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Cross model validation for a diversified cropping system

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ABSTRACT

Crop diversification is gaining traction due to the positive benefits in the delivery of ecosystem services (ESS) and the promotion of biodiversity. Agroecosystem simulation models can contribute to the design of diversified cropping systems but require calibration and validation before they can be applied. However, data availability is still very limited, particularly for diversified cropping systems. Therefore, the main goal of this study was to evaluate the suitability of the Nelder-Mead optimization method and the leave-one-out (LOO) validation method to calibrate and validate a diversified cropping system with a limited dataset, by using either a fixed year combination for calibration and validation for all crops or using a flexible year combination for every crop. Crop phenology was manually calibrated for all year combinations and the best parameter set based on the LOO-validation was selected for the subsequent step. Next, a four-parameter set related to crop growth and biomass dynamics was chosen for parameter optimization in the calibration step. To measure model performance during both steps, the root mean square error (RMSE) in days was used for phenology and a weighed relative RMSE (RRMSE) was used for crop growth, with the intermediate and final biomass contributing to 50% of the error and the other 50% corresponding to grain yield. Data for model comparison was collected at the patch-CROP landscape experiment in Brandenburg, Germany. Observed data included daily weather, soil information, crop phenology, intermediate and final above ground biomass and grain yield for summer seasons 2020, 2021, and 2022 and winter seasons 2020/2021 and 2021/2022 (referred as 2021 and 2022, respectively). Summer crops included maize, soybean, lupine and sunflower, while winter crops were wheat, barley, rye and rapeseed. Results showed that the Nelder-Mead method was successful in reducing the error between observed and simulated data. As for the LOO-validation, the method showed that different year combinations led to a similar RMSE for phenology. However, for crop growth, optimum year combination was critical, as it differed for all summer crops but not for winter crops. For the summer crops, the lowest errors in the LOO-validation were observed in lupine, maize and soybean, with <20.6% RRMSE, while sunflower resulted in a reasonable LOO-validated value with 31.2% RRMSE, but a poor performance in the calibration step with 68.7% RRMSE. For the winter crops, the 2022 calibration year and the 2021 validation year combination resulted in the lowest RRMSE for wheat, barley and rapeseed. However, for rye, both year combinations led to a large error, with the lowest error when using the 2021 season for calibration (65.9% RRMSE) and 2022 season for validation (33.0% RRMSE). The flexible LOO-validation method was useful to make optimal use of the limited dataset as it allowed a more through model testing and pointed to differences among summer and winter crops. The newly validated model has the potential to be used for the design of diversified cropping systems.

1. Introduction

About half of the arable land in Germany is dedicated to cereal production, with wheat (*Triticum aestivum* L.) as the dominant crop, followed by barley (*Hordeum vulgare* L.) and rye (*Secale cereale* L.) (Destatis, 2023), under cropping systems that are highly intensive and productive (Ewert et al., 2005). However, management practices have also led to a series of environmental concerns related to pollutants released to the environment and declines of biodiversity in agricultural areas (Aguiar et al., 2020; Barbieri et al., 2017; Crossley et al., 2021;

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Geiger et al., 2010). Crop diversity is an alternative that offers multiple benefits to the agroecosystems in terms of delivery of ecosystem services (ESS), resource use, productivity and promotion of biodiversity (Beillouin et al., 2021; Dainese et al., 2019; Smith et al., 2023; Tamburini et al., 2020). Moreover, it can improve resilience of cropping systems to better cope with negative impacts of climate change (Marini et al., 2020; Zampieri et al., 2020). Hence, studies on crop diversification have received increasing attention (Hufnagel et al., 2020). Process-based agroecosystem simulation models (or agroecosystem models) can contribute to the design of diversified cropping systems. They have been widely used to understand crop responses to management and environmental factors (Enders et al., 2023; Martre et al., 2017; Thorburn et al., 2018). These models comprise a set of mathematical functions that represent relevant biophysical processes related to crop development and growth (Chenu et al., 2017). When validated, agroecosystem models are flexible tools that can potentially be used for cropping system design, as they allow to conduct virtual experiments that otherwise would not be possible in field conditions due to their cost and management feasibility (Jones et al., 2003). They use input data such as weather data, soil physical and chemical characteristics, crop management, and crop genetic information to simulate crop development, growth and yield (Asseng et al., 2014).

For the current study, the SIMPLACE (Scientific Impact assessment and Modeling Platform for Advanced Crop and Ecosystem management) modelling framework was selected. The framework has been developed during the last decade and main uses include climate change impacts assessments, model uncertainty and crop management (Enders et al., 2023). In the past 10 years, about 60% of the more than 80 published model application studies have been performed for wheat and maize, but the full range of model applications comprise about 22 crops (Enders et al., 2023). The advantage of this modelling framework resides on its flexibility due to its structure, which consists of a set of modules, called SimComponents. SimComponents can be easily exchanged depending on data availability and complexity needed. Each SimComponent contains main mathematical functions for a specific process affecting crop development and growth. An agroecosystem model within the framework is generated by combining a set of SimComponents.

Prior to their application, agroecosystem models need to be calibrated and validated. Model calibration is the process by which a set of model parameters are fitted to field observations to reduce the errors between the simulated and observed results (Wallach et al., 2021). Validation is a next step where the crop model is tested against a new independent set of observed data, that has not been used for calibration (Kersebaum et al., 2015). Calibration is often done by manual trial and error or it can be done in an automatic procedure (Seidel et al., 2018). The quality of model calibration depends on the quantity and quality of the observed data. Often observations can be limited, which may lead to larger errors when validating or applying the model as the calibration may not be representative in wide range of environments.

For model calibration, one approach for parameter optimization is the use of the Nelder-Mead algorithms for unconstrained optimization of non-smooth functions in general (Buis et al., 2011; Cui et al., 2023; Lagarias et al., 1998; Nocedal and Wright, 1999; Wang and Shoup, 2011), its popularity relays on its simplicity and no need for gradient computation (Silva et al., 2018). The method consists of finding the minimum of an objective function (e.g. root mean square error or RMSE), which is evaluated at the vertices of a simplex, moving away from the poorest values (i.e. higher RMSEs) (Nelder and Mead, 1965; Olsson and Nelson, 1975). Despite that the method is common in other research domains, it is not widely adopted for crop or agroecosystem model calibrations. Dumont et al., (2014), showed that the performance of the Nelder-Mead method was comparable with other optimization methods such as the standard least square, the weighted least square, and a transformed likelihood function when using it for parameter identification in the STICS model. Therefore, there is a potential to use the method for parameter optimization for a diverse set of crops.

With regards to model validation, one method is the use of the leave-one-out (LOO) model validation or cross-model validation, a method that can be beneficial when limited data is available. The LOO-validation is a methodology used to choose the model that results in the lowest error of prediction, in the validation step (Wallach et al., 2019). One advantage of this method is that it allows to use all the data in an iterative process for both calibration and validation (Nurulhuda et al., 2022; Thorp et al., 2007). This procedure assumes that each element of the sample is drawn independently at random from the target population (Wallach et al., 2019). Such an approach is contrary to the traditional method of splitting the data and using one fixed set for calibration and one set for validation (Seidel et al., 2018), which may lead to a higher error of prediction in a diversified cropping system. Thorp et al., (2007), used cross-model validation to test how many seasons were sufficient for model calibration of maize grain yield, results showed that the prediction error decreased as the number of seasons were added to the calibration step in the LOO-validation procedure. Xiong et al., (2008) used LOO-calibration instead, for rice yields in China, where the method showed relative higher bias for grain yield estimation, with reasonable results reproducing the spatial variability of yield and phenology. The LOO-validation procedure has been often applied for model selection, but it can be also useful when exploring model performance for different crops in a diversified cropping system. It can help to understand whether there are any model performance patterns depending on the crops and to identify options for model testing and improvement when needed. Therefore, the main goal of this study was to assess the suitability of the Nelder-Mead method for crop growth parameter optimization and apply the LOO-validation method to validate an agroecosystem model for simulating a large range of crops with a limited dataset. The specific objectives were: a) to assess the suitability of the Nelder-Mead optimization procedure to reduce the simulation error in the calibration step, b) to assess whether the application of the LOO-validation method leads to a different result when using fixed year selection or flexible year selection by crop, c) to understand if the year selection of the summer crops can contribute to the parameter selection in the winter crops, with less data available d) to assess for which crops the LOO-method performs best and understand the model limitations when simulations are poor for the optimization and LOO-validation steps. Our hypotheses are that (1) model parameter optimization reduces the error in the calibration and validation set, that (2) a flexible choice of year combination by crop for the LOO-validation gives an improved result (lower simulation error) than fixed year combination choice for all crops in a diversified cropping system setting and that (3) year combination of the crops (here summer crops) with more years of observation can inform on the best year combination for the crops (here winter crops) with less years of observation. Despite that crop diversification of a system may comprise different components such as spatial arrangements and/or temporal aspects of crop rotations with crop types, for the current study, we focus on the component of crop types, and therefore, the calibration and validation are carried out as individual crops.

2. Materials and methods

2.1. Experimental location

The data collection has been carried out in the experimental platform patchCROP, which is located in Tempelberg, Brandenburg, Germany (52.4426° N, 14.1607° E, altitude 68 m). In terms of geomorphology, the site is classified as a young moraine landscape, shaped by past glaciations, and characterized by an undulated relief and heterogeneous soils characteristics (Koch et al., 2023; Meyer et al., 2019). The soil at the top layer is dominantly sandy with an appearance of a clayey layer at different depths in the subsoil, with no immediate influence of ground water (APW, 2023). The area is located in a transition zone between humid oceanic and dry continental climate, long term average temperature from 1980 to 2010 was 9.2 °C, while annual precipitation for the same period was 568 mm. Daily weather data (maximum, mean and minimum temperature, solar radiation, precipitation, wind speed and relative humidity) from the 1st of January 2020–31 st of August 2022 were obtained from two weather stations located in the eastern and western end of the main patchCROP field. Weather stations are maintained by the Leibniz-Centre for Agricultural Landscape Research (ZALF) and undergo yearly calibration procedures. Monthly temperature values and cumulative rainfall for the summer and winter periods are shown in Fig. 1. June and July daily maximum temperature (Tmax) were the highest in 2021, while cumulative precipitation from April to October, shows that 2020 was the wettest season and 2022 was the driest season for summer crops. Similarly, cumulative precipitation from October to end of July shows that season 2020/2021 was the wettest for winter crops.

2.2. The patchCROP experimental platform

The patchCROP is a landscape experiment platform (landscape laboratory) within an on-farm context, which was implemented in spring 2020 (Grahmann et al., 2021). The central experiment was established within a 70-ha field and it consists of 30 "patches" measuring 72×72 m each (Fig. 2a). Patches are subdivisions of a large heterogeneous field into smaller and more homogenous units for site-specific management (Grahmann et al., 2021). In addition, reference patches are established every year in the neighboring fields, having the same crops present as in the diversified patch field, but grown as sole crops in a large field (Fig. 2b). For logistical reasons, the patch is further divided into four centric quadrants of 18×18 m each (Fig. 2c), one for soil related sampling, one for crop related measurements, one for biodiversity measurements and a multi-purpose quadrant for additional measurements. The remaining area around the quadrants is used as a buffer zone (Fig. 2c).

Prior to the experiment, the field was grouped into a high and low yield potential zone to account for spatial differences in long-term yield variability and soil characteristics by applying an advanced cluster analysis (Donat et al., 2022). A specific 5-year crop rotation was established for each yield potential zone. The crop selection was based on the crop market value, crop nutritional requirements and capacity to tolerate abiotic stresses. The high yield potential zone included winter rapeseed (*Brassica napus*, cv. Ambassador), winter barley (cv. Wallace), soybean (*Glycine max*, cv. Acardia), maize (*Zea mays* L., cv. P8349) and winter wheat (cv. Universum), while the low yield potential zone comprised sunflower (*Helianthus annuus* L., cv. Seabird), winter and spring oats (*Avena sativa* L., cv. Fleuron and Delfin, respectively), maize (cv. P8349), lupine (*Lupinus angustifolius*, cv. Boragine) and winter rye (cv. Tayo). Cover crops (phacelia, white mustard-*Sinapis alba*, Ramtill-*Guizotia abyssinica* and a mixture of ramtill and phacelia) were chosen depending on the previous and subsequent crop, harvest date and common agricultural policy regulations.

In addition, three management treatments are considered: i) conventional management ("business as usual"), ii) reduced pesticide management, using crop protection based on control thresholds and iii) reduced management + flower strips, which is also a reduced pesticide treatment surrounded by 12-m wide perennial flower strips to promote beneficiary insects (Dovydaitis et al., 2023). For the current work, the conventional management treatment data from the main field was selected as the agroecosystem model is not capable of simulating reduced pesticide management. The reference patch data was used when high weed pressure was observed in the main field. This was the case for sunflower (2020, 2021 and 2022) and soybean (2021 and 2022). Oats were excluded from the study as different cultivars were used during the 2021 and 2022 harvest seasons. The 2022 year for lupine was excluded as it grew under different soil conditions than the previous two years.

2.3. Field data collection

2.3.1. Soil data

Soil data was collected in the main field using a Pürckhauer soil auger of 1 m length. Two representative samplings, one for the high yield potential zone and one for the low yield potential zone were selected. Soil samples by horizon layer were collected and analyzed for chemical and physical characteristics. Soil layer information regarding bulk density, pH, soil texture, soil organic carbon (SOC), and soil hydraulic properties are shown in Table 1. The soil profile in the high yield potential zone tends to have a lower sand proportion than in the low yield potential zone. In the high yield potential zone, a loamy layer appears at 53 cm soil depth, while the low yield potential profile shows a dominantly sandy soil profile down to 1 m depth. The SOC in the top layer is 0.89% and 0.78% in the high and low yield potential soil, respectively. The lower boundary was extended to 2 m assuming that soil characteristics were the same in deeper soil as the ones found in the last layer of the 1 m soil auger.

2.3.2. Crop data

Crop phenology was visually assessed during the whole growing cycle every one or two weeks using the BBHC scale (Meier, 2018). Selected intermediate above ground biomass samples were collected at

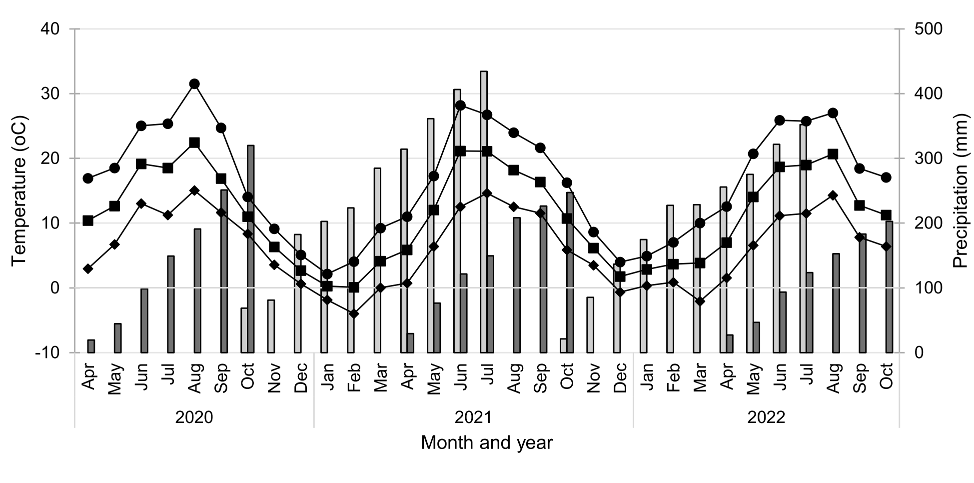

Fig. 1. Cumulative monthly precipitation for summer (April to October) and winter crops (October to August) and monthly minimum (Tmin), mean (Tmean) and maximum (Tmax) temperature from 1st of April 2020–31 st of October, 2022.

Fig. 2. patchCROP landscape experiment set up for the 2023 season. a) main 70 ha field, b) reference fields around the main field c) patch description, soil, biomass, biodiversity and multipurpose quadrants, buffer area of 18 m with around the quadrants.

Table 1
Soil physical and chemical characteristics for two representative soils at the patchCROP, Tempelberg, Brandenburg, Germany. No carbonate presence in the selected profiles.

Yield potential	Bottom depth (m)	Bulk density[1] (g cm^{-3})	pH[2]	Sand[3] (%)	Silt[3] (%)	Clay[3] (%)	SOC[4] (%)	Field capacity[5] (cm^3 cm^{-3})	Wilting point[5] (cm^3 cm^{-3})	Saturation point[5] (cm^3 cm^{-3})
High	0.32	1.5	6.7	68.7	23.0	8.3	0.89	0.170	0.064	0.397
	0.53	1.7	6.3	67.3	23.4	9.3	0.21	0.171	0.075	0.342
	2.00	1.7	7.2	59.8	23.9	16.3	0.30	0.204	0.101	0.346
Low	0.37	1.5	6.5	90.0	7.0	3.0	0.78	0.095	0.034	0.385
	0.75	1.7	6.4	84.3	11.4	4.3	0.18	0.110	0.042	0.333
	2.00	1.7	5.9	90.0	7.0	3.0	0.07	0.089	0.036	0.328

[1]Based on weight of 100 cm^3 of soil volume, measured in a soil pit in the main field; [2] Measured using $CaCl_2$ solution; [3] Sieving-sedimentation method, according the German soil particle classification; [4] Soil organic carbon, measured using an elemental analyzer for C/N model: Euro EA 3000, chromatographic separation; [5] Calculated using HYPRES pedotransfer function for European soils (Wosten et al., 1999, 2001).

BBCH 39, 60/61 (flowering) and 70/71 (end of flowering). For barley, wheat, rye and lupine, 0.5 m^2 were collected per sample, for sunflower, 0.45–1 m^2, for maize between 0.75 and 1.5 m^2, and for soybean between 0.9 and 1 m^2, depending on the year and the phenological stage. Representative samples were collected around the edges of the biomass quadrant by considering the heterogeneity of plant density within the patch. The quadrant central area remained undisturbed for the final biomass collection and grain yield harvest. Four above ground biomass samples were collected during 2020 and 2021 and three samples were collected in 2022 for each measurement date. Above ground biomass samples were oven-dried at 60°C for 48 hours to calculate the dry weight.

The grain yield per patch was determined in the center of the biomass quadrant (18×18 m) in the patches using an experimental plot harvester (Hege 180, Germany) in three sub-plots of 18 m length and 2 m width in 2020 in six sub-plots of 9 m length and 2 m cutting width (harvest area of 18 m^2) in 2021 and 2022. Yields were converted to 9% moisture level for oil seeds and 14% for cereals.

In addition, yield component cuts were collected at physiological maturity (around BBCH 89) for each crop in the biomass quadrant in 2021 (six cuts per patch) and 2022 (four cuts per patch) in an area of 0.25 m^2 for wheat, barley, rye and lupin; 0.125 m^2 for rapeseed; 0.5 m^2 for soybean and sunflower and 0.75 m^2 for maize. Individual plants were counted, as well as the number of spikes, cobs, pods and flowers (crop-specific) and entire samples were dried at 30°C for 5–7 days before further processing. The grain was harvested with a threshing machine (Haldrup LT-35) and dry weight of grain and straw were determined to calculate harvest index, which was then used to calculate final above ground biomass (based on the grain yield per patch) in 2021 and 2022.

2.3.3. *Crop management*

The farm applies conservation agriculture principles; therefore, all crop residues are left in the field and straw is not removed. Additionally, reduced tillage is applied for all crops using a shallow or deep chisel plough from 15 to 25 cm depth, respectively for seed bed preparation. Hence, no ploughing is carried out. Prior to the establishment of the patchCROP experiment in March 2020, the field was planted with narrow crop rotations (rye - rye - rapeseed). Management was carried out using site-specific nitrogen application, potassium and compost fertilization according to soil management zones. Data used for the current study comprises 2020, 2021, and 2022 summer seasons and 2021 (2020/2021) and 2022 (2021/2022) winter seasons. Sowing, emergence, flowering, physiological maturity and harvest dates are presented in Table 2.

The summer crops were planted in the window between the end of March (with lupine being the first sown crop) and early May (for soybean as the last sown), and harvested up to the end of October. While

Table 2
Sowing, emergence, flowering, maturity, and harvest dates for different crops in a diversified cropping system, patchCROP, Tempelberg, Brandenburg, Germany, 2020–2022.

Crop name and cultivar	Sowing date	Emergence date	Flowering date	Maturity date	Harvest date
Grain maize cv. P8329	16/04/2020	07/05/2020	19/07/2020	10/09/2020	20/10/2020
	16/04/2021	11/05/2021	22/07/2021	27/09/2021	10/11/2021
	29/04/2022	09/05/2022	25/07/2022	18/09/2022	20/10/2022
Soybean cv. Acardia	30/04/2020	19/05/2020	08/07/2020	20/08/2020	22/09/2020
	15/05/2021	28/05/2021	06/07/2021	20/09/2021	16/11/2021
	10/05/2022	20/05/2022	09/07/2022	15/09/2022	11/10/2022
Lupine cv. Boragine	03/04/2020	14/04/2020	10/06/2020	10/07/2020	31/07/2020
	30/03/2021	14/04/2021	13/06/2021	15/07/2021	16/07/2021
Sunflower cv. Seabird	06/04/2020	6/04/2020	08/07/2020	14/08/2020	15/09/2020
	01/04/2021	01/04/2021	11/07/2021	19/08/2021	04/10/2021
	31/03/2022	30/03/2022	10/07/2022	25/08/2022	07/09/2022
Winter wheat cv. Universum	28/10/2020	05/11/2020	14/06/2021	14/07/2021	23/07/2021
	15/11/2021	16/12/2021	07/06/2022	12/07/2022	20/07/2022
Winter barley cv. Wallace	21/09/2020	30/09/2020	28/05/2021	24/06/2021	16/07/2021
	20/09/2021	27/09/2021	15/05/2022	14/06/2022	05/07/2022
Winter rye cv. Tayo	02/10/2020	08/10/2020	04/06/2021	13/07/2021	13/07/2021
	13/09/2021	21/09/2021	24/05/2022	05/07/2022	05/07/2022
Winter rapeseed cv.	01/09/2020	09/09/2020	12/05/2021	06/07/2021	23/07/2021
Ambassador	26/08/2021	06/09/2021	10/05/2022	25/06/2022	20/07/2022

winter crops were planted as early as the end of August (e.g. rapeseed), to Mid-November with winter wheat being the last sown crop. Winter crops were harvested in the following year, around the end of July. Split mineral fertilizer applications were carried out according to fertilizer availability, vegetative stage, grain extraction and soil yield potential using solid urea or liquid as urea ammonium nitrate (UAN) as fertilizer source. Additionally, potassium, phosphorus and magnesium fertilizer were occasionally applied to reach fertility class and avoid crop deficiency. Fertilizer application dates and amounts per crop are shown in Table 3.

Table 3
Fertilizer dates and amounts for summer and winter crops in a diversified cropping system, patchCROP, Tempelberg, Brandenburg, Germany, 2020–2022.

Crop name and cultivar	Date	Total N (kg N ha^{-1})
Grain maize cv. P8329	17/04/2020	13.0
	22/05/2020	138.0
	16/04/2021	13.5
	17/04/2021	101.1
	04/06/2021	61.3
	20/05/2022	71.0
	23/06/2022	60.7
Soybean cv. Acardia	-	-
Lupine cv. Boragine	-	-
Sunflower cv. Seabird	24/03/2020	41.0
	06/04/2020	18.0
	01/04/2021	18.0
	08/04/2021	68.3
	30/03/2022	18.0
	05/04/2022	52.6
Winter wheat cv. Universum	14/03/2021	70.7
	27/03/2021	59.9
	07/05/2021	50.0
	19/05/2022	55.1
	11/03/2022	80.0
	05/04/2022	44.3
Winter barley cv. Wallace	17/03/2021	48.2
	08/04/2021	71.1
	07/05/2021	25.0
	11/03/2022	44.9
	05/04/2022	44.8
	10/05/2022	41.7
Winter rapeseed cv. Ambassador	29/09/2020	60.0
	17/03/2021	48.2
	20/03/2021	51.6
	23/04/2021	10.0
	10/08/2021	46.5
	11/03/2022	41.6
	21/03/2022	60.2
Winter rye cv. Tayo	17/03/2021	61.5
	01/04/2021	51.1
	14/05/2021	25.0
	11/03/2022	60.2
	05/04/2022	39.4

2.4. Model description

For the current work the model SIMPLACE <Lintul5, Slim, SoilCN> was used. The Lintul5 SimComponents simulate phenology, potential biomass and biomass production as affected by nutrients and water supply (Wolf, 2012). Simulations are performed in a daily time step. Crop phenological development is based on temperature sum, for winter crops, crop phenology is additionally affected by photoperiod effect. Temperature sum for crop development starts at emergence, the crop reaches flowering when simulated developmental stage (DVS) reaches 1 and physiological maturity occurs once the crop reaches DVS 2. Potential biomass growth is based on the intercepted photosynthetically active radiation and radiation use efficiency (RUE). Potential biomass is then limited by water (TRANRF) and nutrient stress (nitrogen limited, NNI). The stress factors vary from 0 to 1, with 1 meaning no limitation, the lower the stress factor, the higher the magnitude of the stress. The TRANRF is calculated as the ratio of actual evapotranspiration and potential transpiration. Whereas NNI is calculated based on crop nutrient demand and available supply. Both factors affect crop growth, leaf death rate, specific leaf area and crop partition (Wolf, 2012). Daily biomass is then partitioned into the different organs depending on the DVS. Soil water balance and nutrient movement is simulated using SlimWater (Addiscott and Whitmore, 1991), which uses a simple bucket approach by further subdividing the soil profiles in thinner layers of 5 cm thickness. Crop N demand, N turnover and leaching of soil mineral N are calculated using the NPKDemandSlimNP SimComponent. Finally, SoilCN (Corbeels et al., 2005) simulates soil organic carbon and nitrogen turnover in the soil in several storage pools along the soil profile.

2.5. Model initial conditions

Each crop was simulated individually, as the full 5-year rotation length is not completed yet and data available corresponds to the time period from spring 2020 to August 2022. Due to lack of data on the soil initial conditions and given the rainfall patterns in the area, where low rainfall before winter crop sowing is common but soil water tends to be higher when summer crops are planted in spring, we assumed the soil initial water content to be 100% and 30% of the crop usable water

(water between field capacity and wilting point) for summer and winter crops, respectively. Similarly, soil mineral N at the beginning of the experiment was not available, therefore, soil initial mineral N was set to 200 kg/ha and 70 kg/ha for the high and low yield potential soil, respectively, based on end of season measurements during 2020 and 2021, with about 70% allocated to the top soil layer of the 2-m soil profile. The model was reinitialized every season, about 30 days before sowing, which also allows the model to have more realistic soil water and nitrogen conditions in the soil profile at the time of sowing. No residue application from the previous crop was considered. Crops within the high yield potential zone were simulated with the representative high yield potential soil (Table 2). While the low yield potential crops were simulated using the low yield potential soil, except for sunflower, where the crop growth patterns from the reference plots suggested that soil characteristics were better represented by the high yield potential soil.

2.6. Parameter selection for model calibration

For phenology, observed data related to crop emergence, flowering and physiological maturity were used. Phenology parameters for calibration were the temperature sums for the time from sowing to emergence (TSUMEM), from emergence to flowering (TSUM1) and from flowering to physiological maturity (TSUM2). For crop growth, three intermediate biomass cuts in 2020, two intermediate and the final above ground biomass in the rest of the seasons, and grain yield from all seasons were used to compare with the crop growth simulations. The parameter selection for the optimization procedure was done based on previous experience with model applications and sensitivity analyses (Enders et al., 2023; Faye et al., 2023; Gaiser et al., 2013; Seidel et al., 2021), crop growth characteristics of summer and winter crops and the number of observed variables. Table 4 shows a four-crop parameter set related to RUE and leaf area dynamics. The RUETB, is the RUE table as function of developmental stage (DVS), which is a main driver of biomass accumulation, and tends to be the highest during the vegetative stage and declines after flowering. Biomass growth and leaf area index (LAI) are directly related. Potential biomass growth is calculated based on LAI, light interception and the extinction coefficient. Biomass accumulated within a day is then partitioned into the different plant organs, the biomass portion to the leaves is then converted to LAI increase using specific leaf area (SLA), which is the ratio of leaf area to leaf weight. Therefore, the following parameters related to LAI dynamics were additionally chosen: RGRLAI and SLATB (related to increase in LAI), DVSDLT (related to leaf senescence) and RDRL (related to leaf death rate due to water stress). Crop parameter ranges (Table 4) were selected to avoid unrealistic parameters values when the optimization was applied. Initial crop parameter values were extracted from the default crop files of Lintul5 (Wolf, 2012).

The RUETB and SLATB tables as function of DVS are shown in Fig. 3. For these ones, when applying the multiplication factor, the whole curve was equally shifted at every DVS (default value was 1). Default parameters for RGLAI were 0.01 for soybean, 0.029 for maize and sunflower, 0.031 for lupine, 0.0075 for barley, 0.0082 for rye and wheat and 0.08 for rapeseed. While default DVSDLT for all crops was set to 1.1 based on the assumption that, when occurring, crops senescence typically starts after flowering. The RDRL was set to 0.05 for all crops except rye, which was 0.01 due to the crop tolerance to water stress. The RUETB factor, RGRLAI and DVSDLT were optimized for both winter and summer crops, the SLATB factor was optimized just for the summer crops, whereas the RDRL was optimized just for the winter crops (for optimization procedure see Section 2.7).

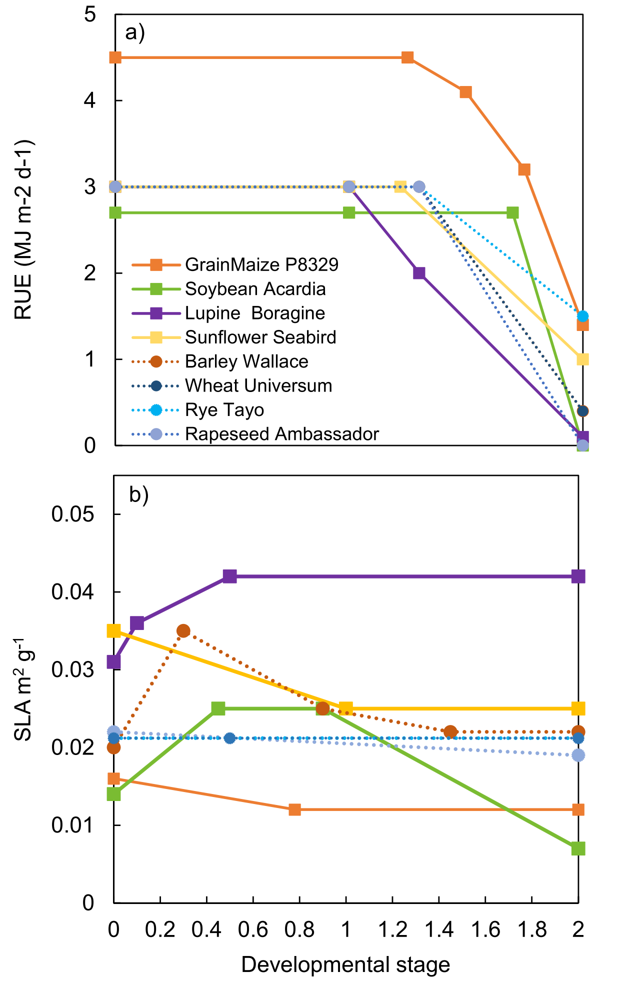

Fig. 3. Model curves for a) default radiation use efficiency (RUETB) and b) specific leaf area (SLATB) as a function of developmental stage for summer and winter crops at the patchCROP landscape experiment.

Table 4
Parameter selection and ranges for crop growth optimization in calibration step using the Nelder-Mead method.

Parameter	Definition	Multiplication factor ranges
RUETB	Radiation use efficiency as function of developmental stage (MJ m^2 d^{-1}).	0.8–1.2
RGRLAI	Daily maximum relative increase in LAI (-).	0.1–0.5
SLATB	Specific leaf area as function of developmental stage (just for summer crops) (m^2 g^{-1}).	0.2–1.0
DVSDLT	Developmental stage above which death of leaves starts in dependence of mean daily temperature (-).	0.9–1.4
RDRL	Maximum relative death rate of leaves due to water stress (just for winter crops) (-).	0.5–1.5

2.7. Parameter optimization

Parameter optimization was done stepwise, by first selecting the optimum parameter set for phenology for each crop. For crop phenology, the model was manually calibrated by modifying the temperature sums for the dates from sowing to emergence (TSUMEM), from emergence to flowering (TSUM1) and from flowering to physiological maturity (TSUM2). As measure of model performance, the average for the root mean square error (RMSE, in days) for emergence, flowering and physiological maturity dates was calculated for calibration and validation. Best phenology parameters were chosen by crop, according to the LOO-validation (described in Section 2.8) and fixed for the crop growth parameter optimization step. The optimized parameter set combination for crop growth for each crop was generated using the

Nelder-Mead method (Nelder and Mead, 1965), the method is implemented within the General-purpose optimization, optim in R (package stats version 4.1.1). The objective function to perform the optimization was a weighed relative root mean square error (RRMSE). This method allows to optimize the four-parameter set simultaneously. The rest of crop parameters was fixed in the model. To measure model performance, a weighed relative root mean square error (RRMSE) was calculated, where the average RRMSE of the intermediate and final (when available) above ground biomass points contributed to 50% of the RRMSE and the other 50% corresponded the final grain yield. Optimized parameters were then used to run the model for the LOO-validation step. The suitability of the Nelder-Mead method for parameter optimization was measured by comparing the RRMSE of the simulated above ground biomass and grain yield when using the default crop parameters vs, the RRMSE when simulations were performed with the optimized parameter resulting from the Nelder-Mead application.

2.8. Leave one out (LOO) or cross-model validation

For a given set of crop seasonal data, one season is picked for model calibration and the rest of the data set is left for model validation. In a following step, another season is picked for calibration and the rest is left for validation, two-year combinations are also performed (in the case of the summer crops), and the left-out year is used for validation. The procedure is repeated until all possible seasonal combinations are performed. Parameter selection is based on the model (or year choice) that gives the lowest predictive error (i.e. lowest error in the validation step). To measure model performance, the average RMSE for phenology (as described in Section 2.7) was used. While for crop growth, the RRMSE (as described in Section 2.7) for above ground biomass and grain yield was used.

For the LOO-validation procedure in the current study, three and two seasons for summer and winter crops, respectively, were used. Therefore, for the summer crops, single year combinations for 2020, 2021, and 2022 were picked for model calibration, as well as the two-year combination 2020+2021, 2020+2022 and 2021+2022, the left-out years for each combination were used then for LOO-validation (Fig. 4). For the winter crops, only a single year combination was possible, 2021 was first calibrated and 2022 remained for LOO-validation and in a second step the opposite combination was performed. The same procedure was applied for each crop, individually.

In order to answer the hypothesis on whether a flexible year combination is more advantageous than a fixed year combination when simulating a diversified cropping system, all possible year combinations for calibration and validation were applied to every crop. For the fixed year combination, the average error by each year combination (RMSE for phenology or RRMSE for crop growth) was calculated. While for the flexible year combination, all year combinations were applied to every crop, solely the best year combination using the LOO-validation method was chosen by crop and the average error for the specific crop combinations was calculated. In a first step, the best phenology parameter set by crop was selected according to the LOO-validation, and then used for

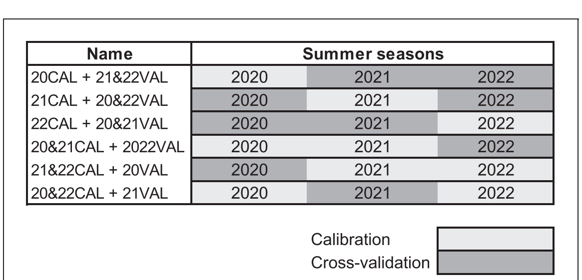

Fig. 4. Names of year combination for LOO-model validation for summer crops comprising 2020, 2021 and 2022 seasons.

the crop growth parameter optimization and validation.

3. Results

3.1. Parameter optimization and LOO-validation for crop phenology

The phenology parameter list and the RMSE for the calibration, as well as the year combination selection according to the LOO-validation are shown in Table 5. Best year combination for the LOO-validation varied among crops. For summer crops, the best year combination RMSEs ranged from 0.7 in soybean with 20&21 calibration (CAL) + 22 validation (VAL) years, to 3 days for sunflower (20&22CAL + 21VAL). For the winter crops, the RMSE was similar for either year combination, except for winter wheat, where season 22CAL+21VAL resulted in the lowest RMSE in the validation with 1.7 days. Often, multiple year combinations led to the same RMSE for the summer and winter crops suggesting that the model was able to capture the year-to-year variability.

3.2. Parameter optimization and LOO-validation for crop growth

Optimized parameter sets for the best year combinations are shown in Table 6. For summer crops, optimized LAI-related parameter RGRLAI decreased close to the minimum allowed range, except for sunflower. Similarly, the SLATB factor parameter was lower than the default value in all crops, except for sunflower. The optimum value for RUETB factor for all summer crops was 0.8, except maize with 0.91. For the winter crops, wheat, rye and rapeseed, the opposite trend was observed, where the parameter optimization often led to a higher RGRLAI value. Similarly, the optimum value for the RUETB factor was higher than the default for most crops, except for rye. The RDRL optimum value for barley, rapeseed and rye was lower than for wheat. The DVSDLT showed more variation among summer and winter crops, with values ranging from 0.99 (soybean) to 1.54 (maize and wheat).

On average, the application of the Nelder-Mead optimization method to calibrate crop growth resulted in a reduction of the average simulation error and its variability (represented as standard deviation) for the calibration and LOO-validation steps. The global average for the RRMSE for the calibration set was reduced from 68.5% when using the default parameter set *vs.* 29.1% when simulating with the optimized parameter set. While for the validation set, the average RRMSE was reduced from 68.5% to 55.0% (Fig. 5).

Fig. 6 shows the LOO-validation results for all the possible year combinations for summer and winter crops. Fixed year combinations typically led to a large RRMSE either in the calibration or LOO-validation step, while a flexible year combination resulted in a lower error in both calibration and LOO-validation steps for both, summer and winter crops. For summer crops, calibration years 2021 and 2022 and their combination led to the highest RRMSE in the LOO-validation step, particularly for soybean and sunflower, despite that the average calibration values by crop were <26%. The lowest errors in the LOO-validation were observed in lupine, maize and soybean, with 11.7, 17.8 and 20.6% RRMSE, respectively. For sunflower, the LOO-validation resulted in a reasonable RRSME value of 31.2%, in spite of a poor performance in the calibration step with 68.7% RRMSE. For the winter crops, optimum year combination for LOO-validation was more stable, with 2022CAL+2021VAL combination resulting in lowest RRMSE for winter wheat, barley and rapeseed. However, for rye, both year combinations led to a large error, with the lowest error obtained in the 2021CAL+2022VAL combination (RRMSE of 65.9% and 33.0% for calibration and LOO-validation, respectively).

Daily outputs of simulations for summer and winter crops corresponding to biomass growth, grain yield and water (TRANRF) and nutrient (NNI) stress are shown in Figs. 7 and 8 respectively. Simulated results show that the dominant stress was due to water limitation in all crops, though summer crops were more affected than the winter crops.

Table 5
Year combinations for LOO-model validation by crop, generated parameter set by year combination and average root mean square error for emergence date (when available), anthesis and maturity date for different crops in a diversified cropping system, patchCROP, Tempelberg, Brandenburg, Germany, 2020–2022.

Crop name and cultivar	Year combination	Parameters (°C d)			RMSE1 (days)	
		TSUMEM[2]	TSUM1[3]	TSUM2[4]	Calibration	Validation
Grain maize cv. P8329	20CAL + 21&22VAL	110	850	750	0.0	5.2
	21CAL + 20&22VAL	100	870	820	0.0	6.6
	22CAL + 20&21VAL	75	900	735	0.0	5.2
	20&21CAL + 2022VAL	100	850	815	2.6	5.0
	21&22CAL + 20VAL	75	890	770	2.7	3.5[5]
	20&22CAL + 21VAL	85	890	765	2.0	5.3
Soybean cv. Acardia	20CAL + 21&22VAL	70	455	520	0.5	10.3
	21CAL + 20&22VAL	70	410	795	0.0	5.7
	22CAL + 20&21VAL	80	445	750	0.0	4.8
	20&21CAL + 2022VAL	70	430	685	4.0	0.7[5]
	21&22CAL + 20VAL	70	440	765	3.9	6.0
	20&22CAL + 21VAL	80	435	680	0.9	6.3
Lupine cv. Boragine	20CAL + 21&22VAL	95	720	590	0.0	1.6
	21CAL + 20&22VAL	90	700	650	0.3	1.7
	22CAL + 20&21VAL	90	700	660	1.7	1.5
	20&21CAL + 2022VAL	95	700	620	0.8	1.3
	21&22CAL + 20VAL	90	710	605	0.9	0.8[5]
	20&22CAL + 21VAL	90	700	620	0.8	1.3
Sunflower cv. Seabird	20CAL + 21&22VAL	130	970	650	0.0	6.1
	21CAL + 20&22VAL	75	980	710	0.0	3.5
	22CAL + 20&21VAL	75	1040	850	0.0	4.3
	20&21CAL + 2022VAL	75	1010	680	0.6	4.0
	21&22CAL + 20VAL	75	1035	765	2.5	3.0
	20&22CAL + 21VAL	75	1015	770	1.9	3.0[5]
Winter wheat cv. Universum	21CAL + 22VAL	80	930	760	0.0	5.3
	22CAL + 21VAL	110	830	670	0.0	1.7[5]
Winter barley cv. Wallace	21CAL + 22VAL	140	820	520	0.0	4.0[5]
	22CAL + 21VAL	100	770	480	0.0	4.3
Winter rye cv. Tayo	21CAL + 22VAL	80	860	780	0.0	4.7
	22CAL + 21VAL	90	980	760	0.0	4.0[5]
Rapeseed cv. Ambassador	21CAL + 22VAL	30	390	740	0.0	5.0[5]
	22CAL + 21VAL	180	440	610	0.0	5.0

1 Root mean square error; [2] Temperature sum from sowing to emergence; [3] Temperature sum from emergence to flowering; [4] Temperature sum from flowering to physiological maturity; [5] Best parameter set based on LOO-model validation (see Section 3.1).

Table 6
Optimized parameter set for summer and winter crops in a diversified cropping system patchCROP when applying the Nelder-Mead method.

Crop name and cultivar	Best year combination1	Parameter type	RGRLAI[2]	DVSDLT[2]	RDRL[2]	SLATB factor[2]	RUETB factor[2]
Grain maize cv. P8329	21&22CAL + 20VAL	Default	0.0294	1.10	0.050	1.00	1.00
		Optimal	0.0029	1.54	0.050	0.75	0.91
Soybean cv. Acardia	20&22CAL + 21VAL	Default	0.0100	1.10	0.050	1.00	1.00
		Optimal	0.0010	0.99	0.050	0.60	0.80
Lupine cv. Boragine	20CAL + 21VAL	Default	0.0310	1.10	0.050	1.00	1.00
		Optimal	0.0031	1.16	0.050	0.94	0.80
Sunflower cv. Seabird	20&22CAL + 21VAL	Default	0.0294	1.10	0.050	1.00	1.00
		Optimal	0.0229	1.26	0.050	1.11	0.80
Winter wheat cv. Universum	22CAL + 21VAL	Default	0.0082	1.10	0.050	1.00	1.00
		Optimal	0.0094	1.54	0.043	1.00	1.14
Winter barley cv. Wallace	22CAL + 21VAL	Default	0.0075	1.10	0.050	1.00	1.00
		Optimal	0.0100	1.17	0.010	1.00	1.20
Rye cv. Tayo	21CAL + 22VAL	Default	0.0082	1.10	0.010	1.00	1.00
		Optimal	0.0107	1.28	0.005	1.00	0.80
Rapeseed cv. Ambassador	22CAL + 21VAL	Default	0.0800	1.10	0.050	1.00	1.00
		Optimal	0.0852	1.08	0.013	1.00	1.20

1 see definitions in Fig. 4; [2] see parameter definition in Table 4

Best year combinations in summer crops showed that years with lower simulated stress in the calibration, performed better in both the calibration and LOO-validation step. The model tends to perform well with the optimized parameters. In sunflower the model showed strong water stress and was not able to capture the increasing grain yield trend shown in the observations. Similarly for rye, both seasons show a very high degree of water stress limiting crop growth and resulting in poor RRMSE in the calibration step. For the winter crops, the model shows stronger simulated water stress during the 2022 season. Despite that the model tends to capture the above ground biomass and final yield reasonably well, the model was not able to capture the increasing yield trend in the 2022 season.

Error contribution for above ground biomass and grain yield is shown in Fig. 9. Error contribution varied for summer and winter crops,

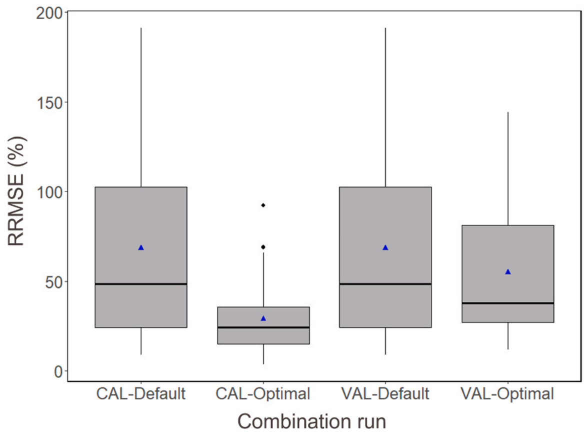

Fig. 5. Box plot for relative root mean square error (RRMSE) for intermediate and final (when available) above ground biomass and final grain yield, for model calibration (CAL) and validation (VAL) when running the model with the LOO-validated phenology parameter set either with the default crop growth parameter set or the optimized parameter set using the Nelder-Mead method for all year combinations for summer (maize, soybean, lupine and sunflower) and winter (wheat, barley, rye and rapeseed) crops at the patchCROP landscape experiment. For each box plot, horizontal lines represent, from top to bottom, the 10th percentile, 25th percentile, median, 75th percentile and 90th percentile, and the average (triangle). Circles represent the single year combination by crop.

in general above ground biomass contributed in higher magnitude to the total error in the summer crops, but the opposite was observed in the winter crops, where grain yield often contributed the most to the total error. In summary, for phenology LOO-validation showed that many different year combinations can lead to a reasonable result. However, for crop growth, particularly for summer crops, the year combination was key to pick the best model parameter set, as results showed that year combination differed for every crop.

4. Discussion

4.1. Parameters optimization

Manual calibration of the phenology data successfully reduced the model error (RRMSE) for all crops. As for the crop growth parameters, the Nelder-Mead method was successful in reducing the average error between observed and simulated above ground biomass and grain yield data for all summer and winter crops. Results are similar to Cui et al., (2023), who reported that the Nelder-Mead method reduced the normalized RMSE from 10.3% to 6.4% from a 30-year sole winter wheat grain yield data. The four-parameter set selected for the optimization step was below the median number of 6 reported by Seidel et al., (2018). The parameter selection and ranges was based on the amount of data per crop, previous model knowledge and expert opinion, however, there is a risk that the selected parameter number and choice can compensate for model errors (Seidel et al., 2018; Wallach, 2011). Higher incidence of simulated water stress in rye and sunflower resulted in limited improvement of the model performance in the calibration or validation step. However, it is known that rye tends to be more resistant to water stress than other winter cereal crops like wheat (Uprety and Sirohi, 1987), which is not currently considered in the model. More detailed data sets from different environments and further model testing would be useful to improve model performance for these crops. With regards to number of included years for model optimization, Thorp (2007) suggested that adding more seasons to the calibration step reduced the error, in the current study, this was true for summer crops (except lupin, where two years were used). The use of an optimized function for model optimization for crop growth parameters helped to reduce the personal bias compared to manual calibration approach and it also speeds up a procedure that is typically time consuming, especially when having multiple crops or long time series (Röll et al., 2020).

4.2. LOO-validation

Applying the LOO-validation for phenology resulted in similar RMSE for the different year combinations, suggesting that the model was able to capture the year-to-year variability and that year combination selection may not be crucial for the success of the validation procedure for phenology. Nurulhuda et al., (2022) reported that, for the same crop, multiple parameter combination sets lead to a similar result or equifinality, which was true for crop phenology; but not for the simulated above ground biomass and grain yield, where the LOO-validated values would often drastically change from one year combination to another. Minimizing RRMSE for summer crops was heavily dependent on the year combinations for calibration and validation, whereas for winter crops RRMSE values were less dependent on year combinations except for rye. Therefore, a LOO-validation with flexible years combination offered an advantage over a fixed years combination, especially for the summer crops. This was possibly due to the fact that summer crop phenological development and timing of sensitive stages during the vegetative and grain filling phases occur during a different period of the year for each

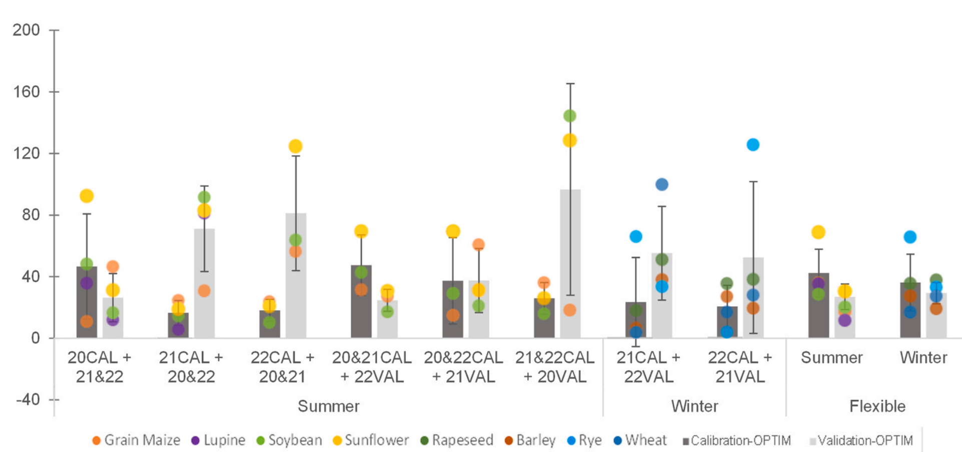

Fig. 6. Average relative root mean square error (RRMSE) for intermediate and final (when available) above ground biomass and final grain yield, for each year selection (bars) and by crop (points) for model calibration (CAL) and validation (VAL) for the optimized parameter set for summer (maize, soybean, lupine and sunflower) and winter (wheat, barley, rye and rapeseed) crops at the patchCROP landscape experiment for the seasons from 2020–2022, when using a fixed year combination or when using a flexible year combination by crop. Error lines represent standard deviation.

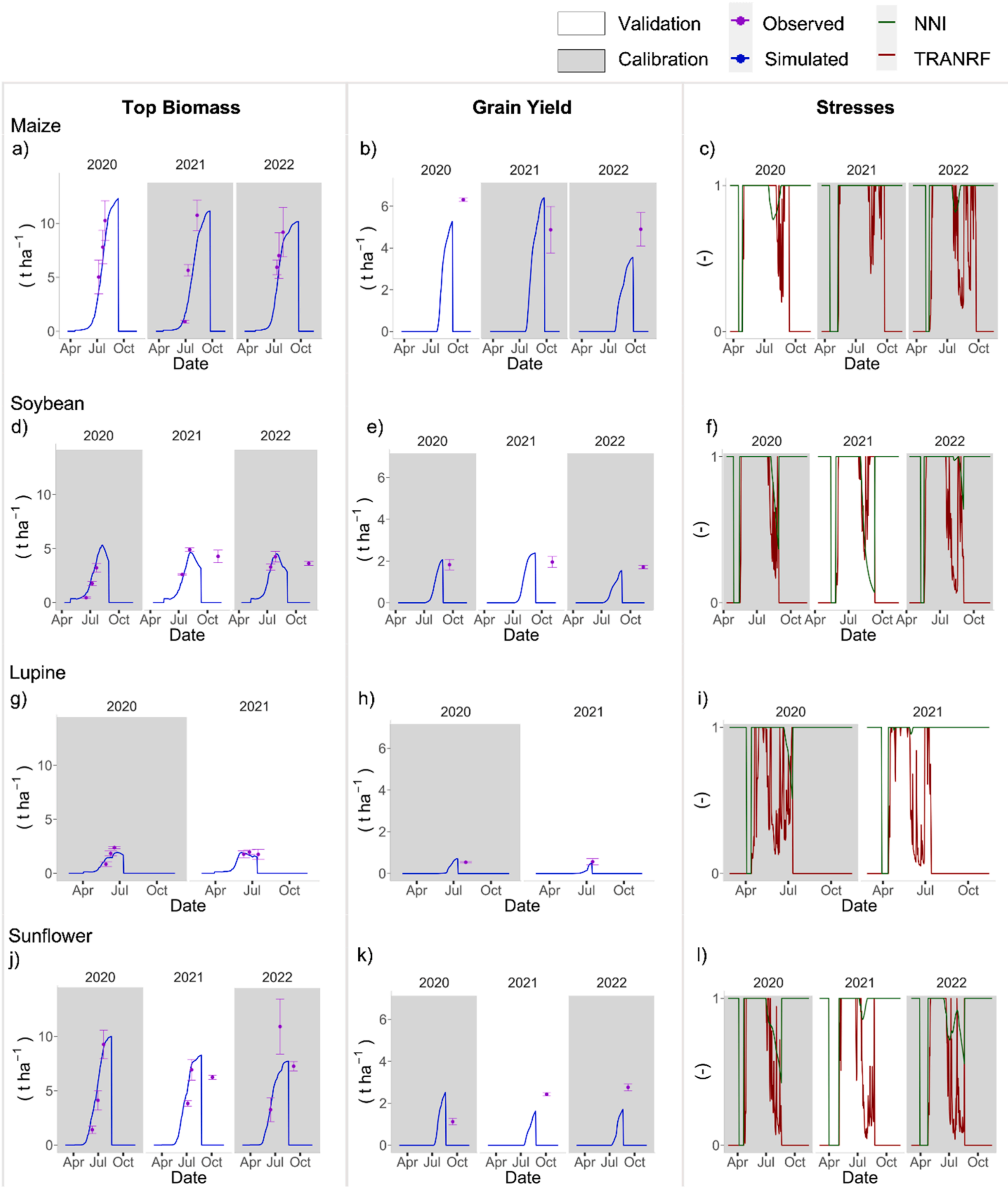

Fig. 7. Daily simulations for crop growth, grain yield and water (TRANRF) and nutrient (NNI) stress for the best year combination (parameter set in Table 6) according to the LOO-validation method for summer crops (maize, soybean, lupine and sunflower) at the patchCROP experiment for the 2020–2022 seasons. Error lines represent standard deviation or 3–4 replicates per sampling date.

crop. Also, their season is much shorter, contrary to the winter crops which have a longer growing season with less inter-annual variability in growth and yield. This trend was also observed in regionally observed crop data for spring and winter crops in Central Europe by Hlavinka et al., (2009), who reported that spring crops were more sensitive to water stress than winter crops, as the latter tend to have a more extensive rooting system and a longer growth period. The fact that years with lower simulated stress in the calibration, performed better in both the

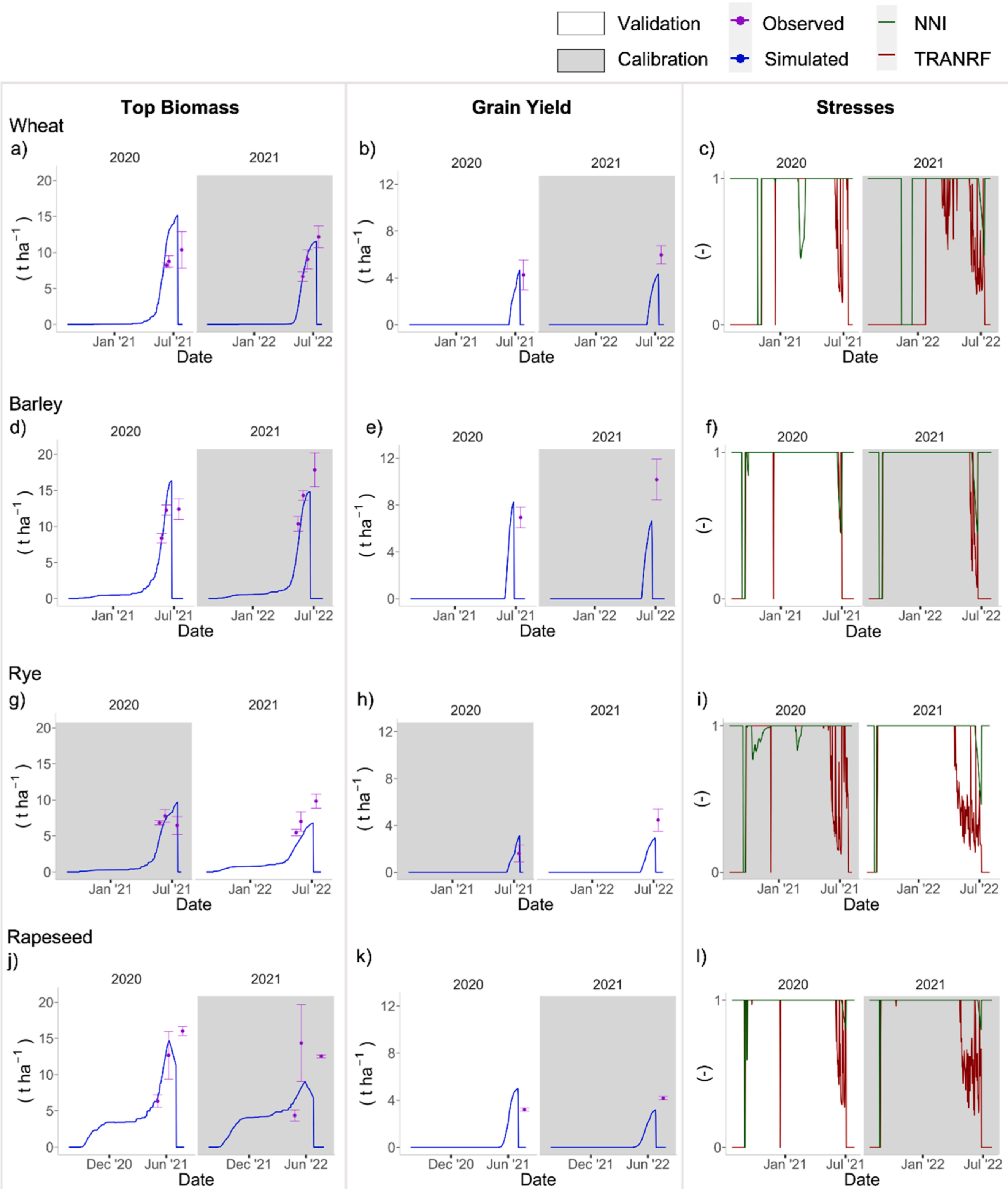

Fig. 8. Daily simulations for crop growth, grain yield and water (TRANRF) and nutrient (NNI) stress for the best year combination (parameter set in Table 6) according to the LOO-validation method for winter crops (wheat, barley, rye and rapeseed) at the patchCROP experiment for the 2020–2022 seasons when applying the LOO-model validation method. Error lines represent standard deviation or 3–4 replicates per sampling date.

calibration and LOO-validation step confirms, that data for calibration should be close to optimal crop growth conditions especially for crops where stress response functions are not already known (Kersebaum et al., 2015). The LOO-validation allows a more thorough use of the data when the amount of data is limited, which is a common limitation when crop models are calibrated (Seidel et al., 2018). By conducting both the calibration and validation procedures, we can get a better confidence on how the calibrated parameters perform during the validation. Moreover,

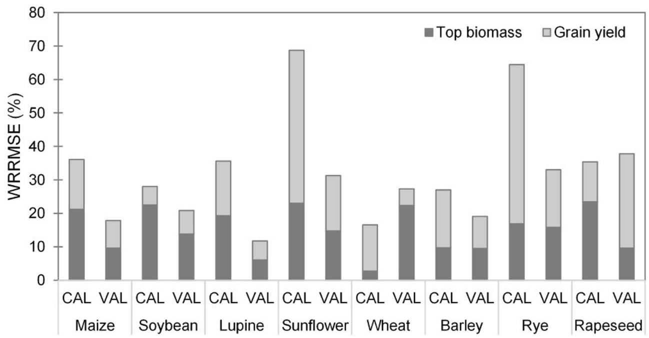

Fig. 9. Contribution of intermediate and final (when available) above ground biomass and grain yield to the weighed relative root mean square error (RRMSE) for the optimized parameter set for the calibration (CAL) and LOO-validation (VAL) for the summer (maize, soybean, lupine and sunflower) and winter (wheat, barley, rye and rapeseed) crops at the patchCROP experiments for the seasons from 2020 to 2022.

as year combination selection for LOO-validation in the summer crops varied by crop, it did not provide useful information on the year combination choice for the winter crops.

4.3. Other influences of modeling results

The model optimization for growth parameters and LOO-validation performed reasonably well for lupine, maize and soybean crops, as well as wheat, barley and rapeseed. However, model performance for less studied crops such as sunflower was less satisfactory. Other factors not accounted in the model may have contributed to this, such as the use of two soil profiles for a large field, which may not be fully representative for all plots in the low and high yield potential zones. The model showed very strong water stress particularly in the low yield potential soil, which also may suggest that the model needs to be more thoroughly tested on whether it can properly simulate water stress dynamics in extreme conditions such as entirely sandy soil profiles. The selected crops for the study are currently growing in a rotation mode, but the current simulations neglected the potential carry-over effects between crops, as well as the effects of cover crops and residues. As for the carry-over effects, residual mineral N and N released right after harvest of the previous crop is rapidly leached out in the dominantly sandy soils, such as the ones at the study site, and fertilization is typically the major source of N supply to the crops. Therefore, no considerable effect on crop parameter estimation was expected. Moreover, carry-over effects tend to play a bigger role in low input systems, but rotation effects may be reduced when N fertilizer and water supply are adequate (Kollas et al., 2015). In terms of soil carbon, changes due to rotation tend to be minimal in the short term, but have a significant impact in the long term (Basso et al., 2018; Grosz et al., 2017; Teixeira et al., 2015). Basso et al., (2018) reported that simulated soil organic carbon declined from 0.7% to 4.4% (relative to the initial value) within a 30-year period under different temperature scenarios in different locations. Moreover, results for Teixeira et al., (2015) and Faye et al., (2023), suggest that model sensitivity to consideration of carry over effects in crop rotation was higher for soil-related variables (such as soil water and soil nitrogen) than for crop productivity variables like grain yield. Similarly, crop residues may not have a significant impact on model performance for crop growth in the short term, but for long term model applications it should be considered as it can have important impacts on soil aggregates, soil carbon and soil moisture conservation (Basso et al., 2020; Kollas et al., 2015). In this case, soil model routines also need to be validated.

4.4. Future research priorities

Results were poor sunflower in the calibration step, mostly due to strong water limitations. Further field experimentation and model testing would be helpful to improve model performance. The same applies to winter rye, where the better resistance to drought may need to be accounted for, on the basis of more experimental data. Moreover, once the first five-year cycle of the current rotation is completed, further model testing would be needed to test the model capabilities in terms of simulating the temporal aspects of crop rotations such as the carry over effects and implications of crop residues crop productivity, resource use and soil dynamics related to water, nutrients, and organic carbon.

5. Conclusions

The current study showed the value of using the Nelder-Mead method and the LOO model validation for a more efficient data utilization when data is limited for model calibration and validation, which is often the case in multi-crop studies. Also, it points to the relevance of using a LOO model validation for diversified cropping systems with multiple crops, which can contribute to reduce the simulation error, especially for crops with a larger inter-annual yield variability like summer crops in Germany. For winter crops, the LOO-validation showed less sensitivity. Further field experimentation and model testing for under-represented crops (such as sunflower and cover crops) can also contribute to improve model performance. The newly calibrated and validated crop model has the potential to be used to conduct virtual experiments to understand the tradeoffs and synergies of diversified cropping systems in regards to the delivery of ESS and crop productivity for multifunctional and resilient cropping systems of the future.

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CRediT authorship contribution statement

Anna Engels: Writing – review & editing, Visualization. **kathrin Grahmann:** Writing – review & editing, Data curation. **Thomas Gaiser:** Writing – review & editing, Methodology, Data curation, Conceptualization. **Ixchel Manuela Hernandez-Ochoa:** Writing – original draft, Methodology, Formal analysis, Data curation, Conceptualization. **Frank Ewert:** Writing – review & editing, Methodology, Conceptualization. **Sabine Seidel:** Writing – review & editing. **Christian Kersebaum:** Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

Data will be made available on request.

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References

Addiscott, T.M., Whitmore, A.P., 1991. Simulation of solute leaching in soils of differing permeabilities. Soil Use Manag. *7* (2), 94–102. https://doi.org/10.1111/j.1475-2743.1991.tb00856.x.

Wallach, D., Makowski, D., Jones, J.W., Brun, F. (Eds.), 2019. Working with dynamics crop models. Academic Press.

Aguiar, S., Texeira, M., Garibaldi, L.A., Jobbágy, E.G., 2020. Global changes in crop diversity: trade rather than production enriches supply (Article). Glob. Food Secur. -Agric. Policy Econ. Environ. *26*, 100385. https://doi.org/10.1016/j.gfs.2020.100385.

APW. (2023). Auskunftsplattform Wasser. Land Brandenburg. Retrieved 20.09.2023 from https://apw.brandenburg.de/?feature=showNodesInTree%7C%5b%5b256.399,256.444,256.411,256.445%5d,true&th=zr_gw_me#.

Asseng, S., Zhu, Y., Basso, B., Wilson, T., Cammarano, D., 2014. Simulation Modeling: Applications in Cropping Systems. In: Van Alfen, N.K. (Ed.), Encyclopedia of Agriculture and Food Systems. Academic Press, pp. 102–112. https://doi.org/10.1016/B978-0-444-52512-3.00233-3.

Barbieri, P., Pellerin, S., Nesme, T., 2017. Comparing crop rotations between organic and conventional farming (Article). Sci. Rep. *7*, 13761. https://doi.org/10.1038/s41598-017-14271-6.

Basso, B., Dumont, B., Maestrini, B., Shcherbak, I., Robertson, G.P., Porter, J.R., Rosenzweig, C., 2018. Soil organic carbon and nitrogen feedbacks on crop yields under climate change, 5 pp, Article Unsp 180026 Agric. Environ. Lett. *3* (1). https://doi.org/10.2134/ael2018.05.0026.

Basso, B., Martinez-Feria, R.A., Dumont, B., 2020. Modeling crop rotations: capturing short-and long-term feedbacks for sustainability and soil health (pp). In: Boote, K. (Ed.), Advances in Crop modelling for a sustainable agriculture. Burleigh dodds Science publishing, p. 22.

Beillouin, D., Ben-Ari, T., Malezieux, E., Seufert, V., Makowski, D., 2021. Positive but variable effects of crop diversification on biodiversity and ecosystem services. Glob. Change Biol. *27* (19), 4697–4710. https://doi.org/10.1111/gcb.15747.

Buis, S., Wallach, D., Guillaume, S., Varella, H., Lecharpentier, P., Launay, M., Justes, E., 2011. The STICS crop model and associated software for analysis, parameterization, and evaluation. Methods Introd. Syst. Models into Agric. Res. 395–426.

Chenu, K., Porter, J.R., Martre, P., Basso, B., Chapman, S.C., Ewert, F., Asseng, S., 2017. Contribution of crop models to adaptation in wheat. Trends Plant Sci. *22* (6), 472–490. https://doi.org/10.1016/j.tplants.2017.02.003.

Corbeels, M., McMurtrie, R.E., Pepper, D.A., O'Connell, A.M., 2005. A process-based model of nitrogen cycling in forest plantations Part I. Structure, calibration and analysis of the decomposition model. Ecol. Model. *187* (4), 426–448. https://doi.org/10.1016/j.ecolmodel.2004.09.005.

Crossley, M.S., Burke, K.D., Schoville, S.D., Radeloff, V.C., 2021. Recent collapse of crop belts and declining diversity of US agriculture since 1840. Glob. Change Biol. *27* (1), 151–164. https://doi.org/10.1111/gcb.15396.

Cui, W.A., Nie, Z.G., Li, G., Yuan, J.Y., 2023. Optimization of parameters related to grain growth of spring wheat in dryland based on the next-generation APSIM. Article 1915 Agron. -Basel *13* (7), 1915. https://doi.org/10.3390/agronomy13071915.

Dainese, M., Martin, E.A., Aizen, M.A., Albrecht, M., Bartomeus, I., Bommarco, R., Steffan-Dewenter, I., 2019. A global synthesis reveals biodiversity-mediated benefits for crop production. Article eaax0121 Sci. Adv. *5* (10), eaax0121. https://doi.org/10.1126/sciadv.aax0121.

Destatis. (2023). Agriculture and forestry, fisheries. Field crops and grassland. Federal Statistical Office of Germany. 2023 ⟨https://www.destatis.de/EN/Themes/Economic-Sectors-Enterprises/Agriculture-Forestry-Fisheries/Field-Crops-Grassland/_node.html⟩.

Donat, M., Geistert, J., Grahmann, K., Bloch, R., Bellingrath-Kimura, S., 2024. Patch cropping- a new methodological approach to determine new field arrangements that increase the multifunctionality of agricultural landscapes. Comput. Electron. Agric. (In press.).

Dovydaitis, E., Kunze, T., Born, F., Ewert, F., Dachbrodt-Saaydeh, S., Grahmann, K., 2023. Assessing pollen beetle dynamics in diversified agricultural landscapes with reduced pesticide management strategies. J. Sustain. Org. Agric. *74* (1), 1–24. https://doi.org/10.5073/LBF.2023.01.03.

Dumont, B., Leemans, V., Mansouri, M., Bodson, B., Destain, J.P., Destain, M.E., 2014. Parameter identification of the STICS crop model, using an accelerated formal MCMC approach. Environ. Model. Softw. *52*, 121–135. https://doi.org/10.1016/j.envsoft.2013.10.022.

Enders, A., Vianna, M., Gaiser, T., Krauss, G., Webber, H., Srivastava, A.K., Ewert, F., 2023. SIMPLACE-a versatile modelling and simulation framework for sustainable crops and agroecosystems (Article). Silico Plants *5* (1), diad006. https://doi.org/10.1093/insilicoplants/diad006.

Ewert, F., Rounsevell, M.D.A., Reginster, I., Metzger, M.J., Leemans, R., 2005. Future scenarios of European agricultural land use I. Estimating changes in crop productivity. Agric. Ecosyst. Environ. *107* (2-3), 101–116. https://doi.org/10.1016/j.agee.2004.12.003.

Faye, B., Webber, H., Gaiser, T., Müller, C., Zhang, Y., Stella, T., Ewert, F., 2023. Climate change impacts on European arable crop yields: sensitivity to assumptions about rotations and residue management. Eur. J. Agron. *142*, 126670.

Gaiser, T., Perkons, U., Kupper, P.M., Kautz, T., Uteau-Puschmann, D., Ewert, F., Krauss, G., 2013. Modeling biopore effects on root growth and biomass production on soils with pronounced sub-soil clay accumulation. Ecol. Model. *256*, 6–15. https://doi.org/10.1016/j.ecolmodel.2013.02.016.

Geiger, F., Bengtsson, J., Berendse, F., Weisser, W.W., Emmerson, M., Morales, M.B., Inchausti, P., 2010. Persistent negative effects of pesticides on biodiversity and biological control potential on European farmland. Basic Appl. Ecol. *11* (2), 97–105. https://doi.org/10.1016/j.baae.2009.12.001.

Grahmann, K., Reckling, M., Hernandez-Ochoa, I., Ewert, F., 2021. An agricultural diversification trial by patchy field arrangements at the landscape level: the landscape living lab "patchCROP". Asp. Appl. Biol. *146*, 385–391.

Grosz, B., Dechow, R., Gebbert, S., Hoffmann, H., Zhao, G., Constantin, J., Ewert, F., 2017. The implication of input data aggregation on up-scaling soil organic carbon changes. Environ. Model. Softw. *96*, 361–377. https://doi.org/10.1016/j.envsoft.2017.06.046.

Hlavinka, P., Trnka, M., Semeradova, D., Dubrovsky, M., Zalud, Z., Mozny, M., 2009. Effect of drought on yield variability of key crops in Czech Republic. Agric. For. Meteorol. *149* (3-4), 431–442. https://doi.org/10.1016/j.agrformet.2008.09.004.

Hufnagel, J., Reckling, M., Ewert, F., 2020. Diverse approaches to crop diversification in agricultural research. A review, 17 pp, Article 14 Agron. Sustain. Dev. *40* (2). https://doi.org/10.1007/s13593-020-00617-4.

Jones, J.W., Hoogenboom, G., Porter, C.H., Boote, K.J., Batchelor, W.D., Hunt, L.A., Ritchie, J.T., 2003. The DSSAT cropping system model. Article Pii s1161-0301(02)00107-7. Eur. J. Agron. *18* (3-4), 235–265. https://doi.org/10.1016/s1161-0301(02)00107-7.

Kersebaum, K.C., Boote, K.J., Jorgenson, J.S., Nendel, C., Bindi, M., Fruhauf, C., Wegehenkel, M., 2015. Analysis and classification of data sets for calibration and validation of agro-ecosystem models. Environ. Model. Softw. *72*, 402–417. https://doi.org/10.1016/j.envsoft.2015.05.009.

Koch, T., Deumlich, D., Chifflard, P., Panten, K., Grahmann, K., 2023. Using model simulation to evaluate soil loss potential in diversified agricultural landscapes (Article). Eur. J. Soil Sci. *74* (1), e13332. https://doi.org/10.1111/ejss.13332.

Kollas, C., Kersebaum, K.C., Nendel, C., Manevski, K., Muller, C., Palosuo, T., Wu, L.H., 2015. Crop rotation modelling-A European model intercomparison. Eur. J. Agron. *70*, 98–111. https://doi.org/10.1016/j.eja.2015.06.007.

Lagarias, J.C., Reeds, J.A., Wright, M.H., Wright, P.E., 1998. Convergence properties of the Nelder-Mead simplex method in low dimensions. Siam J. Optim. *9* (1), 112–147. https://doi.org/10.1137/s1052623496303470.

Marini, L., St-Martin, A., Vico, G., Baldoni, G., Berti, A., Blecharczyk, A., Bommarco, R., 2020. Crop rotations sustain cereal yields under a changing climate (Article). Environ. Res. Lett. *15* (12), 124011. https://doi.org/10.1088/1748-9326/abc651.

Martre, P., Yin, X.Y., Ewert, F., 2017. Modeling crops from genotype to phenotype in a changing climate. Field Crops Res. *202*, 1–4. https://doi.org/10.1016/j.fcr.2017.01.002.

Meier, U. (Ed.). (2018). Growth stages of mono- and dicotyledonous plants. Julius Kühn-Institut (JKI). https://doi.org/10.5073/20180906-074619.

Meyer, S., Kling, C., Vogel, S., Schröter, I., Nagel, A., Kramer, E., … Ruehlmann, J. (2019). Creating soil texture maps for precision liming using electrical resistivity and gamma ray mapping. Precision Agriculture'19, Conference Proceedings, 9 pp. https://doi.org/https://doi.org/10.3920/978-90-8686-888-9.

Nelder, J.A., Mead, R., 1965. A simplex algorithm for function minimization. Comput. J. *7*, 308–313. https://doi.org/10.1093/comjnl/7.4.308.

Nocedal, J., Wright, S.J., 1999. Numerical optimization. Springer, New York.

Nurulhuda, K., Muharam, F.M., Shahar, N.A.N., Hashim, M.F.C., Ismail, M.R., Keesman, K.J., Zulkafli, Z., 2022. ORYZA (v3) rice crop growth modeling for MR269 under nitrogen treatments: assessment of cross-validation on parameter variability (Article). Comput. Electron. Agric. *195*, 106809. https://doi.org/10.1016/j.compag.2022.106809.

Olsson, D.M., Nelson, L.S., 1975. The Nelder-Mead simplex procedure for function minimization. Technometrics *17*, 45–51.

Röll, G., Memic, E., Graeff-Hönninger, S., 2020. Implementation of an automatic time-series calibration method for the DSSAT wheat models to enhance multi-model approaches. Agron. J. *112* (5), 3891–3912. https://doi.org/10.1002/agj2.20328.

Seidel, S.J., Gaiser, T., Ahrends, H.E., Huging, H., Siebert, S., Bauke, S.L., Ewert, F., 2021. Crop response to P fertilizer omission under a changing climate-experimental and modeling results over 115 years of a long-term fertilizer experiment. Article 108174 Field Crops Res. *268*, 108174. https://doi.org/10.1016/j.fcr.2021.108174.

Seidel, S.J., Palosuo, T., Thorburn, P., Wallach, D., 2018. Towards improved calibration of crop models - where are we now and where should we go? Eur. J. Agron. *94*, 25–35. https://doi.org/10.1016/j.eja.2018.01.006.

Silva, K.G., Aloise, D., Xavier-de-Souza, S., Mladenovic, N., 2018. Less is more: simplified Nelder-Mead method for large unconstrained optimization. Yugosl. J. Oper. Res. *28* (2), 153–169.

Smith, M.E., Vico, G., Costa, A., Bowles, T., Gaudin, A.C.M., Hallin, S., Bommarco, R., 2023. Increasing crop rotational diversity can enhance cereal yields. Article 89 Commun. Earth Environ. 4 (1). https://doi.org/10.1038/s43247-023-00746-0.

Tamburini, G., Bommarco, R., Wanger, T.C., Kremen, C., van der Heijden, M.G.A., Liebman, M., Hallin, S., 2020. Agricultural diversification promotes multiple ecosystem services without compromising yield. Article eaba1715 Sci. Adv. *6* (45), eaba1715. https://doi.org/10.1126/sciadv.aba1715.

Teixeira, E.I., Brown, H.E., Sharp, J., Meenken, E.D., Ewert, F., 2015. Evaluating methods to simulate crop rotations for climate impact assessments - a case study on the

Canterbury plains of New Zealand. Environ. Model. Softw. *72*, 304–313. https://doi.org/10.1016/j.envsoft.2015.05.012.

Thorburn, P.J., Boote, K.J., Nendel, C., Rötter, R.P., Ewert, F., 2018. Recent advances in crop modelling to support sustainable agricultural production and food security under global change. Eur. J. Agron. *100*, 1–3. https://doi.org/10.1016/j.eja.2018.10.009.

Thorp, K.R., Batchelor, W.D., Paz, J.O., Kaleita, A.L., DeJonge, K.C., 2007. Using cross-validation to evaluate CERES-Maize yield simulations within a decision support system for precision agriculture. Trans. Asabe *50* (4), 1467–1479.

Uprety, D.C., Sirohi, G.S., 1987. Comparative study on the effect of water stress on the photosynthesis and water relations of triticale, rye and wheat. J. Agron. Crop Sci. -Z. Fur Acker Und Pflanzenbau *159* (5), 349–355. https://doi.org/10.1111/j.1439-037X.1987.tb00113.x.

Wallach, D., 2011. Crop model calibration: A statistical perspective. Agron. J. *103* (4), 1144–1151. https://doi.org/10.2134/agronj2010.0432.

Wallach, D., Palosuo, T., Thorburn, P., Hochman, Z., Gourdain, E., Andrianasolo, F., Seidel, S.J., 2021. The chaos in calibrating crop models: lessons learned from a multi-model calibration exercise (Article). Environ. Model. Softw. *145*, 105206. https://doi.org/10.1016/j.envsoft.2021.105206.

Wang, P.C., Shoup, T.E., 2011. Parameter sensitivity study of the Nelder-Mead simplex method. Adv. Eng. Softw. *42* (7), 529–533. https://doi.org/10.1016/j.advengsoft.2011.04.004.

Wolf, J. (2012). User guide for Lintul5: Simple generic model for simulation of crop growth under potential, water limited and nitrogen, phosphorus and potassium limited conditions.

Wosten, J.H.M., Lilly, A., Nemes, A., Le Bas, C., 1999. Development and use of a database of hydraulic properties of European soils. Geoderma *90* (3-4), 169–185. https://doi.org/10.1016/s0016-7061(98)00132-3.

Wosten, J.H.M., Pachepsky, Y.A., Rawls, W.J., 2001. Pedotransfer functions: bridging the gap between available basic soil data and missing soil hydraulic characteristics. J. Hydrol. *251* (3-4), 123–150. https://doi.org/10.1016/s0022-1694(01)00464-4.

Xiong, W., Holman, I., Conway, D., Lin, E., Li, Y., 2008. A crop model cross calibration for use in regional climate impacts studies. Ecol. Model. *213* (3-4), 365–380. https://doi.org/10.1016/j.ecolmodel.2008.01.005.

Zampieri, M., Weissteiner, C.J., Grizzetti, B., Toreti, A., van den Berg, M., Dentener, F., 2020. Estimating resilience of crop production systems: From theory to practice. Article 139378 Sci. Total Environ. *735*, 139378. https://doi.org/10.1016/j.scitotenv.2020.139378.