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## Assessing the effect of intercropped leguminous service crops on main crops and soil processes using APSIM NG

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## HIGHLIGHTS

## G R A P H I C A L A B S T R A C T

- Crop modules for oats, winter wheat and red clover were calibrated to simulate intercrops in Sweden in APSIM NG.
  Effects of intercropping cereals (oats-
- Effects of intercropping cereals (oatswinter wheat) and a legume service crop on cereals and soil processes were assessed.
- Calibration resulted in satisfactory endbiomass, but poor simulation of biomass during leaf development and tillering.
- Intercropping with a service crop had positive effects from an ecosystem service perspective.
- Drawbacks were elevated N losses in winter wheat and fallow, indicating a need for long-term N management.

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## ABSTRACT

*CONTEXT*: To improve agricultural sustainability, alternative cultivation methods and assessment tools need to be developed. Integrating service crops (SC) can potentially increase cropping system multifunctionality and mitigate negative climate and environmental impacts of agriculture.

*OBJECTIVES:* (1) Calibrate oats, winter wheat and red clover SC, grown as sole crops and intercrops, in the cropping system model APSIM NG for northern Europe climate conditions. (2) Use the calibrated crop modules to assess ecosystem processes from an intercropping system. (3) Discuss the role of mechanistic crop models in assessing ecosystem services and disservices from complex cropping systems.

*METHODS*: The crops were calibrated with data from an oats-winter wheat cropping sequence at two field sites. Thirty weather datasets were created from historical weather data to generate weather-dependent variability in crop performance and related processes. The assessment compared two scenarios, with or without an intercropped red clover SC sown in oats and terminated the following spring in winter wheat. Outputs representing processes related to important ecosystem services were extracted from the simulations.

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*RESULTS AND CONCLUSIONS:* Calibration of the three crops resulted in satisfactory biomass levels at the end of the growing season. Including a SC reduced oat yield, but increased winter wheat yield in two-thirds of simulations. Model outputs showed that including a SC resulted in 33–79% more fresh soil organic carbon, depending on site, compared with no SC. Nitrogen (N) uptake by both crops was highest in the SC scenario. In oats, N losses did not differ between the two scenarios, while in winter wheat the SC scenario had approximately 50% lower N leaching losses and 30% higher gaseous N emissions. However, in the fallow period from winter wheat harvest through to spring, both types of N losses were elevated in the SC scenario. The SC scenario had only a minor effect on water dynamics, causing a small reduction in soil water content.

*SIGNIFICANCE:* In this paper we give an example of how APSIM NG can be used to assess ecosystem services from complex agricultural systems using a case study with intercropping of cereals and leguminous SCs. APSIM NG was useful in providing a holistic assessment, and we show that intercropping with a SC can improve cropping system performance and reduce negative impacts, but long-term strategic management of N is required to prevent increased losses. To further improve simulation of intercrops more accurate simulation of early growth is needed for all crops included.

## 1. Introduction

Intensive agricultural systems, focusing on growing few crops in pure stands, reliant on fertilisers and agrochemicals, can have negative effects on the soil and surrounding environment and contribute to climate change. Since the mid-20th century, inputs of nitrogen (N) and phosphorus have greatly increased (Davidson, 2009; Yuan et al., 2018), and substantial quantities of these nutrients can be lost via leaching, runoff or gaseous emissions (Billen et al., 2021; Mekonnen and Hoekstra, 2018). These losses alter the chemical balance in water bodies and the atmosphere, contributing to climate change (Hong et al., 2021), eutrophication (Wurtsbaugh et al., 2019) and air pollution (Townsend et al., 2003). The intensification of agriculture has also led to separation of animal husbandry and crop production (Garrett et al., 2020), leading to reduced access to manure and less incentive to grow leys in cropdominated areas. An associated reduction in organic matter inputs through manure and leys has led to a decline in soil organic matter and soil biota (D'Hose et al., 2018; Peyraud et al., 2014).

Service crops (SCs), i.e. crops grown to provide supporting and regulating ecosystem services to the cropping system, have been proposed as a measure to reduce the negative effects of agriculture on the environment and climate and the cropping system itself (Gardarin et al., 2022). Compared to leaving the soil bare between main crops, SCs can increase water infiltration (Chalise et al., 2018), reduce nutrient losses via leaching and runoff (Blanco-Canqui, 2018; Vogeler et al., 2021), increase soil organic matter content (Frasier et al., 2016; Poeplau and Don, 2015), promote soil microorganisms (Muhammad et al., 2021), add N through dinitrogen (N<sub>2</sub>) fixation (Guiducci et al., 2018) and mine deep soil layers for nutrients (Wendling et al., 2016). The ability of SCs to improve in-field nutrient cycling and reduce competition from weeds can also improve yield of the following crop (Hallama et al., 2019; Jensen et al., 2021; Toukabri et al., 2020). Due to these positive aspects, SCs have recently been included in the European Union's subsidy system for environmentally friendly practices, as catch and cover crops (EC, 2021). However, SCs may also cause negative effects, sometimes referred to as "disservices" (Zhang et al., 2007). For example, SCs sown postharvest may take up too much N and water, causing pre-emptive competition, leading to poor growth of subsequent crops (Peterson et al., 2019; Thorup-Kristensen, 1993), or propagate pests and diseases (Acharya et al., 2020; Dunbar et al., 2016). Frost killed SCs can also cause increased nutrient losses when their biomass decays (Liu et al., 2019). For SCs to be a useful component in sustainable agriculture, better understanding of their positive and negative impacts on the main crop, field and surrounding environment is needed, as well as of the extent to which varying SC performance affects the provision of service and disservice.

Service crops are normally grown between two main crops, in autumn or from autumn to spring. When sown late at northern latitudes, they are exposed to deteriorating growing conditions, which can hamper their growth and consequently the services they deliver (Hashemi et al., 2013; Kumar et al., 2023b). As an alternative, early establishment of SCs by intercropping in a main crop extend their growth period and can increase biomass production (De Notaris et al., 2019). The main drawback of intercropping is competition between the two crops, with the risk of reduced main crop yields (Blackshaw et al., 2010).

Service crop productivity and impacts on main crops and environment are most commonly studied in field experiments. However, the high costs associated with running field experiments and the equipment and labour required for data collection and analysis often limit the amount of data that can be collected. Field experiments also often run over a short period, limiting the ability to study temporal variability in SC growth and the services and disservices they deliver. Due to these limitations, crop models are valuable complements to field data. Mechanistic crop models simulate the interactions of climate, biophysical processes and management practices on crop development and growth, and are helpful in assessing the potential effects of crop management on agroecosystems (Böldt et al., 2021; Sapkota et al., 2012). They can complement field experiments by providing estimates for: (i) variables that are difficult to measure in the field (Basche et al., 2016; Büchi et al., 2018); (ii) effects of climate change on crop production (Araya et al., 2015; Chimonyo et al., 2020); and (iii) screening the effects of alternative management and novel cropping systems (Amarasingha et al., 2017; Mupangwa and Jewitt, 2011; Ripoche et al., 2011; Xin and Tao, 2020) to guide future research. The ability to run the models over many years also makes it possible to assess annual variability in crop growth and soil processes due to weather conditions. The mechanistic crop models APSIM (Githui et al., 2023), DSSAT (Pierre et al., 2023) and STICS (Vezy et al., 2023) are the most commonly used models for simulating annual intercropping systems. Out of these models, APSIM has the most documentation of its performance simulating crops at northern latitudes in Europe (Kumar et al., 2023a; Morel et al., 2020; Vogeler et al., 2019a), although not for intercropping. However, APSIM has previously been used to simulate intercropping of maize and SC in the US with satisfactory results (Bartel et al., 2020), while studies on intercropping two main crops have found simulation of biomass and LAI of the crops to fit poorly to observed values (Berghuijs et al., 2021; Knörzer et al., 2011b; Nelson et al., 2021).

The aim of this study was to investigate the possibility of using APSIM NG (Holzworth et al., 2018) to assess ecosystem services from a cereal-SC intercropping system. Specific objectives were to: (i) calibrate modules for each crop in the intercropping system; (ii) assess the impact of SCs on simulated processes affecting important ecosystem services, using 30 weather datasets to generate weather-dependent variability in crop performance and related processes; and (iii) discuss the role of mechanistic crop models in assessing ecosystem services and disservices from complex cropping systems. We hypothesised that intercropping with SCs would slightly reduce biomass production and yield of the crop grown in the establishment year (oats), but increase biomass, yield and N uptake of the following crop (winter wheat), due to a residual N effect, and inputs of fresh organic carbon (FOC) to the soil. Furthermore, we

hypothesised that N and water would be utilised more efficiently in the APSIM NG-simulated system, owing to a reduction in losses and increased uptake by plants.

## 2. Materials and methods

## 2.1. Model description

The cropping system model APSIM uses daily weather data (maximum and minimum temperatures, precipitation and solar radiation) to simulate crop development and growth, and corresponding carbon, water, and nitrogen dynamics in the soil. In APSIM, different crop and management modules can be combined, allowing simulation of a wide range of agricultural systems, including sole crops, pastures, agroforestry and intercropping (Holzworth et al., 2014). APSIM NG was developed to better handle more complex cropping systems and higher demand on model software (Holzworth et al., 2018). In APSIM NG, the Microclimate and SoilArbitrator modules accounts for resource sharing if two crops grow together. Aboveground competition is simulated based on the height of the crops, their extinction coefficients and leaf area index (LAI) of both live and dead leaves (Githui et al., 2023). For utilisation of belowground resources the model uses a fourth order Runge-Kutta solution at a daily time step (Huth et al., 2024). Furthermore, as a default, the crops are simulated as growing in the same row (Wu et al., 2021).

The default module for simulating soil water dynamics in APSIM, SoilWat, uses a cascading approach (Probert et al., 1998), and was used in this study. APSIM has been used to accurately simulate fluctuations in soil water in Midwestern US (Archontoulis et al., 2014; Kivi et al., 2022), and to simulate evaporation in humid environments (Guo et al., 2021; Vogeler et al., 2020). The module Nutrient simulates turnover of organic matter, with special focus on nitrogen pathways (Probert et al., 1998). However, studies suggests that default decomposition rates are slightly under-estimated both in Oceania and in northern Europe (Smith et al., 2020; Vogeler et al., 2019a). Denitrification rates are simulated as a function of soil moisture, temperature, nitrate and active carbon content, a set denitrification coefficient and the ratio between N<sub>2</sub> and N<sub>2</sub>O (Thorburn et al., 2010).

## 2.2. Study system

The study system comprised a two-crop sequence with oats (Avena sativa L.) and winter wheat (Triticum aestivum L.) intercropped with a SC of forage legumes (squarrose clover (Trifolium squarrosum L.) and red clover (T. pratense)). Oats and SC were sown together in spring, while winter wheat was sown between SC rows approximately one month after oat harvest. The SC was terminated by row hoeing in spring the second year. The analysis was based on data from experiments at two sites in south-east Sweden (hereafter referred to as Site1 and Site2) located 14

## Table 1

km from each other (58°5N 15°4″E and 58°4N 15°5″E, respectively). Site1 had a heavy clay soil, while Site2 had a silty clay loam with a higher proportion of stones (Table 1). The 30 years average mean annual temperature is 7.1 °C at Site1 and 7.2 °C at Site2, while during the main growing season (May–August) it is 12.2 °C and 12.4 °C, respectively. The 30 years average annual precipitation is 565 mm at Site1 and 597 mm at Site2, while during the main growing season it is 222 mm and 225 mm, respectively.

## 2.3. Experimental design

The experiments at Site1 and Site2 had a randomised block design, with data collected from four blocks. Experiments ran between 2019 and 2020. The experiment was two factorial. The first factor was a combination of SC sowing dates and the presence or absence of the SC. The second factor was N rate, with either recommended N rate or half of the recommended. In this study, only data from treatments with the recommended nitrogen rate (120 kg N ha<sup>-1</sup> in oats and 160 kg N ha<sup>-1</sup> in winter wheat) with SCs sown at the same time as oats and corresponding treatments without SCs were considered. Plots were 2.5 m × 36 m.

Mineral fertilisers were applied to the experiments the day before sowing, on 18 April at Site1 and 16 April at Site2. The day after, oats were sown at a seed rate of 140 kg ha<sup>-1</sup> (Site1) and 176 kg ha<sup>-1</sup> (Site2) at 60 mm depth and row spacing of 250 mm. The SC was sown in the same operation and in the same row as oats, at 10 mm depth, with a seed rate of 13.8 kg ha<sup>-1</sup>. Oats were harvested on 27 August at Site1 and 16 August at Site2. Winter wheat was sown on 25 and 26 September at Site1 and Site2, respectively, following the same depth and row spacing as with oats. Seeding rate was 241 kg ha<sup>-1</sup> at both sites. The SC was terminated on 22 April and 17 April at Site1 and Site2, respectively and SC aboveground biomass was left on the soil surface. Mineral fertilisers were applied on 18 and 17 April at Site1 and Site2, respectively. Winter wheat was harvested on 14 August and 24 August at Site1 and Site2, respectively.

## 2.4. Field data collection

Data on phenological development and aboveground biomass of oats were collected during the growing season in 2019, on 29 May, 18 June and 10 July at Site1 and 27 May, 17 June and 9 July at Site2. Winter wheat phenology and aboveground biomass were measured at both sites on 24 October 2019, 5 April 2020, 27 May 2020 and 28 June 2020. Data on SC aboveground biomass were collected on the same occasions as data collection on oats, and on the two first sampling dates in winter wheat. For biomass samples, 10 individual shoots (cereals) or plants (SC) were collected randomly in each plot. When applicable, the biomass samples were divided into stem, leaf and head before ovendrying at 60 °C for 48 h and weighing. Plants per m<sup>2</sup> were counted in four 50 cm × 50 cm squares for SC and cereals at first sampling, while

Soil texture and chemical parameters at the two experimental sites.											
Site/soil layer	Clay <sup>§</sup> [%]	Silt [%]	Sand [%]	Stone [%]	Organic carbon* [%]	P-AL [mg 100 g <sup>-1</sup> ]	P-HCl [mg 100 g <sup>-1</sup> ]	pH**			
Site1											
0–20	70.4	24.7	4.8	0.1	3.2	6.75	54.5	6.8			
20-60	75.1	22.3	2.6	0	0.59	16.56	54.5				
60-80	76.6	21.5	1.9	0	0	20.33	54.5				
Site2											
0–20	39.2	45.2	14.3	1.3	2.5	4.31	62.7	6.4			
20-60***	24.1	39.2	27.8	8.9	0.53	3.06	62.7				

<sup>§</sup> Soil texture was determined by the sieving and sedimentation method (ISO 11277, 2020).

\* Measured as ignition loss after oven drying at 105 °C over-night followed by 4 h at 550 °C. Organic matter content was then calculated with a reduction factor related to clay content and divided by 1.7 to obtain organic carbon content.

\*\* pH measured in water solution. Only measured in the topsoil.

\*\* 60-80 cm was not sampled due to too many stones.

shoots per  $m^2$  of cereals were counted in four 1 m rows in each plot. The average number of shoots and plants per  $m^2$  were used to calculate plant biomass per plot. This approach was used as there was no space for repeated destructive sampling of larger areas in the plots.

Harvesting was done from a  $26 \text{ m}^2$  area central in the plot with a combine harvester. For yield determination, a subsample of 400–500 g grain was taken from the continuous flow in the combine and cleaned. Grain moisture content and grain N concentration were then analysed using the near-infrared transmittance (NIT) method (InfratecTM 1241 Grain Analyzer, Foss, Denmark).

Leaf area index of oat sole crop was measured on 9–10 July 2019 and LAI of winter wheat sole crop on 26 June 2020. Measurements were made across the crop rows using a SunScan type SS1 sensor (Delta-T Devices Ltd., Burwell, England). Five measurements were made per plot and the average value per plot was estimated.

## 2.5. Preparation of modelling data

Soil texture and chemical properties were determined for one pooled sample per site, consisting of 12 subsamples covering the experimental area. Hydraulic properties were obtained from the APSIM soil database (APSIM Initiative, 2022) by comparing the impacts of different sets of soil hydraulic properties on crop growth, grain yield and soil water (see Supplementary Material (SM) 1).

Daily weather data for the period 1983–2020 on minimum and maximum temperature, precipitation and solar radiation were obtained from the closest weather stations, Glyttinge (Site1) and Fornåsa (Site2), 1.6 and 7.2 km, respectively, from the sites. If data were missing for one day, the average of five previous and five subsequent days was used. Longer periods of missing data were filled with data from the closest station with available data, mainly Norrköping weather station. During the calibration years, no data were missing. Data for Glyttinge and Norrköping were obtained from the Swedish Meteorological and Hydrological Institute (SMHI, https://www.smhi.se/data, latest access date: 1 December 2022), while data for Fornåsa was obtained from SLU Lantmet (https://www.slu.se/fakulteter/nj/om-fakulteten/centrumbi ldningar-och-storre-forskningsplattformar/faltforsk/vader/lantmet/).

Weather data for 2019–2020 were used for calibration against experimental data, while the whole dataset was used to generate 30 individual three-year weather datasets for scenario assessment (see Section 2.7.1).

## 2.6. Crop model set up and calibration

## 2.6.1. Crop management simulation

The crop management operations in the field experiments described above were replicated in the simulation set up. Some modifications were however needed. Fertiliser type was set to NO<sup>3</sup>-N. Starting populations of oats and winter wheat were set to 200 plants m<sup>-2</sup>, and for the SC to 80 plants m<sup>-2</sup>. The SC was sown at 1.5 mm depth, adjusted from the field depth to compensate for slow simulated germination. Defoliation of the SC, to simulate the effect of cutting at harvest of oats, was set to 20 September, to avoid cutting before oat harvest in any simulation. Defoliation was simulated as cutting of biomass with a residual dry matter (ResidualDM) content of 30 g m<sup>-2</sup>, which corresponds to 10–15 cm height in APSIM. Termination of the SC was set to occur 343 and 345 days after sowing at Site1 and Site2, respectively, using an end-crop command in APSIM. Service crop aboveground biomass was left as surface residues.

## 2.6.2. Crop calibration

Calibration was performed stepwise, in the order phenology, biomass and grain yield, for oats and winter wheat, using a trial and error approach by changing one parameter at a time (Seidel et al., 2018). The two clover species were considered a single species in APSIM for calibration of SC biomass, using the red clover module that was previously validated with Danish data (Cichota, 2022). The crops were first

calibrated as sole crops and then as intercrops, testing if light interception had to be modified. Field data for calibrating the cereals as sole and intercrops, and SC as intercrop, were obtained from the experiments as described earlier. An initial evaluation of red clover growth as a sole crop at northern latitudes was done using published data from three other experiments (Dhamala et al., 2017, 2018; Höök, 1993), before calibration against our intercropping data. Details of crop calibration can be found in SM2.

As few changes as possible were made to the starting parameters, and all observed data were used for calibration, as this increases calibration strength and ensures broad applicability of models calibrated with data from different environments (Brown et al., 2018; Raymundo et al., 2017). In our case, the small dataset also made it important to use all data for calibration. Oats and SC were calibrated starting from default parameter values, while winter wheat was calibrated starting from parameter values of a cultivar (Rosario) already calibrated for Northern Europe (Brown et al., 2022).

Calibration of phenology, yield and LAI of sole crop oats and sole crop winter wheat was performed by comparing observed data with simulation outputs. The biomass calibrations were evaluated by comparing observed and simulated values using model determinants (mean of simulated and observed biomass, adjusted R<sup>2</sup>, mean absolute error (MAE), relative root mean squared error (RRMSE)). The goal was to achieve adjusted R<sup>2</sup> > 0.7 and RRMSE <0.3.

#### 2.7. Cropping system scenarios

Two scenarios were created: (i) with and (ii) without a SC in the oatwinter wheat sequence (the latter used as control). The assessment period ran for 24 months, from sowing of oats in mid-April to when a third-year spring crop would normally be sown in mid-April two years later (Fig. 1). The assessment period included the oat growing period up to sowing of wheat, the winter wheat growing period of exactly one year, and a fallow period after winter wheat until spring of the next year.

## 2.7.1. Generating weather datasets

To better account for the annual variability in crop performance and soil processes caused by weather, and prevent conclusions being drawn based on specific weather events, 30 different combinations of weather data (not chronological) used in the simulation covering the scenario assessment period were generated based on the data extracted from 1983 to 2020 (Section 2.5) per site. No further modification of the data was done.

Before the assessment years, the model was initialised and run for 15



Fig. 1. Schematic timeline for the scenario assessment and the time points and ranges of data extraction. Length of crop periods: oats = 149 days, winter wheat = 365 days, fallow = 216 days.

years alternating oats and winter wheat without SC in order to stabilise soil water and pools of organic C and N, adjusting the water balance to precipitation and avoiding flushes of N in the assessment period. A 15year period was chosen because annual N mineralisation stabilised after this amount of time. All 30 weather datasets had the same initial 15 years of weather data, which were the 15 years prior to the calibration years in the original dataset, i.e. 2003–2017. Year 2018, the year just before the calibration, was however excluded due to an extreme drought in the region that year. The weather files and replicated scenario simulations were created in R Studio using the *apsimx* package (Miguez, 2022) and R version 4.2.2 (R Core Team, 2022), which was also used to run all simulations.

## 2.7.2. Assessment of outputs

The assessment of outputs was based on crop productivity, FOC input, and N and water dynamics in each scenario (Fig. 1). Crop productivity was assessed as main crop (oats and winter wheat) aboveground biomass and yield at harvest, and SC aboveground biomass at harvest of oats and at SC termination in spring. Organic matter input was assessed as average soil FOC at 0-35 cm depth at the end of the oat period (August-September) and at SC termination. In this system, FOC mainly represented C in dead root biomass, as aboveground residues were not incorporated into the soil. To assess how well N and water were utilised in the two scenarios, N and water uptake (from all growing crops) were compared with simulated losses of N and water, calculated as sums of all daily outputs over each period (Fig. 1). Losses of N were estimated as nitrate (NO<sub>3</sub>) leaching and gaseous N<sub>2</sub> and nitrous oxide (N<sub>2</sub>O) emissions, and water losses as drainage, runoff and evaporation. The proportion of N<sub>2</sub> fixation by the SC was also estimated, based on outputs of N<sub>2</sub>-fixation and uptake of soil mineral N (SMN) over the whole lifespan of the SC. The sum of N mineralisation and average daily soil water was estimated for four seasons: spring (March-May), summer (June–August), autumn (September–November) and winter (December-February).

#### 2.7.3. Statistical analysis

To test our hypotheses, the statistical significance of differences between scenarios with and without a SC was analysed for all considered output variables, using linear mixed effect models (lme4 package; Bates et al., 2022). Most data required power transformation according to the Box-Cox test (car package; Fox et al., 2022), but the appropriate power transformation varied depending on output variable. Transformations were needed for main crop biomass, regression between SC biomass and winter wheat biomass at both sites, regression between SC biomass and winter wheat yield at Site1, FOC, all nitrogen dynamics variables and all water dynamics variables except plant water uptake. The runoff data were still quite poor after transformation and hence these results should be interpreted with caution. Two outliers, one per site, that strongly affected the regression between SC biomass and oat biomass were removed from all analyses. Scenario and site, and if applicable period or season, were fixed effects, while simulation replicate (different weather datasets) nested in site was the random effect. Analysis of variance was performed using the Anova() function (car package). Pairwise comparisons between scenarios were made using the emmeans() function (emmeans package; Lenth et al., 2022). Visualisation was performed using the ggplot() function (ggplot2 package; Wickham et al., 2023).

## 2.8. Limitations of the study

In our paper we use APSIM, in its current form, to assess multiple ecosystem services and compare different cropping systems to show the potential of this approach, but also to highlight areas that need further development. Therefore, as much as possible, measured parameter values were used and only a minimum of crop calibration was done, to improve the most critical aspects of simulating the system based on our small dataset. Soil processes were not validated and, knowing they are not perfectly simulated, absolute values should be interpreted with caution. The focus is on the direction of change in the SC scenario, assuming that the model simulates these processes reasonably well. In the discussion we also relate the outputs to field observations and validations in other studies, and highlight potential model weaknesses.

#### 3. Results

#### 3.1. Crop calibration

Simulation of the phenological development of oats and winter wheat was improved by increasing the rate of early development and prolonging the maturation phase (Figure SM2.1, Table SM2.10). All three crop calibrations resulted in satisfactory simulation of biomass at the last sampling time (Fig. 2 and Table 2). However, to fit simulated final biomass to that observed of all simulated crops, crop parameters that overestimated biomass at previous sampling times had to be used, resulting in acceptable adjusted R<sup>2</sup> but a rather high RRMSE (Table 2). Excluding the first data points led to RRMSE <0.30 for most crops, while adjusted R<sup>2</sup> was slightly lower than desired, showed in parenthesis in Table 2. Since final biomass of the crops was the most important variable in scenario assessment, the calibration of the crops were considered satisfactory. Simulated yields were similar to observed yields or slightly overestimated at Site2, while at Site1 yields were underestimated (Table 2).

## 3.2. Assessment of cropping system scenarios

#### 3.2.1. Productivity of cereals and service crop

In the SC scenario, oat biomass production and yield were significantly reduced (p < 0.001), by approximately 4% and 12%, respectively, relative to the control scenario as a mean of all simulated years (Fig. 3ab). Winter wheat showed large variation in relative biomass and yield, ranging from a 50% increase to a 50% reduction. Winter wheat biomass was not significantly different between the two scenarios, but winter wheat yield was 14% higher in the SC scenario than in the control without SC (p = 0.01).

Service crop biomass did not differ by much between the two sites. At oat harvest SC biomass (mean and standard deviation over the 30 simulations) was 421  $\pm$  156 and 419  $\pm$  166 kg ha<sup>-1</sup> at Site1 and Site2, respectively. Before termination in spring, SC biomass was 989  $\pm$  399 and 924  $\pm$  289 kg ha<sup>-1</sup> at Site1 and Site2, respectively. There were no significant relationships between SC biomass and biomass and yields of oats (Fig. 3c-d). There was a significant positive relationship between SC biomass and winter wheat biomass at Site2 (Fig. 3e), while for yield the relationship was significant at both sites (Fig. 3f). Main crop productivity was higher at Site1, with clayey soil, than at Site2, with silty clay loam.

#### 3.2.2. Soil fresh organic carbon

The input of FOC at 0–35 cm soil depth at oat harvest was 19% and 15% higher (p < 0.001) in the SC scenario than in the control at Site1 and Site2, respectively (Fig. 4a). At SC termination in spring (winter wheat period) the difference was even greater, with 80% and 68% (p < 0.001) more soil FOC in the SC scenario than in the control at Site1 and Site2, respectively (Fig. 4b). The larger difference in FOC at termination could be because root biomass only becomes FOC when the plant dies, and at oat harvest FOC is mainly derived from oats.

## 3.2.3. Nitrogen dynamics

At Site1 (clayey soil), crop N uptake was slightly higher and N losses were lower than at Site2 (silty clay loam) (Fig. 5). Nitrogen uptake by all crops was 27 and 34 kg ha<sup>-1</sup> higher in the SC scenario than in the control scenario at Site1 and Site2, respectively (p < 0.001). Most of this N was utilised by the main crops, 91 ± 3% and 90 ± 2%, at Site1 and Site2, respectively. The SC obtained 75 ± 6% and 73 ± 7% of its N from N<sub>2</sub>-



**Fig. 2.** Observed versus simulated aboveground biomass (dry weight, DW) of oats and winter wheat as sole crops (top) and intercrops (bottom), and of the red clover service crop as intercrop in oats followed by winter wheat (data from May–October). The line within the boxplot represents the median value. Dots represent potential outliers. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

## Table 2

Model determinants, calculated as mean observed and simulated aboveground biomass (dry weight, DW), adjusted  $R^2$ , mean absolute error (MAE) and relative root mean squared error (RRMSE), and observed (Obs) and simulated (Sim) crop yield. Values in parenthesis are based only on observations in June and July for the cereals and in July, August and October for the service crop, i.e. excluding the first observations where biomass was greatly overestimated in simulations.

	Model determinants						Yield [Mg DW ha <sup>-1</sup> ]		
	Mean observed	Mean simulated	Adjusted R <sup>2</sup>	MAE	RRMSE	Site1		Site2	
Sole crop	[Mg DW ha <sup>-1</sup> ]	[Mg DW ha <sup>-1</sup> ]		[Mg DW ha <sup>-1</sup> ]		Obs	Sim	Obs	Sim
Oats	4.6 (6.7)	5.3 (7.3)	0.78 (0.62)	1.4 (1.2)	0.35 (0.22)	5.0	3.9	4.0	4.5
Winter wheat	3.4 (5.3)	4.6 (7.3)	0.88 (0.88)	1.3 (1.3)	0.48 (0.28)	7.6	8.2	6.2	5.9
Intercrop									
Oats	4.1 (6.0)	4.8 (6.8)	0.81 (0.63)	1.3 (1.1)	0.37 (0.24)	5.2	3.1	3.9	4.3
Winter wheat	3.2 (5.1)	3.0 (4.6)	0.90 (0.85)	0.72 (0.99)	0.37 (0.29)	8.1	6.7	6.3	5.1
Service crop	0.23 (0.41)	0.20 (0.34)	0.81 (0.71)	0.074 (0.13)	0.50 (0.39)				

fixation at Site1 and Site2, respectively, corresponding to approximately 100  $\pm$  50 kg N ha^{-1} at both sites. In oats, the difference in N losses between the SC and control scenarios was <10%. However, in the winter wheat period, the SC scenario leached 60% and 48% less NO<sub>3</sub> than the control at Site1 and Site2, respectively (p < 0.001), while gaseous emissions were 27% and 35% higher than in the control scenario at Site1 and Site2, respectively (p < 0.001). In the fallow period, leaching was 76% and 88% higher (p < 0.001), and gaseous emissions were 95% and 131% higher (p < 0.001), in the SC scenario at Site1 and Site2, respectively. Over the whole assessment period, difference in N losses were rather small, with about 22.5%, or 5 kg ha^{-1}, larger N losses in the SC scenario.

Nitrogen mineralisation was in general similar at both sites and in both scenarios, except in winter wheat during the second summer where it was slightly higher in the SC scenario (p < 0.01) (Fig. 6).

## 3.2.4. Water dynamics

In the oat period, crop water uptake at both sites was slightly higher (p < 0.001), and total water losses slightly lower, in the SC scenario compared with the control (Fig. 7). In contrast, in the winter wheat period, crop water uptake was slightly higher in the control scenario, but water losses were also higher. Evaporation was significantly lower in the

SC scenario at both sites (p < 0.001). In the fallow period, water losses were slightly higher in the SC scenario, mainly in the form of drainage losses. Losses via surface runoff were minor in all periods. Over the whole simulation period, water losses were 4% and 3% lower in the SC scenario compared with the control at Site1 and Site2, respectively. Hence, this difference could be considered negligible.

Volumetric soil water was not greatly affected by including a SC. In oats, soil water content was lower (p < 0.001) in Autumn1 in the SC scenario compared with the control scenario (Fig. 8). In winter wheat, on the other hand, the control scenario had less water in the soil profile in summer (p = 0.05). During the fallow period, soil water was recharged in both scenarios. The soil at Site1 held more soil water than that at Site2, but the seasonal pattern in soil water content was similar at the two sites.

#### 4. Discussion

#### 4.1. Crop calibration

Crop calibration for the APSIM NG model provided satisfactory simulations of biomass production aboveground at later sampling times for all three crops, in both sole crop and intercropping, and was



**Fig. 3.** (a) Aboveground biomass and (b) yield of oats and winter wheat grown as intercrops with a service crop relative to when grown as sole crop (control scenario) at the two sites. The line at y = 1 indicates biomass or yield in the control scenario. Small dots around the boxes indicate relative biomass/yield in each simulation (different weather data), while large dots indicate potential outliers. The line within the boxplot represents the median value. (c-f) Relationship between service crop dry weight (DW) biomass and main crop DW biomass (c and e) and yield (d and f), with regression lines. The grey area indicates the 95% confidence interval, and only significant linear regressions are plotted (p < 0.05).



**Fig. 4.** Fresh organic carbon (FOC) at 0-35 cm soil depth at (a) oat harvest (averages for August–September) and (b) service crop termination (31 March) in the two cropping scenarios at two sites. Small dots around the boxes indicate FOC in each simulation (different weather data), while large dots indicate potential outliers. The line within the boxplot represents the median value. SC = service crop scenario, Control = scenario without service crop.

therefore considered suitable for the purpose of scenario assessment. However, the model overestimated biomass production of cereals at early development stages (during leaf development and stem elongation). This could have affected the calibration of SC growth, as competition from oats would have been lower. Changing the specific leaf area of the simulated SC greatly improved the biomass simulation in July and August (Figure SM2.7, Figure SM2.8, Table SM2.7). The changes in temperature response and radiation use efficiency, were made to improve the simulation of the SC as sole crop (Figure SM2.5, Figure SM2.6), and the change in biomass partitioning resulted in better



**Fig. 5.** Fate of nitrogen (N) in different crop periods and scenarios, with losses divided into gaseous emissions ( $N_2$  and  $N_2O$ ), leaching ( $NO_3$ ) and N uptake by all growing plants at the two sites. SC = service crop scenario, Control = scenario without service crop. The line within the boxplot represents the median value, while dots indicate potential outliers.



**Fig. 6.** Sum of soil nitrogen (N) mineralisation at 0–35 cm depth in the different seasons of the assessment period. Spring = March–May, summer = June–August, autumn = September–November (winter season not shown due to low mineralisation). The grey dashed lines indicate the seasons to which crop periods belong. The line within the boxplot represents the median value, while dots indicate potential outliers. SC = service crop scenario, Control = scenario without service crop.

model accuracy (Figure SM2.8).

Similarly to our observations, Kumar et al. (2023a) found that APSIM Classic provided better simulations of biomass and N uptake by winter wheat grown in Denmark at a late growth stage (bolting) than during early development (tillering and stem elongation). The trade-off between precision in simulation of early and late biomass production could be due to the inability of the model to appropriately capture the long days in spring and summer (May–July) and the impact of diffuse light at high latitudes (Campbell and Aarup, 1989; Morel et al., 2020; Rodriguez and Sadras, 2007). Most of the crop cultivars available in APSIM are calibrated based on data on crops grown in Oceania (mainly Australia), where annual temperatures are higher, days during summer are shorter and diffuse light is less prevalent than in Northern Europe. However, early growth has also been overestimated by APSIM and DSSAT for crops grown in Germany (Knörzer et al., 2011a, 2011b), which could be because models have mainly been calibrated against data sampled at harvest. Similarly to our calibration process, Knörzer et al. (2011b) reduced the thermal time response and extended time to maturity to increase the speed of early development and prolong the grain filling period when adapting a German wheat cultivar in APSIM Classic. In our study, the partitioning of biomass between different plant organs was also not optimal, with underestimation of grain yield (Table 2) and overestimation of leaf biomass and LAI (SM 2). Knörzer et al. (2011b) improved grain and N yield simulations by increasing the rate of leaf senescence, but we did not have available data to justify such a change. However, the overestimation of leaf biomass and LAI in our simulations suggests that the model overestimated the proportion of biomass allocated to leaves, which has also been observed in other studies (Berghuijs



**Fig. 7.** Losses of water (drainage, evaporation and runoff) and water uptake by all growing plants in different crop periods and scenarios at the two sites. SC = service crop scenario, Control = scenario without service crop. The line within the boxplot represents the median value, while dots indicate potential outliers.



Fig. 8. Mean daily soil water content in the 0-100 cm soil profile in the different seasons of the assessment period (spring = March–May, summer = June–August, autumn = September–November, winter = December–February). The line within the boxplot represents the median value, while dots indicate potential outliers. The grey dashed lines indicate the seasons to which crop periods belong. The blue solid lines indicate soil field capacity (upper line) and wilting point (lower line). SC = service crop scenario, Control = scenario without service crop.

et al., 2021; Nelson et al., 2021). This might be due to Australian wheat cultivars (for which the model was initially developed) generally having lower harvest index than European cultivars (Hoogmoed et al., 2018; Porker et al., 2020; Pronin et al., 2020). Hence, further work to improve simulations of crops grown at northern latitudes should focus on the trade-off between early and late growth and biomass partitioning, especially with regard to leaves and heads. This would probably also have a positive effect on simulation of intercropping systems in both cases.

For winter wheat, simulated intercropping drastically reduced early growth, which generally improved model performance compared with winter wheat as sole crop, but this was not observed in the field. This disparity could be due to APSIM simulating intercropping based on the two crops being grown in the same row, while in the field experiments winter wheat was sown between the rows of the SC, as narrow-strip intercropping (Lagerquist et al., 2022). Hence, competition between crops was likely lower in the field than in the simulations, where the two crops were assumed to be perfectly mixed and competed directly for incoming solar radiation. Wu et al. (2021) solved this by introducing a small change in the script of the module used when simulating intercropping in APSIM Classic (Canopy) to take into account that the two crops grow in separate strips and hence do not compete directly for light. A comparison between the abilities of DSSAT and APSIM to simulate a wheat-maize intercrop found that DSSAT performed better, which was attributed to its shading algorithm (Knörzer et al., 2011b). Hence, simulations of both resource sharing and crop responses to interspecific competition need to be revised to improve simulations of multispecies interactions in APSIM.

## 4.2. Assessment of cropping system scenarios

## 4.2.1. Biomass and yield

The varying effect on relative yield depending on intercropping reflects observations from other studies. In some studies intercropping reduced main crop yield (Cheriere et al., 2020; Pridham and Entz, 2008), while others found similar or even higher grain yields, regardless of SC biomass (Blackshaw et al., 2010). Similar to our observations in the establishment year, Pridham and Entz (2008) reported that red clover sown in conjunction with winter wheat reduced grain yields by 12-34% depending on the year. In the experiments this study is based on, oat yields were generally not negatively affected (Bergkvist, 2021), but in other experiments using the same system but slightly different SCs we found both neutral and great negative effects on oat yields (Lagerquist et al., 2022). In our simulations, oat yield was always negatively affected, although sometimes by <5%. The relationship between SC biomass and oat biomass and yield was neutral, indicating that when the SC grew well there were often sufficient resources for the main crop to grow as well. Although the effects of SCs on winter wheat were predominantly positive, intercropping with SCs reduced winter wheat biomass and yield in approximately one-third of years. These results aligns well with the general pattern of leguminous SCs to most often increase yield of the subsequent crop in field studies (Shackelford et al., 2019). However, there is probably a bias in reporting positive effects of both intercropping and SC performances, with negative effects less likely to be reported. In the present experiments there were no significant effect of the SC on winter wheat yields (Bergkvist, 2021), but in previous experiments we have found effects ranging from positive to negative (Lagerquist et al., 2022), with negative effects being due to SCs surviving termination, something that never occurred in the model.

Service crop biomass varied greatly between years, as a result of weather conditions. Weather conditions are one of the main drivers of SC growth (Peterson et al., 2021; Vrignon-Brenas et al., 2016), leading to large annual variation in SC biomass production (Dorn et al., 2015; Leoni et al., 2022) and the competitive ability of crops grown in intercropping systems (Amossé et al., 2013; Blackshaw et al., 2010; Gabriel and Quemada, 2011). In the present study, the APSIM NG model and the approach of simulating the system with 30 different weather datasets managed to capture a realistic pattern of crop growth, although the specific weather-crop growth dynamics could not be verified.

The positive effect of SC biomass on winter wheat performance was greater at Site2 than at Site1. Site2 has a slightly poorer soil, with lower water-holding capacity, lower organic matter content and lower pH compared with the soil at Site1. Similarly, field studies have shown that on less fertile soils, leguminous SCs generally have a more positive effect on performance of the main crop (Plumhoff et al., 2022; Sjursen et al., 2012). Combining legumes and non-legumes has been shown to have the highest overall productivity on soils with high fertility (Plumhoff et al., 2022), and this was reflected in our scenario assessment since biomass production of all crops were slightly higher at Site1.

## 4.2.2. Soil fresh organic carbon

As expected, intercropping with SCs increased FOC inputs to the soil, especially at termination when the SC had been growing for a longer time. However, there was quite large variation in soil FOC between years. The range of simulated FOC was in line with mean annual C sequestration from SCs in agricultural soils ( $320 \pm 80 \text{ kg C ha}^{-1}$ ) according to a meta-analysis by Poeplau and Don (2015). However, not all FOC enters the more stable C pool, since some are lost by microbial respiration during different breakdown cycles (Dynarski et al., 2020), but root-derived organic matter, what FOC mainly constitute of, is the main contributor to soil organic matter (Kätterer et al., 2011).

The C pool in the soils only stabilised during model calibration if the initial C content was set to 8–9.5% (SM 1). In Swedish agricultural soils the C content is often much lower, around 2–3% (Eriksson, 2021). Running simulations with higher annual temperatures than in Sweden

(APSIM examples for oats and winter wheat simulated in Australia, data not shown), this problem was not observed and soil C stabilised at similar initial C levels as measured in our experiments. APSIM Classic has been shown to capture long-term C dynamics in Australian cropland and grasslands with good accuracy (Luo et al., 2011; O'Leary et al., 2016), but Vogeler et al. (2019a) found that outputs on N release agree poorly with observed data from Danish cropping systems. This indicates that decomposition of organic matter is poorly simulated in colder regions and outputs related to organic matter decomposition needs to be interpreted with care. APSIM uses first-order kinetics to simulate organic matter turnover (Probert et al., 1998), which are commonly used in crop models but are vulnerable to overestimation of soil organic matter stocks (Campbell and Paustian, 2015).

## 4.2.3. Nitrogen dynamics

Over the whole simulation period, the difference in N losses between the two scenarios was small (5% larger losses in the SC scenario). However, the scenario that was best in preventing N losses varied depending on crop period, especially for leaching losses, which were lower in the SC scenario in winter wheat but higher in the SC scenario during the fallow period. Studies in the field (De Notaris et al., 2018; Vogeler et al., 2019b) and in microcosms (Fernandez Pulido et al., 2023) have shown that living leguminous SCs reduce NO<sub>3</sub> leaching compared with bare soil. However, when leguminous SCs die off and decay, the SMN pool immediately starts to increase (Amossé et al., 2013; Bergkvist et al., 2011), which may increase both leaching and gaseous emissions (Olofsson and Ernfors, 2022; Storr et al., 2021). Hence, gaseous emissions and leaching both need to be reduced in this system to make leguminous SCs a more robust practice for N management. Residual effects of SCs in terms of N leaching can be managed by keeping the period during which no crop is growing at a minimum. Nitrous oxide emissions are more difficult to target, but could be reduced by improved soil structure and soil aeration (Robertson and Groffman, 2015). Soil structure could be improved e.g. by growing deep rooted crops (Ball et al., 2005), promoting earthworm activity (Kim et al., 2017), and reducing traffic-induced soil compaction (Schjønning et al., 2002).

## 4.2.4. Water cycling

The SC scenario gave lower water losses than the control scenario, in both oats and winter wheat. The lower losses with SCs in these periods were mainly due to reduced evaporation. In oats, larger water uptake by oats and SC also contributed to lower losses. In winter wheat, lower soil water content at the start of the winter wheat period also contributed to lower water losses, as the two scenarios had similar plant water uptake during this period. In the fallow period, drainage amount was larger in the SC scenario compared with the control scenario, probably due to the greater soil water content in the SC scenario at the start of the fallow period. Almost no runoff occurred in our simulations, due to efficient infiltration. In conditions where runoff is a problem, living SCs have been shown to efficiently reduce water losses via runoff (Griffith et al., 2020; Machiwal et al., 2021; Muñoz-Ventura et al., 2022). However, others have seen no effects of SCs on the amount of runoff (Gongora et al., 2022) or increased runoff losses when the SC causes greater snow accumulation (Weyers et al., 2021). Frost-killed SCs are poor at reducing runoff (Muñoz-Ventura et al., 2022), so in areas where frost can be expected and runoff risks are large, it is necessary to choose frost-tolerant SCs to substantially reduce runoff risks.

A common concern regarding cultivation of SCs is that they may deplete the soil of water. In this study, an effect of the SC in soil water depletion was only observed after the first summer, while from autumn until the following spring soil water storage was recharged despite SC biomass almost doubling. Similarly, other modelling studies have observed soil water recharge after termination of a wheat SC, with similar or slightly higher soil water content during the growing period of the subsequent main crop (cotton, maize or soybean) and maintained crop yields (Himanshu et al., 2022; Yang et al., 2020). In our simulation study, volumetric soil water content varied more within than between the scenarios, indicating that weather-year had a larger impact on soil water than scenario. Even in a dry year, the SC did not have a large effect on soil water compared with the control. Hence, growing SCs at sites similar to those in this study does not seem to greatly reduce soil water content as long as there is a period of soil water recharge.

# 4.3. Using APSIM to assess ecosystem service delivery from cropping systems

We used APSIM NG to assess processes related to crop productivity, C input to the soil, and N and water dynamics in two cropping systems, with and without inclusion of a SC in an oats-winter wheat sequence. These output variables were chosen as they represent important processes of key ecosystem services and disservices in crop production. We compared point estimates, cumulative values or average flows, but the model could also be used to compare differences in daily flows over years or specific periods, or to calculate N or water use efficiency, as done by Ma et al. (2022). APSIM also provides information on different N forms and simulates daily rates of transformation between different N pools, which could be valuable when assessing measures to mitigate different N losses, or management of SCs as green manures. However, for reliable detailed assessments of N dynamics under cold temperate conditions, the decomposition module in APSIM needs to be improved (Vogeler et al., 2019a).

Mechanistic models have great potential for long-term assessments of cropping systems, provided that simulations of organic matter decomposition are reasonable. APSIM also simulates microbial C and N pools, which increase with increasing organic matter resources. However, these pools only reflect what is sometimes called active C and N, and not the soil microbial community (Maharjan et al., 2018), which varies in functionality depending on management practices, such as type of tillage and use of SCs and organic amendments (Martínez-García et al., 2018; Schmidt et al., 2018). Moreover, conventional farming systems, which are often the basis for model development, are generally poorer at supporting soil microorganisms than organic farming systems (Banerjee et al., 2019; Lori et al., 2017; Lupatini et al., 2017). With growing understanding of the importance of the microbial community and its contribution to sustainable agriculture (Bender et al., 2016), crop-soil-atmosphere models should preferably take these into account to a greater extent and on a more detailed level. This could be done e.g. by distinguishing different functional groups or taxa of the microbial community and assigning them different decomposition rates or other functions (Crowther et al., 2019), and by acknowledging that management practices affect different soil organisms differently (Li et al., 2020). Similarly, APSIM does not take into account changes in soil physical properties over time, preventing appropriate evaluation of management practices that have an impact on these (Maharjan et al., 2018; Peng et al., 2022).

As the type of SC species used may vary with the service required, e. g. legume or non-legume, and with their suitability for a specific location in terms of e.g. growth and winter hardiness, many different SC modules may be needed to cover the range of functions and growth conditions. Crop modules in APSIM consist of many parameters that can be adjusted to specify cultivar growth on a very detailed level, which allows calibration of locally used cultivars. It also means that many individual crop modules with several cultivars need to be developed to meet the diversity of crops that are used, which is both costly and time-consuming. Currently it is common to use crop modules for main crops to also simulate SCs, e.g. Vogeler et al. (2019a) used the oilseed rape module to simulate fodder radish with APSIM, Gupta et al. (2022) modified the wheat module in DSSAT to better tolerate cold temperatures for simulating cereal rye. In contrast, STICS can simulate several commonly used SCs, fodder radish, cereal rye and mustard, with good accuracy in French cropping systems, for which the model has been thoroughly tested (Coucheney et al., 2015). An alternative to developing speciesand cultivar-specific modules in APSIM and DSSAT would be to focus on certain functional characteristics of SCs that are important for the delivery of specific services. APSIM NG currently includes modules for oilseed rape, chicory, cereals (except cereal rye) and perennial clovers that could be used for simulating SCs. Developing modules for herbs without a taproot, cereal rye, non-cereal grasses and annual clovers would be useful to better cover the common types of SCs used today.

## 5. Conclusions

The calibrated crop modules in this study simulated the crops grown, both as sole crops and in the intercropping system, with reasonable accuracy. Short-term assessment of services (crop productivity, C inputs, N and water dynamics) showed that the SC generally had a positive effect on the cropping system, improving yield of subsequent winter wheat, increasing C inputs and reducing water losses in both crops. However, these effect varied substantially depending on prevailing weather conditions. Over all simulations, the negative effects were rather small, such as a slight reduction in oat yield and increase in N losses. The results indicated a larger build-up of the soil N pool by the SC, leading to larger N losses in the fallow period from autumn until spring after winter wheat. Hence, future studies on SC cultivation should consider long-term N leaching and investigate options where the soil is never left without vegetation, or growing mixtures that provide more recalcitrant residues. Further work is also needed to improve simulation of organic matter decomposition at northern latitudes, to better reflect the dynamics of both C and N, and simulation of early biomass production and biomass partitioning in the crops, to improve the model's ability to simulate intercropping systems. Improving the ability of process-based crop models to simulate intercropping systems, especially with regards to crops grown in different rows, can increase understanding of interactions of these complex systems, due to the detail with which these models can simulate crop-soil-atmosphere interactions.

### CRediT authorship contribution statement

**Elsa Lagerquist:** Writing – original draft, Visualization, Methodology, Formal analysis, Data curation, Conceptualization. **Iris Vogeler:** Writing – review & editing, Supervision, Methodology, Conceptualization. **Uttam Kumar:** Writing – review & editing, Supervision, Methodology, Conceptualization. **Göran Bergkvist:** Writing – review & editing, Supervision, Funding acquisition, Conceptualization. **Marcos Lana:** Writing – review & editing, Supervision, Methodology, Conceptualization. **Christine A. Watson:** Writing – review & editing, Software, Methodology, Conceptualization. **David Parsons:** Writing – review & editing, Supervision, Methodology, Formal analysis, Conceptualization.

## 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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#### Appendix A. Supplementary data

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