
11 Asseng et al., 2014; Bassu et al., 2014; Li et al., 2014; Martre et al., 2014). Palosuo et al. (2011)  
12 showed that, with minimal calibration, none of the models involved were robust enough and  
13 sufficiently accurate across a range of environments in a winter-wheat crop model comparison  
14 exercise. Furthermore, all of the above studies showed that the multi-model mean of simulations  
15 is a better estimator of the mean crop yield than single-model simulations.

16 However, most climate impact studies on crop production focus methodologically on simulating  
17 single years and single crops (Asseng et al., 2013; Bassu et al., 2014; Palosuo et al., 2011; Rötter  
18 et al., 2012), although *in situ* crop performance depends strongly on the crop's position within the  
19 sequence of crops (see arguments above). In these studies, the initial conditions of the soil in  
20 terms of water, organic matter and nutrients were kept constant at the onset of each of the  
21 growing seasons; carry-over effects such as N mineralising from the harvest residues of the  
22 previous year or altered soil water content due to evaporation from cover crops were ignored,  
23 which is viewed as a drawback of climate impact studies (Ewert et al., 2014). In contrast,

1 Teixeira et al. (in press) recently demonstrated the advantage of simulating continuous crop  
2 rotations compared to single crops and years for a single location in new Zealand, particularly  
3 under limited growing conditions. Here, we hypothesise that the continuous simulation of crop  
4 growth across years will improve yield predictions at different locations across Europe and  
5 rotations compared to simulating crop growth in single years only.

6 All of the multi-model comparisons were undertaken for the globally most important staple  
7 crops, such as wheat, barley, rice and maize (Asseng et al., 2013; Bassu et al., 2014; Li et al.,  
8 2014; Palosuo et al., 2011; Rötter et al., 2012); less attention was paid to other key crops such as  
9 sugar beet and oat (White et al., 2011). Moreover, intermediate crops are largely disregarded in  
10 crop simulation studies. With a few exceptions (i.e. some legumes), these crops generate a  
11 limited or no direct commercial product, but have a significant impact on soil fertility and the  
12 growth of the following crop (Blombäck et al., 2003). Consequently, many current crop models  
13 exhibit a limited ability to simulate continuous farming systems.

14 In the present study, therefore, we ask the following research questions concerning a minimal  
15 model calibration of fifteen crop growth simulation models:

16 (1) How accurately can a crop model ensemble simulate the crop yields of various crop rotations?  
17 Furthermore, which of the two modes of simulation – continuous or year-by-year – performs  
18 better in terms of accuracy?

19 (2) Which crops common to European agriculture are simulated more accurately, and which  
20 crops create major deficiencies in reproducing yields?

21 (3) Is a crop model ensemble capable of reproducing the effects of sites and treatments on crop  
22 yield?



## 1        2. Methods

### 2        2.1. Experimental crop rotations

3        Five experimental crop rotation datasets, each containing a different set of treatments (Table 1),  
4        were selected for the present study. The datasets cover the European environmental zones of the  
5        Atlantic North, Atlantic Central, Continental and Pannonia (lowlands, valleys and mountain  
6        peripheries on the Middle- and the Lower-Danube Plains and the Black Sea area), according to  
7        Metzger et al. (2005, Fig. 1). Overall, the study provided experimental data on 301 growing  
8        seasons and ten distinct crops.

9        At the experimental site in Foulum, Denmark, the effects of catch crops in crop rotations and the  
10       strategies of tillage and crop residues at harvest were investigated from 2002 to 2012. For our  
11       study, six treatments encompassing two rotations were selected, namely a rotation of winter  
12       barley (*Hordeum vulgare* L.)–winter oilseed rape (*Brassica napus* L.)–winter wheat (*Triticum*  
13       *aestivum* L.) and a rotation of winter wheat/grass (*Lolium perenne* L.)–spring barley/grass–pea  
14       (*Pisum sativum* L.)–winter wheat–winter wheat–spring barley/oilseed radish (*Raphanus sativus*  
15       var. *oleiformis*)–spring oat (*Avena sativa* L.); two tillage regimes (ploughed and no tillage); and  
16       two residue managements (retention of straw at the site and removal of straw). The experimental  
17       site and setting are described in detail in Munkholm et al. (2008).

18       A second experiment in Müncheberg, Germany, was designed to study management intensities,  
19       irrigation, biomass development and inter-annual variation in crop rotations (Mirschel et al.,  
20       2007). The dataset, consisting of one crop rotation from 1992 to 1998, is composed of sugar beet  
21       (*Beta vulgaris* L.), winter wheat, winter barley, winter rye (*Secale cereale* L.) and oilseed radish  
22       (catch crop). The rotation was carried out in four parallel plots with a shift of one year to  
23       establish each crop each year. Treatments included rainfed agriculture versus an irrigated regime.



1 The Braunschweig Free-Air Carbon Dioxide Enrichment (FACE) experiment was set up to study  
2 the interactive effects of CO<sub>2</sub> concentration and N fertilisation on crop production (Weigel and  
3 Manderscheid, 2012). The crop rotation consisted of winter barley – a mixture of three different  
4 ryegrass cultivars (*Lolium multiflorum Lam.*) as a cover crop – sugar beet–winter wheat, a  
5 sequence grown in two consecutive cycles starting in autumn 1999. Treatments included an  
6 ambient (374 ppm) and an enriched (550 ppm) concentration of atmospheric CO<sub>2</sub>, both with a  
7 standard and a reduced (-50 %) supply of nitrogen (N) fertiliser.

8 The fourth experiment focused on agricultural management practice concerning soil water  
9 drainage and nitrate leaching, using lysimeters in the agricultural region in Marchfeld, Austria  
10 (Eitzinger et al., 2004). Here, the crop rotation involved mustard (*Sinapis alba*, catch crop)–  
11 spring wheat–mustard–barley–winter wheat–mustard–potato (*Solanum tuberosum L.*)–winter  
12 wheat–maize (*Zea mays L.*)–winter wheat. The crops were grown on three soil types (Calcic  
13 Chernozem, shallow and sandy Calcaric Phaeozem and Gleyic Phaeozem) in order to study the  
14 water cycle, and the influence of soil type and rotation.

15 Finally, the Thibie experiment in France combined the effects of catch crops (catch crop vs. no  
16 autumn/winter crop cover) and nitrogen fertiliser (conventional vs. reduced N fertilisation) on  
17 yields involving a medium-term experiment from 1991 to 2003 (Constantin et al.; 2010, 2012). It  
18 consisted of a split-plot design of pea, winter wheat and sugar beet crops in rotation. All crops  
19 were present each year. The catch crops grown during the period under investigation included  
20 grass, oilseed radish and barley.

## 21 **2.2. Crop models**

22 Fifteen European modelling teams participated in the present study. The models varied  
23 considerably in complexity and functionality, ranging from a dynamic global vegetation model to

1 agroecosystem models designed for field-scale application (Table 2). A list describing the  
2 physiological processes and approaches taken by the models can be found in Supplement A. The  
3 models were grouped according to their capability of simulating continuous crop growth. Three  
4 models (Theseus, SWIM and APSIM) performed continuous runs only, i.e. they simulated the  
5 multi-year datasets without reinitialising subroutines at the onset of each growing season,  
6 hereafter called ROTATION. The five models DSSAT1/DSSAT2, LPJmL, SPACSYS and  
7 WOFOST performed single-season crop growth only, i.e. they simulated each crop in the rotation  
8 separately, hereafter called SINGLE. Crops were simulated separately either because the model  
9 was unable to reproduce rotations (e.g. cover periods without crop) or because specific crops had  
10 not yet been implemented in that respective model. In the latter case, models skipped the  
11 corresponding crop or dataset. Finally, half of the models (DAISY, FASSET, HERMES,  
12 MONICA, STICS, LINTUL and CROPSYST) provided results for both modes, ROTATION and  
13 SINGLE (Table 2).

### 14 2.3. Simulation task with standardised input data

15 The simulation task for all modellers was designed to reproduce the field experimental  
16 treatments. Hence, the modelling teams were requested to simulate each treatment at each site,  
17 using observed information on daily weather (precipitation, minimum and maximum  
18 temperature, mean relative humidity, global radiation and mean wind speed), information on  
19 daily field management (previous crops, tillage, sowing, irrigation, fertilisation and harvest) and  
20 soil properties (bulk density, texture, organic matter and water capacity parameters) as the driving  
21 variables for the models. All of the variables were provided synchronously. In order to evaluate  
22 any differences between the SINGLE and ROTATION modes of simulation, the modelling teams  
23 were supplied with initial values of soil water content and soil mineral N (at a date close to

1 sowing) for each treatment for the first year only. Thus, the ROTATION simulation was set up  
2 once using the specified initial values, and crop growth was subsequently simulated for the period  
3 of the rotation. In contrast, the modellers set up the SINGLE mode of simulations by using the  
4 initial values to set up and run the first year of simulations and subsequently used estimates of the  
5 initial values to calculate the subsequent year's crops separately.

6 The modelling teams were additionally asked to provide information on how initial values were  
7 estimated at the beginning of the growing seasons in the SINGLE mode of calculation. The  
8 modellers also provided information on how “experienced” the model was in simulating each  
9 crop in terms of the number of seasons it had been applied and calibrated in the past.

#### 10 **2.4. Model calibration**

11 In addition to the input data described above, the modellers were provided with limited data  
12 (separately for each site and dependent on the availability of observation data) to perform a  
13 minimal calibration of local crop varieties. The data, i.e. the variable subject to calibration for  
14 each site, is shown in Table 1. This method followed the idea of a “blind test” in order to mimic  
15 modelling practice in the event of scarce data, which is often encountered in regional climate  
16 impact studies (Palosuo et al. 2011; Rötter et al. 2012; Asseng et al. 2013; Bassu et al. 2014). The  
17 calibration data consisted of key phenological observations (dates of emergence, anthesis and  
18 maturity) for one single treatment of the datasets for Foulum and Hirschstetten (Table 1), harvest  
19 dates in Thibie, final biomass observations for Müncheberg as well as phenological observations  
20 for the first four years at Braunschweig.

1 After calibration, the modelling teams ran their models for all other years and treatments in the  
2 two simulation modes (ROTATION and SINGLE), and the model outputs were gathered for  
3 statistical analysis.

4

## 5 **2.5. Evaluation of model performance**

### 6 *2.5.1. Crop rotations*

7 Model performance was evaluated by calculating complementary performance indicators, as  
8 proposed by Bennett et al. (2013). The selection of indicators enables the magnitude of errors to  
9 be quantified and bias to be detected. The following model performance indicators were  
10 calculated for each model, site and mode of simulation (ROTATION and SINGLE), and then  
11 averaged for each site: mean absolute error (MAE), index of agreement (IOA), percent bias  
12 (PBIAS) and root mean square error (RMSE). MAE is calculated as the average of the absolute  
13 errors. It provides the magnitude of deviation by ignoring the direction of the deviation. IOA is a  
14 standardised measure of the degree of model prediction error, ranging from 0 to 1, with the latter  
15 indicating a perfect fit (Willmott, 1982). PBIAS (%) was calculated as:

$$16 \quad \text{PBIAS} = 100 * \frac{\sum_{i=1}^n (S_i - O_i)}{\sum_{i=1}^n O_i} \quad \text{eq. 1}$$

17 where  $s_i$  is simulated crop yield and  $o_i$  observed crop yield at each harvest date. PBIAS measures  
18 the tendency of the model to overestimate or underestimate the measured values. An optimal  
19 PBIAS value is 0.0; positive values indicate an overestimation and negative values are indicative  
20 of an underestimation. Finally, RMSE represents the sample standard deviation of the differences  
21 between simulated and observed values. In contrast to MAE, the main drawback of RMSE is that

1 it is sensitive to outliers. Nonetheless, it was calculated here to enable the results to be compared  
2 with earlier modelling studies. Further, we partitioned RMSE into its systematic part:

$$3 \quad \text{RMSE}_s = \sqrt{1/n \sum_{i=1}^n (\bar{S}_i - O_i)^2} \quad \text{eq. 2}$$

4 which describes the linear bias, and its unsystematic part, where  $\bar{S}_i$  is derived from the linear  
5 regression between observed and simulated values. The random error was calculated according to  
6 Willmott (1982):

$$7 \quad \text{RMSE}_u = \sqrt{1/n \sum_{i=1}^n (S_i - \bar{S}_i)^2} \quad \text{eq. 3}$$

### 8 *2.5.2. Performance of crop rotation vs single-year simulations*

9 Student's t-tests were conducted separately on the three main analyses (per site, per crop, per  
10 treatment) of this study ( $\alpha = 0.05$ ). We compared the mean of performance indicators in the  
11 ROTATION mode of simulation against the mean in SINGLE mode. In the site-specific analysis,  
12 we used performance indicators for each site as a pair in the paired t-test. In the crop-specific  
13 analysis, we used performance indicators for each crop as pairs in the paired t-test. Finally, in the  
14 treatment-specific analysis, we tested each treatment separately, using performance indicators for  
15 each model as pairs in the paired t-test.

16

### 17 *2.5.3. Crop-specific yield*

18 In order to evaluate the quality of the crop-specific simulation, we calculated performance indices  
19 on yield prediction (in tonnes dry matter per hectare; t DM ha<sup>-1</sup>) for each crop across all models,  
20 treatments and sites. Final aboveground biomass was only evaluated for oilseed radish and grass  
21 vegetation because biomass was a better proxy for growth in these catch crops. Mustard was

1 excluded from this analysis because no observations were available for this crop. In order to  
2 detect any differences between the predictability of crops, the normalised mean absolute error  
3 (nMAE) was calculated as follows:

$$4 \quad \text{nMAE} = \frac{\frac{1}{n} \sum_{i=1}^n |s_i - o_i|}{\bar{o}_i} \quad \text{eq. 4}$$

5 where  $\bar{o}_i$  is the mean of observations of all datasets and treatments. Here, normalisation is  
6 required because mean observed yields vary considerably from crop to crop. In addition, we  
7 selected the indicator PBIAS because it measures the average tendency to overpredict or  
8 underpredict. We consciously decided against using the index of agreement or modelling  
9 efficiency (Nash and Sutcliffe, 1970), since both indicators determine the variance of the  
10 simulated and observed dataset. Since the yield simulation of each model for a certain crop type  
11 varies around a certain level/mean but observations vary on one level only, the ensemble of  
12 simulations will obviously invariably exhibit greater variance than observations.

13

#### 14 *2.5.4. Management treatments*

15 The capability of models to reproduce a wide range of treatments (Table 1) was tested.  
16 Differences between yields of the standard treatment and the above-mentioned treatments were  
17 calculated for observations and for the ROTATION and SINGLE modes of simulation.  
18 Differences were expressed as percentages of the yields of the standard treatment, and averaged  
19 per model. In addition, performance indicators RMSE, MAE and IOA were calculated on the  
20 level of the simulations of each model, and averaged per treatment.

## 1 **3. Results**

### 2 **3.1. Crop rotations**

3 Yield simulations of both ROTATION and SINGLE runs of each model were compared to  
4 observations of all seasons, treatments and sites covered by the individual model. Figure 2  
5 provides an overview of all modelling results per site and crop. Overall, the models provided  
6 similar results for ROTATION and SINGLE simulations, and the model results showed higher  
7 yield variability than the observed results, especially in Foulum. Notable differences between the  
8 observed and simulated yields were detected for several crops, such as oat and pea at Foulum,  
9 sugar beet at Müncheberg and Thibie, and wheat and potato at Hirschstetten. The closest match  
10 between the observed and simulated mean results was achieved for crops at Braunschweig.

11 The largest deviations (highest RMSE and MAE values) between simulated and observed yields  
12 occurred at Thibie, which was the most diverse dataset, followed by Müncheberg, although the  
13 IOA values for these two sites were high (Table 4). In contrast, the models performed best at  
14 Braunschweig and Foulum, as shown by performance indicators RMSE and MAE, although the  
15 results of these two sites had the lowest IOA values. Here, the low IOA values were due to the  
16 fact that IOA evaluates the variance of the observations and simulations such that large variances  
17 are favoured. Since the variance of yields in Foulum is very low (no sugar beet), the index of  
18 agreement is influenced negatively in this case.

19 With regard to the crop yield datasets, those from Müncheberg and Thibie were systematically  
20 underestimated in ROTATION mode by 11 % and 18 % , respectively, whereas those from  
21 Hirschstetten were overestimated considerably (by 43 % mean per site across all models).  
22 Systematic errors regularly exceeded unsystematic errors, with the exception of Foulum. This

1 indicates that crop growth processes were reflected successfully by the models, but predictions of  
2 crop yields were considerably biased due to the minimal calibration.

3 The simulation accuracy of the single best model resembled the accuracy of the multi-model  
4 mean simulations (Tables 4 & 6). One out of three indicators (IOA) exhibited significantly more  
5 accurate results when the ROTATION simulation mode was compared to the SINGLE mode  
6 (Table 4).

7

### 8 **3.2. Crop-specific yields**

9 Each crop type was simulated by at least five (ROTATION) or four (SINGLE) models (Table 3).  
10 However, more models provided results for main crops such as wheat and rye, whereas fewer  
11 models were capable of simulating intermediate crops such as oilseed radish or grass vegetation.  
12 Of the crops simulated, oilseed radish and oat were simulated by seven modelling teams for the  
13 first time (Table 3), using proxies for the crop-specific parameter setting. Wheat and barley were  
14 present in each dataset and thus grown under varying environmental conditions, whereas crops  
15 such as maize, potato, rye and oat were grown at one site each only (Table 3).

16 RMSE and nMAE showed that, across all crops, the ROTATION mode of simulation resulted in  
17 slightly more accurate results than those generated in SINGLE mode (Fig. 3, Table 5). In  
18 addition, the multi-model mean again produced good accuracy compared to the results generated  
19 by single crops (rRMSE of 0.31 and nMAE of 0.26 in ROTATION mode). With the exception of  
20 maize, yields of the main cereals (wheat, barley, rye and oat) were reproduced reasonably well  
21 with nMAE<0.5, meaning errors less than 50 % of the mean observed crop yield. Notably, sugar  
22 beet (occurring in three datasets and modelled by nine groups in ROTATION mode and ten



1 teams in SINGLE mode) was simulated with a high degree of accuracy, as shown by the two  
2 normalised measures of accuracy (nMAE=0.32 and rRMSE=0.42), whereas in absolute terms it  
3 was the crop with the highest simulation error (RMSE: 6.9 t ha<sup>-1</sup> DM). Potato exhibited a low  
4 deviation in ROTATION and a high deviation in SINGLE simulation mode. In contrast,  
5 intermediate crops (oilseed radish and grass vegetation) were generally simulated with a rather  
6 low degree of accuracy (nMAR>0.5). Overall, both ROTATION and SINGLE agreed on bias  
7 across all crops with the exception of maize, where ROTATION overestimated (PBIAS>0) yield  
8 and SINGLE underestimated it (PBIAS<0; Table 5). A notable systematic underestimation of  
9 yields was found for oat, sugar beet (in Müncheberg and Thibie) and grass vegetation and, to a  
10 lesser extent, for rye, pea and oilseed radish; in contrast, yields were overestimated for potato and  
11 barley.

12

### 13 **3.3. Management treatments**

14 The observed and simulated treatment effects on crop yields are shown in Table 6, separated by  
15 modes of simulation (ROTATION and SINGLE). The DM yield change (in %) is calculated from  
16 the yields of a zero-treatment as a reference. The three indicators of simulation quality (RMSE,  
17 MAE and IOA) exhibited no significant difference between ROTATION and SINGLE simulation  
18 modes for treatment effects.

#### 19 *3.3.1. Irrigation*

20 The observations at Müncheberg indicated a 19.6 % mean yield increase due to irrigation (Table  
21 6). However, the mean irrigation effect of the simulation of all models was 12.2 % (ROTATION)  
22 and 8.1 % (SINGLE). Hence, although the positive effect of irrigation on crop yield was

1 simulated by the models, it was underestimated for all crops, particularly for wheat and sugar  
2 beet. The rainfed treatments were simulated more accurately than the irrigated treatments.

### 3 4 3.3.2. *CO<sub>2</sub>*

5 At Braunschweig, an 11.3 % mean yield increase was observed due to a 176 ppm increase in  
6 atmospheric CO<sub>2</sub> concentration. This effect was captured well by the models (Table 6, Fig. 4).  
7 The simulated mean effect was 10.9 % (ROTATION) and 12.3 % (SINGLE).

### 8 3.3.3. *Nitrogen*

9 The observed effect of the increased N application rate on yields was 12.7 % in Braunschweig  
10 and 2.5 % in Thibie (Table 6). This effect was captured especially well by the results generated  
11 using the ROTATION mode. In contrast, the SINGLE simulation mode underestimated this  
12 effect at Braunschweig, generating an effect of about 7 %, and approximately 2 % at Thibie. The  
13 accuracy of simulations was the same for both N application treatments.

### 14 3.3.4. *Tillage and residues*

15 At Foulum, the observed effect of conventional tillage on the crop yield compared to no tillage  
16 was -3.7 %. The mean results generated by the models exhibited virtually no effect on yields,  
17 although there was a 0.6% simulated yield increase when using the ROTATION mode. The  
18 observed effect of residue handling (retention of straw on the field compared to removal of straw)  
19 on crop yield was negligible during the investigated period (1.5 %). This was confirmed by the  
20 ROTATION simulation mode (0.6 %), but not by the SINGLE mode of yearly calculations  
21 (-9.7 %).

### 22 3.3.5. *Soil*

1 At Hirschstetten, the significantly lower crop yields on the Calcaric Phaeozem soil (−51.1 %)   
2 compared to yields on the Gleyic Phaeozem soil were captured poorly by the simulations (−11.4   
3 % and −5.1 % for ROTATION and SINGLE mode, respectively). The observed strong negative   
4 effect of the sandy soil was underestimated by the models for all crops, with the largest errors   
5 occurring for wheat and barley. In addition, the majority of errors emerged from the simulation of   
6 yields at the Calcaric Phaeozem (sandy texture) rather than from the simulation of yields at the   
7 Gleyic Phaeozem. Four models showed no effect or even an opposite soil effect on yields; five   
8 other models exhibited only very minor effects on yield reduction. Observed yields at the Calcic   
9 Chernozem differed insignificantly from the Gleyic Phaeozem (0.9 % change), which was   
10 reproduced by both modelling modes (ROTATION and SINGLE).

### 11 *3.3.6. Intermediate crops*

12 The model ensemble failed to capture the slightly positive effect of introducing intermediate   
13 crops (oilseed radish and grass vegetation) on yields of the following main crops (+3.5 %). The   
14 model ensemble yielded effects of 0 % and −2.5 % for ROTATION and SINGLE, respectively.   
15 Only two models in the ROTATION mode were able to reproduce the small positive effect.

16

## 17 **4. Discussion**

18 This study compared for the first time the accuracy of fifteen minimally calibrated crop models in   
19 simulating yields of various crop rotations. The overall results showed that the simulation of an   
20 entire rotation is better at estimating crop yields than single-year simulations. The study also   
21 revealed that not all crops, i.e. their yields, are simulated equally well, highlighting focal areas for   
22 future field studies and potential improvements to the models. Likewise, treatments, i.e. field

1 management practices, were identified that require attention when represented in the models.  
2 Since the study includes a large number of models that simulate a variety of field experiments, it  
3 must be noted that individual model errors may cancel each other out (see, e.g. Fig. 2). Hence the  
4 conclusion drawn from our analysis refers to the ensemble, and cannot be related to a single  
5 model. The field experiments used in this study were originally designed to address specific  
6 questions that were of interest to stakeholders. In practice, crop rotations are often simpler and,  
7 under certain circumstances, cause environmental problems.

8

#### 9 **4.1. Crop rotations**

10 In the present study, the site-specific index of agreement (IOA) across all models varied between  
11 0.45 and 0.87 (per site), and is thus comparable to reported IOA values of 0.4 to 0.7 per model  
12 found in a single-crop study with very limited calibration (Palosuo et al., 2011). However, the  
13 IOA values determined are lower than the IOA values of 0.9 to 0.99 per model reported in a  
14 calibrated single-site study (Kersebaum et al., 2007).

15 Large simulation errors in sugar beet yields were the main driver of the high discrepancies  
16 between modelled and observed yields for the Thibie dataset. Since five modelling teams  
17 parameterised sugar beet for the first time using proxies such as potato crop parameters, these  
18 models were responsible for the wide range of simulated yields (between 0.2 and 29.2 t ha<sup>-1</sup>)  
19 differing greatly from observed yields (12.8 to 21.2 t ha<sup>-1</sup>). Thus, we identified the need to  
20 accurately parameterise sugar beet in several models in order to improve the simulation results  
21 and to meet study demands, since this crop is agro-economically and environmentally important  
22 in large parts of Europe. The best modelling results were achieved for the Braunschweig dataset,

1 which contained only one of the less accurately simulated crops (grass vegetation), homogenous  
2 soil conditions and a relatively small number of treatments. Uncertainties between sites were  
3 therefore driven mainly by the ability of the models to capture minor crops and soil conditions.  
4

#### 5 **4.2. Crop rotation vs. single-year simulation**

6 Simulating continuous crop rotations has the potential to increase the precision of yield estimates  
7 compared to simulations of crop growth on a single-year basis. This is due to the fact that soil  
8 water, soil organic matter and nutrient conditions can be predicted more accurately in rotation , as  
9 this mode continuously updates soil conditions daily, and does not assume any soil conditions at  
10 the beginning of the growing season, as is the case in single-year simulations.

11 In the five selected field experiments, crops were grown under nutrient-rich conditions and  
12 generally adequate water supply, especially during the onset of the growing period, when soils  
13 were usually at field capacity. Thus, most crops began to grow under close-to-optimal  
14 environmental conditions. Under these conditions, the presumed carry-over effects, such as water  
15 and nutrient savings and transfer from the previous crop (reproduced in ROTATION mode only),  
16 could only affect the growth of the next crop to a low degree. While rotation effects under  
17 nutrient-limited conditions turned out to be significant (Smith et al. 2008), studies for wheat and  
18 maize, for instance, showed that the positive rotation effect decreased with increasing fertilisation  
19 levels (Angus et al., 2001; Berzsenyi et al., 2000; Sieling et al., 2005) and better water supply  
20 (Nevens and Reheul, 2001). Similar results were obtained by Teixeira et al. (in press) for New  
21 Zealand where consideration of continuous rotation was more important under water- and  
22 nitrogen-limited conditions. From the aspect of crop yields, at least, there was therefore limited

1 potential for ROTATION simulation, which explicitly takes into account carry-over effects, to  
2 achieve more superior predictions than SINGLE simulations.

3 Nevertheless, we found that continuous simulations performed slightly better when the two  
4 methods of simulating yield (ROTATION vs. SINGLE) were compared site by site, crop by crop,  
5 and treatment by treatment (Tables 4, 5 and 6). This means that the conditions of water and  
6 nutrients in the soil, and thus the emerging yield, were simulated better across all models by the  
7 continuous mode of simulation than the single-year mode. In the latter case, most modellers  
8 manually or automatically estimated soil water content and nutrients less accurately at the  
9 beginning of each growing season. We expect to see greater contrast between continuous and  
10 single-year simulations (i) when other model outputs such as water and matter fluxes are  
11 investigated; (ii) when long-term effects (>20 years) are studied; (iii) when all crops are well  
12 parameterised; and (iv) when low-fertilised/water-limited crop datasets are investigated.

13 Although the beneficial effect of continuous simulation on crop yield results was not pronounced,  
14 the general need for continuous simulations to assess ecosystem services from cropping systems  
15 cannot be ignored.

16

### 17 **4.3.Crop-specific yields**

18 Considering that the calibration data provided for this modelling study was minimal, the yield  
19 simulations of the widely grown and simulated cereals wheat, barley and rye were good (RMSE  
20 between 2.4 and 2.6 t ha<sup>-1</sup> DM in the ROTATION mode). Errors are comparable with reported  
21 errors under similar conditions (Beaudoin et al., 2008). This high level of accuracy is probably  
22 due to the great deal of experience that modellers have with these crops since the development of

1 the first crop growth simulation models in the late 1960s (e.g. Wit, 1965). In contrast, the low  
2 simulation quality in maize yields is due to the fact that modellers have little experience in  
3 simulating the wide range of maize varieties (FAO, 2015). Maize parameterisation in European  
4 models is often poor, possibly due to the calibration of crop models with observations a) from  
5 nearby field sites only, b) under ample water and nutrient supply, and c) generated decades ago  
6 with lower yield potentials (Reidsma et al., 2009; Manevski et al., 2014).

7 Nonetheless, the RMSE of  $3.9 \text{ t ha}^{-1}$  DM in maize is consistent with findings by Bassu et al.  
8 (2014), who compared maize crop models. Furthermore, the results of yield simulations in maize  
9 are probably biased because this crop was grown in Hirschstetten only, where yield was  
10 measured only once on three different soils. As shown below, most of these models failed to  
11 reproduce crop growth on these soils.

12 Yields of intermediate crops (oilseed radish and grass vegetation) were generally reproduced with  
13 a lower degree of accuracy than main crop yields. According to information provided by the  
14 modelling teams, this is mainly due to their lack of experience in dealing with these crops. This is  
15 explained by their low economic value and the fact that they are not considered as highly  
16 influential on the growth of main crops. Only about half of the modelling teams were experienced  
17 in specifically simulating oilseed radish and grass vegetation. Those who simulated intermediate  
18 crops reported difficulties in reproducing the emergence date of these crops under summer  
19 conditions.

20

#### 21 **4.4. Management treatments**

22 *CO<sub>2</sub> / nitrogen / tillage / residues*

1 Thanks to the provision of calibration data concerning both ambient and increased CO<sub>2</sub>  
2 concentration, the model results were in good agreement with the measured effect of increased  
3 CO<sub>2</sub> concentration on yield in the FACE experiment at Braunschweig. Thus, by applying a 15-  
4 model ensemble (where most models used the approach of radiation use efficiency), we were able  
5 to reproduce the results generated in other modelling studies that simulated the effect similarly  
6 well (Kartschall et al., 1995; Nendel et al., 2009; Tubiello et al., 1999).

7 The fertilisation experiments at Braunschweig and Thibie reduced the “normal” dose of N  
8 fertilisation to 50 % and 69 %, respectively. In both datasets, the effect of fertiliser was generally  
9 well reproduced, albeit underestimated slightly by 2 to 3%. This indicates that the models  
10 successfully reflect the effects of varying crop N nutrition. Notably, in the case of Braunschweig,  
11 the growth response to the complex interaction of CO<sub>2</sub>, available soil water and N (see review in  
12 Wu and Kersebaum, 2008) was simulated well.

13 According to field data from Foulum, reducing tillage and remaining harvest residuals on the  
14 field had no short-term effect on yield. This was reproduced by the models. It is worth noting that  
15 several models did not specifically simulate ploughing, whereas those able to simulate ploughing  
16 (e.g. DAISY) do not include any effects of ploughing on the soil organic matter turnover, which  
17 has direct implications for the simulation of soil processes in ROTATION over time. Similar  
18 observations were found under comparable climatic conditions at two sites in Denmark and  
19 Germany (Deike et al., 2008), whereas short-term tillage effects have been reported under  
20 warmer and drier climatic conditions (Fischer et al., 2002; López-Bellido and López-Bellido,  
21 2001).

22 Thus, we conclude that simulated responses to fertiliser and residues are described well in the  
23 models.



1

2 *Irrigation / soil / intermediate crop*

3 In general, dynamic crop simulation models are able to successfully reproduce irrigation effects  
4 because they were developed in order to respond to key environmental drivers such as  
5 precipitation, temperature and radiation. However, the model ensemble we evaluated strongly  
6 underestimated the effect of irrigation for all crops in the Müncheberg dataset. In particular,  
7 simulations of the irrigated treatment exhibited a high discrepancy to observations because half of  
8 the models demonstrated no or virtually no effect of irrigation. We found that the erroneous  
9 reproduction of the soil water dynamics was responsible for the mismatch. However, when  
10 comparing multi-model simulations of wheat in the same dataset, Palosuo et al. (2011) reported  
11 similarly underestimated yields due to a poor representation of the soil water dynamics. These  
12 mismatches cannot be explained by the various water limitation approaches taken by the models.  
13 Instead, it seems that water dynamics driven by light spring and/or summer drought were not well  
14 reproduced by the models for the sandy soil of Müncheberg. Four models used implausible  
15 values of field capacity; for two models, the underestimation of soil water content was related to  
16 the underestimation of yields; and one model simulated implausibly high soil water contents.

17 Similarly, in Hirschstetten most models failed to reproduce the very low yields of all crops on the  
18 Calcaric Phaeozem. For this dataset, minimal calibration data was provided for a rotation on  
19 Gleyic Phaeozem. When applying the same rotation to the shallow and sandy Calcaric Phaeozem,  
20 which contains >50 % gravel from below 95 cm soil depth, the limited availability of measured  
21 data for a proper soil parameter calibration turns out to be responsible for the reduced response.  
22 In particular, the reduced water holding capacity provoked by the high stone content was not  
23 considered by most models. This is confirmed by the models' inaccurate soil water simulations in

1 Hirschstetten (Supplementary B). Of the four datasets where soil water measurements were  
2 available, the simulation accuracy of this variable was lowest at Hirschstetten. In addition, the  
3 interpretation of models differed regarding rooting depth. While some models used an  
4 exponential distribution function over depth with decreasing uptake from the subsoil, others  
5 interpreted depth as an “effective rooting depth”, allowing full extraction of water down to 2 m,  
6 which was the maximum rooting depth. In view of the sandy soil and the high stone content in  
7 the profile, this seems unrealistic, and led to a lower response to dry periods. Examples from  
8 precision agriculture show that models usually respond well to differences in soil conditions if  
9 rooting depth is properly considered (Kersebaum et al. 2005).

10 In the experiment, the effect of growing intermediate crops (oilseed radish and grass vegetation)  
11 instead of leaving the soil bare during the non-growing season resulted in higher quantities of  
12 biomass generated by the following sugar beet and winter wheat (Constantin et al., 2010). This  
13 was not reproduced by the model results (ROTATION and SINGLE mode). There may be two  
14 main reasons for the lack of model response: a) the generally low accuracy of biomass simulation  
15 for intermediate crops (Fig. 3) due to limited experience and minimal calibration data, and b)  
16 uncertainty in the simulated N release from mineralisation of soil organic matter and from the  
17 decomposition of crop residues, both of which contribute to the N supply to the main crop under  
18 N-limited conditions. Under the conditions of minimal calibration, a poor model performance  
19 does not coercively imply model deficiencies, as modellers were forced to assume certain  
20 conditions and processes. Thus, the question as to which model process requires improvement  
21 may better be answered after full calibration of each individual model.

22

23

## 5. Conclusion

Past model inter-comparisons focused on single crops only and usually on single years when drawing conclusions on the uncertainty of applying models at sites for which they had not been calibrated. In this study, we accommodate the fact that crop production is generally driven by crop rotations, where preceding crops influence the growth of the following crop due to a number of processes. As such, we raise the complexity of crop modelling to a higher system level.

The results suggest that it is a matter of urgency to model crop rotations in order to evaluate the resilience of cropping systems and their contribution to ecosystem services under changing climate conditions. However, none of the models involved was capable of reliably simulating yields of all crop species in all datasets when data for calibration was sparse. Hence, the multi-model ensemble approach minimised the error arising from simulations of single models. As hypothesised, the continuous simulation of multi-year crop rotations slightly outperformed simulations of single years with regard to crop yield. Finally, a better functional understanding and parameterisation of intermediate crops is required, especially in order to reproduce their effects on main crops.

Based on the results we obtained and the authors' expert knowledge, we propose taking the following steps in priority order when addressing future challenges in crop rotation modelling:

- (1) Knowledge of carry-over effects in crop rotations remains sparse. We suggest a literature review of the various effects of the preceding crop on yields in the following crop, as well as of soil water and nutrient balances from an agro-ecosystem modeller's perspective.
- (2) High-quality experimental data (potential growth and water-/nutrient-limited growth) is required as the "backbone" for developing and improving models. We identified a high

1 demand for crop rotation datasets including measurements of soil conditions at high  
2 temporal resolution and for datasets of crops that have so far been investigated  
3 inadequately (e.g. rape seed, radish, sugar beet, oat, potato). Kersebaum et al. (2015)  
4 recently stressed the need for consistent datasets in order to improve models.

5 (3) We propose the careful review and improvement of existing models towards the  
6 continuous simulation of multi-year crop growth (rotations) because technical limitations  
7 continue to exist for some models.

8 (4) More specifically, the following processes were identified as seeming to be represented  
9 inadequately in many models and therefore in need of improvement/implementation for a  
10 sound representation of crop rotations and their treatments: N release from mineralisation  
11 of residues, effects of tillage, dynamics of soil organic matter, parameterisation of under-  
12 studied crops, low temperature and frost effects on intermediate crops.

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## 1 **Acknowledgements**

2 The present study was carried out in the context of CropM within the FACCE-MACSUR  
3 knowledge hub. We thank the experimenters involved in the Thibie experimental dataset:  
4 ARVALIS Institut du Végétal (G. Briffaux, G. Aubrion) and INRA (J. Duval). KCK, CK, CN,  
5 MW and WM acknowledge financial support from the FACCE MACSUR project  
6 (2812ERA147), funded by the German Federal Ministry of Food and Agriculture (BMEL). CN  
7 received additional support by BMBF via the CARBIOCIAL research project (01LL0902M).  
8 CM, KW and TC acknowledge financial support from the FACCE MACSUR project  
9 (031A103B), funded by the German Federal Ministry of Education and Research (BMBF). CM  
10 acknowledges financial support from the KULUNDA project (01LL0905L), funded by the  
11 BMBF. TP and RPR were supported by the NORFASYS project, funded by the Academy of  
12 Finland (decision no. 268277) and MTT strategic projects MACSUR and MODAGS, funded by  
13 the Finnish Ministry of Agriculture and Forestry. HH, TG and FE acknowledge financial support  
14 from the FACCE MACSUR project (2812ERA115), funded by the German Federal Ministry of  
15 Food and Agriculture (BMEL). RM and HJW acknowledge financial support by BMEL. JEO,  
16 KM, IÖ, SR and BS were funded from the FACCE MACSUR project by Innovation Fund  
17 Denmark. CMAH, NB, JC, IGCA, ML, BM, DRW, FR were funded from the FACCE MACSUR  
18 project by INRA ACCAF Metaprogramme.

## Tables

Table 1: Characteristics of the study sites.

Location	Position (latitude/longitude/elevation a.s.l.)	Precipitation <sup>a</sup> [mm year <sup>-1</sup> ]	Temperature <sup>b</sup> [°C]	Soil type	Period	Crop rotation <sup>c</sup>	Treatment (all)	Treatment (tested)	Minimal calibration <sup>d</sup>
Foulum (FO)	56.49/9.57/52 m	670	7.9	Mollic Luvisol	2002-2012	BAR/RAP/WHB WHB/GRV/BAR/GRV/PEA/WHB/WHB/BAR/RAD/OAT/WHB/RAD/BAR/RAD/OAT	6 (tillage, rotation, residuals)	No till vs. plough Retention of resid. vs. removal of resid.	Phen/1 treat
Münchenberg (MU)	52.52/14.12/62 m	564	8.4	Eutric Cambisol	1992-1998	SBT/WHB/BAR/RYE/RAD	8 (irrigation, inter-year variation)	Irrigated vs rainfed	Biom/1 treat
Braunschweig (BR)	52.3/10.45/79m	642	10.0	Luvisol	1999-2005	BAR/GRV/SBT/WHB	4 (fertiliser, CO <sub>2</sub> )	Elevated CO <sub>2</sub> vs ambient concentr. High vs. low fertilisation	Phen/4 years
Hirschstetten (HI)	48.2/16.57/150m	495	11.0	Gleyic phaeozem/ Calcic phaeozem/ Calcic chernozem	1998-2004	MUS/WHB/MUS/BAR/WBH/ MUS/POT/WHB/MAZ/WHB	3 (soil type)	cPhaeo vs. gPhaeo Cherno vs. gPhaeo	Phen/1 treat
Thibie (TH)	48.93/4.23/110 m	657	10.9	Eutric Cambisol	1991-2003	PEA/WHB/SBT PEA+GRV/WHB/RAD/SBT/BAR	12 (catch crops, inter-year variation, fertiliser)	High vs. low fertilisation Catch crops vs. bare soil	Harv/1 treat

<sup>a</sup> Average annual precipitation during period of observation.

<sup>b</sup> Average annual temperature during period of observation.

<sup>c</sup> BAR = barley, RAP = oilseed rape, WHB = wheat, GRV = grass vegetation, PEA = pea, RAD = oilseed radish, OAT = oat, RYE = rye, MUS = mustard, POT = potato, MAZ = maize, SBT = sugar beet

<sup>d</sup> Phen = phenology, treat = treatment, Biom = biomass, Harv = harvest date

Table 2: Models applied in this study and the web addresses of their websites.

<b>Model</b>	<b>Abbreviation</b>	<b>Version</b>	<b>Key reference</b>	<b>SINGLE/ ROTATION</b>	<b>Web address</b>
DSSAT1	DS	4.6	(Jones et al., 2003)	yes/no	<a href="http://dssat.net">http://dssat.net</a>
HERMES	HE	4.26	(Kersebaum, 2011; Kersebaum and Nendel, 2014)	yes/yes	<a href="http://www.zalf.de/en/forschung/institute/lsa/forschung/oekomod/hermes">http://www.zalf.de/en/forschung/institute/lsa/forschung/oekomod/hermes</a>
MONICA	MO		(Nendel et al., 2011)	yes/yes	<a href="http://monica.agrosystem-models.com/">http://monica.agrosystem-models.com/</a>
LPJmL	LP		(Bondeau et al., 2007)	yes/no	<a href="http://www.pik-potsdam.de/research/projects/lpjweb">http://www.pik-potsdam.de/research/projects/lpjweb</a>
Daisy	DA	5.16	(Hansen et al., 2012)	yes/yes	<a href="https://code.google.com/p/daisy-model">https://code.google.com/p/daisy-model</a>
FASSET	FA		(Olesen et al., 2002)	yes/yes	<a href="http://www.fasset.dk">www.fasset.dk</a>
SPACSYS	SP	5.0	(Wu, et al., 2007)	yes/no	
Theseus	TH		(Wegehenkel, 2002)	no/yes	Request from <a href="mailto:mwegehenkel@zalf.de">mwegehenkel@zalf.de</a>
STICS	ST	8.3.1	(Brisson et al., 2003)	yes/yes	<a href="http://www6.paca.inra.fr/stics_eng/">www6.paca.inra.fr/stics_eng/</a>
SIMPLACE, LINTUL2, SoilCN, SLIM	LI	svn327	(Addiscott and Whitmore, 1991; Angulo et al., 2013; van Oijen and Lefelaar, 2008)	yes/yes	<a href="http://www.simplace.net">www.simplace.net</a>
CROPSYST	CR	3.02	(Stöckle et al., 2003)	yes/yes	<a href="http://www.sipeaa.it/ASP/ASP2/CropSyst.asp">www.sipeaa.it/ASP/ASP2/CropSyst.asp</a>
SWIM	SW		(Krysanova et al., 2000)	no/yes	<a href="https://www.pik-potsdam.de/research/climate-impacts-and-vulnerabilities/models/swim">https://www.pik-potsdam.de/research/climate-impacts-and-vulnerabilities/models/swim</a>
WOFOST	WO	7.1.5		yes/no	<a href="http://www.wofost.wur.nl">http://www.wofost.wur.nl</a>
			(Boogaard et al., 1998; Jylhä et al., 2004; Supit et al., 1994; van Ittersum et al., 2003)		
DSSAT2	DT	4.5	(Jones et al., 2003)	yes/no	<a href="http://www.icasa.net/dssat">www.icasa.net/dssat</a>
APSIM	AP	7.5	(Keating et al., 2003)	no/yes	<a href="http://www.apsim.info">www.apsim.info</a>

Table 3: Crop-specific observations and the abilities of each model, stating the abbreviation of the crop, the number of models able to simulate the crop in multi-year (ROTATION) and single-year (SINGLE) mode, the number of models that predicted this crop for the first time, the number of datasets in which the crop appears and the number of yield observations.

<b>Crop</b>	<b>Code</b>	<b>No. of models ROTATION/ SINGLE</b>	<b>No. of models first time</b>	<b>No. of datasets</b>	<b>No. of observations</b>
Maize	MAZ	7/7	2	1	3
Winter wheat	WHB	10/12	1	5	96
Winter barley	BAR	10/11	3	5	37
Rye	RYE	10/9	5	1	12
Oat	OAT	7/7	7	1	8
Sugar beet	SBT	10/9	5	3	64
Potato	POT	7/6	5	1	3
Oilseed radish	RAD	5/4	7	3	42
Pea	PEA	8/9	4	2	52
Grass vegetation	GRV	7/6	5	3	14



Table 4: Model evaluation indices describing the goodness of fit between observed and simulated yields for all sites. The results are given as the mean per site (across models), the best performing model over all sites (best model mean) and the goodness of fit of the mean of predictions by all models (multi-model mean).

Site	RMSE [t ha <sup>-1</sup> DM]		MAE [t ha <sup>-1</sup> DM]		IOA		PBIAS [%]	
	ROTATION**	SINGLE	ROTATION	SINGLE	ROTATION *	SINGLE *	ROTATION	SINGLE
FO	2.5 (1.7+1.8)	2.8 (1.9+1.9)	2.1	2.4	0.45	0.45	+10	-1
MU	3.3 (2.6+1.8)	3.2 (2.6+1.9)	2.5	2.5	0.71	0.66	-11	-10
BR	2.9 (2.1+1.7)	2.5 (1.7+1.7)	2.2	1.9	0.87	0.80	-5	-5
HI	3.1 (2.4+1.8)	3.5 (2.6+2.2)	2.7	2.7	0.66	0.54	+43	+22
TH	4.4 (3.5+2.3)	4.3 (3.6+1.9)	3.3	3.4	0.78	0.68	-18	-16
Best model mean	2.1(1.2+1.6)	2.1(1.3+1.4)	1.6	1.7	0.81	0.82	0	3
Multi-model mean	2.2	2.1	1.7	1.6	0.78	0.83		

\* p-value<0.05 for significance of the mean.

\*\* values in brackets indicate the systematic part plus random error of RMSE.

Table 5: Crop-specific performance indicators describing the accuracy of yield predictions generated by the models involved and the multi-model ensemble.

Crop	RMSE [t ha <sup>-1</sup> DM]		rRMSE		nMAE		PBIAS [%]	
	ROTATION*	SINGLE*	ROTATION	SINGLE	ROTATION *	SINGLE *	ROTATION	SINGLE
MAZ	3.9	3.6	0.68	0.63	0.53	0.48	25.8	-11.8
WHB	2.6	2.9	0.40	0.44	0.31	0.36	-0.1	2.3
BAR	2.5	2.8	0.51	0.56	0.40	0.45	16.1	9.8
RYE	2.4	2.5	0.34	0.35	0.28	0.29	-18.2	-12.3
OAT	2.3	3.7	0.37	0.59	0.30	0.48	-25.5	-41.9
SBT	6.9	6.7	0.42	0.41	0.32	0.30	-21.1	-23.4
POT	3.7	7.1	0.44	0.84	0.35	0.70	16.7	40.0
RAD	1.4	1.8	0.87	1.11	0.65	0.87	-18.0	-4.0
PEA	2.1	2.3	0.51	0.57	0.41	0.47	-2.5	-16.7
GRV	2.3	3.3	0.67	0.95	0.54	0.56	-27.1	-20.6
Multi model mean	1.8	2.1	0.31	0.35	0.26	0.31		

\* p-value<0.05

Table 6: Observed (O) and simulated (R-ROTATION, S-SINGLE) treatment effects on crop yield. DM yield change (%) is calculated from yields of a zero-treatment as a reference. Three model performance indicators are included viz. Root Mean Squared Error (RMSE), Mean Absolute Error (MAE) and Index of Agreement (IOA). BR-Braunschweig dataset and TH-Thibie dataset. Note that there were no significant differences in performance indicators between ROTATION and SINGLE.

Treatment	Yield change [%]			RMSE [%]		MAE [%]		IOA	
	OBSERVED	ROTATION	SINGLE	ROTATION	SINGLE	ROTATION	SINGLE	ROTATION	SINGLE
Irrigation	19.6	12.2	8.1	35	31	27	25	0.41	0.51
CO <sub>2</sub>	11.3	10.9	12.3	13	15	10	12	0.36	0.28
N (BR)	12.7	13.3	7.5	22	19	18	15	0.37	0.41
N (TH)	2.5	2.8	0.1	16	13	10	9	0.39	0.43
Soil cPhaeo	-51.1	-11.4	-5.1	42	49	38	45	0.33	0.30
Soil Chernozem	0.86	-0.1	2.1	28	23	20	15	0.28	0.43
Tillage	-3.7	0.6	-0.1	28	26	18	16	0.10	0.11
Residues	1.5	0.6	-9.7	13	22	9	19	0.15	0.19
Intermediate crop	3.5	0	-2.5	19	17	12	13	0.33	0.33
Best model mean				18	18	14	13	0.37	0.54
Multi model mean				18	19	14	15	0.36	0.40

## Figure captions

Fig. 1: Locations of the five experimental study sites in Europe.

Fig. 2: Yield predictions (R-ROTATION, S-SINGLE) of 15 models and observation (O) of all treatments of the five datasets. Final biomass predictions are shown in GRV and RAD. Boxes of the box-and-whisker plots show the upper and lower quartile of the distribution and the median. The whiskers extend to the most extreme data points (minimum/maximum), which are no further away than 1.5 times the inter-quartile range whereas the circles represent outliers. For crop abbreviations, see Table 1.

Fig. 3: Crop-specific errors (normalised mean absolute errors) of yield prediction across all models, sites and treatments. Final biomass was predicted in RAD and GRV. The area above the dashed line indicates errors exceeding 50 % of mean observed yields.

Fig. 4: Treatment effects reproduced by all models and observation (on the basis of percent yield change). H<sub>2</sub>O = irrigation, CO<sub>2</sub> = increased CO<sub>2</sub> concentration, N = fertilisation, Soil cPhaeo = Calcaric Phaeozem compared to Gleyic Phaeozem, Soil Chernozem = Calcic Chernozem compared to Gleyic Phaeozem, Tillage = no tillage compared to common plough, Residues = retention of residues compared to removal of residues, Catch crop = catch crop use compared to bare soil. Red stars indicate the median of observations, boxplots show the median response of each model. Boxes of the box-and-whisker plots show the upper and lower quartile of the distribution and the median. The whiskers extend to the minimal/maximal data points. Left bars: ROTATION, right bars: SINGLE.

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**Supplementary Table A.** Modeling approaches of 15 crop simulation models contributing to the study.

<b>Process/Model</b>	<b>DT</b>	<b>SP</b>	<b>TH</b>	<b>DA</b>	<b>HE</b>	<b>FA</b>	<b>LI</b>	<b>CR</b>	<b>SW</b>	<b>LP</b>
Light conversion <sup>a</sup>	RUE	PR	PR	PR	PR	RUE, PR,	RUE	TE/RUE	RUE	PR
Yield formation <sup>b</sup>	B, Gn	Prt	Prt	Prt	Prt	B, Prt	B, Prt	HI_mw/B	HI, Prt	B,HI
Phenology <sup>c</sup>	T, DL, V	T, DL, V, O	T	T, DL, V, O	T, DL,	T, O	T, DL, V, O	T, DL, V	T	T,DL,V
Root growth <sup>d</sup>	EXP	EXP/Call/O	LIN	EXP	Call,	Lin, EXP	Call, O	EXP	EXP	EXP
Water limitation <sup>e</sup>	E, S	S	S	E,S	E, S	E, S	E, S	E	S	E, S
N limitation <sup>f</sup>	R	R	-	R,O	R	R, O	R, O	R	R	NA
Heat stress <sup>g</sup>	R	N/A	R	-	R	O	O		O	NA
Water dynamics <sup>h</sup>	C	R	R	R	C		R, (D)	C/R	R	C
Evapotranspiration	PT, PM	PM	P	PM, MAK,	PM, PT,	MAK, P	P	PT,PM	TI	PT
Soil C / N model <sup>j</sup>	CN( Century,	CN, P(6), B	-	CN, N, P(5), B(2)	N, P(2)	CN, P(x), B	CN P(10), B	N, P(4)	N, P(1)	none
CO <sub>2</sub> effect <sup>k</sup>	RUE	RUE, TE	-	-	F, TE	TE, GY, somewhat	RUE	RUE, TE	RUE	F
# of crop-specific parameters	~50			~80	16 + 12 x #dev.stag	~66	31	~50	2	12
Climatic drivers (variables) <sup>l</sup>	R, Tx, Tn, Rd, RH, W	Ta, Rd, Day length, T <sub>Soil</sub>	R, Tx, Tn, RD, RH, W	R, Ta, Rd, e, RH, W	R, Ta, Tx, Tn, Rd, RH, W	R, Tx, Tn, Td, Rd, e, RH, W	R, Tx, Tn, Ta, Rd, W	R, Tx, Tn, Rd, RH, W	R, Tx, Tn, Ta, Rd, RH	R, Ta, Rd

a RUE, radiation use efficiency approach; PR, gross photosynthesis – respiration; TE, transpiration efficiency biomass growth.

b HI, fixed harvest index; B, total (above-ground) biomass; Gn, number of grains; Prt, partitioning during reproductive stages; HI\_mw, harvest index modified by water stress.

c T, temperature; DL, photoperiod (day length); V, vernalization; O, other water/nutrient stress effects considered.

d LIN, linear, EXP, exponential, SIG, sigmoidal, Call, carbon allocation; O, other approaches.

e E, actual to potential evapotranspiration ratio; S, soil available water in root zone.

f R, assimilates reduction factor, O, others

g R, assimilates reduction factor, O, others

h C, capacity approach; R, Richards approach; D, Darcy approach.

i P, Penman; PM, Penman-Monteith; PT, Priestley –Taylor; TW, Turc-Wendling; MAK, Makkink; HAR, Hargreaves; SW, Shuttleworth and Wallace (resistive model); EB, energy balance (“bold” indicates approached used during the study).

j CN, CN model; N, N model; P(x), x number of organic matter pools; B, microbial biomass pool.

k RUE, radiation use efficiency; TE, transpiration efficiency; GY, grain yield; CLN, critical leaf N concentration; F, Farquhar model.

l Cl, cloudiness; R, precipitation; Tx, maximum daily temperature; Tn, minimum daily temperature; Ta, average daily temperature; Td, dew point temperature; Rd, radiation; e, vapor pressure; RH, relative humidity; W, wind speed.

<b>Process/Model</b>	<b>ST</b>	<b>WO</b>	<b>AP</b>	<b>DS</b>	<b>MO</b>
Light conversion <sub>a</sub>	RUE	PR	RUE+TE	RUE	RUE
Yield formation <sub>b</sub>	HI(Gn),B	Prt	HI, Gn, Prt	B, Gn, Prt, HI_mw	Prt
Phenology <sub>c</sub>	T, DL, V, O	T, DL	T, DL, V, O	T, DL, V	T, DL, V, O
Root growth <sub>d</sub>	LIN, SIG	LIN	O, LIN	EXP	EXP
Water limitation <sub>e</sub>	E, S	E, S	S	E/S	E
N limitation <sub>f</sub>	R	-	R, O	R,O	R
Heat stress <sub>g</sub>	R	-	R, O	R	R
Water dynamics <sub>h</sub>	C	C	C, R	C	C
Evapotranspiration <sub>i</sub>	SW	P	PT	PT	PM
Soil C and N model <sub>j</sub>	CN, P(4), B	-	CN, P(3)	CN/P(4)	CN, P(6), B
CO <sub>2</sub> effect <sub>k</sub>	RUE, TE	-	RUE,TE,CLN	RUE, TE	F
# of crop-specific parameters	Yes, the main part of the crop parameters are specific	21		39	15
Climatic drivers (variables) <sub>l</sub>	R, Tx, Tn, Rd, e, W	R, Tx, Tn, Rd, e, W	Tx, Tn, Rd, R	R, Tx, Tn, Rd	R, Tx, Tn, Rd, RH, W

Site	Treat ment	ROTATION						SINGLE				Mean per site
		AP	DA	HE	MO	ST	SW	DA	HE	MO	ST	
TH	1	180	22	100	NA	30	NA	16	119	NA	44	
TH	2	180	22	98	NA	31	NA	14	117	NA	47	
TH	3	188	51	100	NA	29	NA	NA	116	NA	39	
TH	4	198	48	98	NA	31	NA	NA	114	NA	37	
TH	5	201	82	109	NA	40	NA	90	124	NA	36	
TH	6	201	81	106	NA	39	NA	89	122	NA	36	<b>89</b>
TH	7	199	84	111	NA	41	NA	76	116	NA	36	
TH	8	200	83	109	NA	40	NA	76	116	NA	36	
TH	9	180	79	118	NA	37	NA	80	122	NA	32	
TH	10	178	77	116	NA	37	NA	78	119	NA	32	
TH	11	186	79	118	NA	33	NA	47	118	NA	27	
TH	12	186	78	118	NA	32	NA	NA	117	NA	26	
MU	1	40	17	23	19	40	98	17	20	19	41	
MU	2	NA	24	26	27	40	100	24	24	28	41	
MU	3	47	20	22	21	35	114	23	25	27	36	
MU	4	38	20	23	23	36	108	23	22	25	37	<b>36</b>
MU	5	44	16	18	16	40	111	21	21	23	41	
MU	6	47	21	21	25	38	107	23	20	27	38	
MU	7	35	21	17	12	45	106	24	22	17	46	
MU	8	42	29	24	23	48	102	32	29	27	50	
BR	1	93	22	23	51	37	161	22	23	51	42	
BR	2	84	22	23	51	38	163	22	22	51	44	<b>52</b>
BR	3	86	21	21	50	44	150	21	21	50	49	
BR	4	78	21	21	50	46	151	21	21	50	51	
HI	1	42	68	70	145	281	NA	NA	65	NA	233	
HI	2	57	86	87	170	175	NA	NA	91	NA	151	<b>118</b>
HI	3	85	65	67	133	214	NA	NA	36	NA	149	
<b>Mean</b>		<b>119</b>	<b>47</b>	<b>66</b>	<b>54</b>	<b>58</b>	<b>122</b>	<b>40</b>	<b>70</b>	<b>33</b>	<b>55</b>	

Supplementary table B: The prediction accuracy (RMSE [mm]) of soil water content (0-measurement depth) is given for all sites and treatments (where measurements were available) and for all models providing this output variable.