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Highlights

- Sustainability of converting grassland to arable depends on soil workability
- Workability and trafficability is controlled by weather and soil type
- Low probability of successfully sowing winter wheat in converted lands in SW UK
- CO_2eq emissions from the converted arable land are higher than those from grassland
- Soil carbon stocks decline after conversion under current and future climates

Graphical Abstract

CONTEXT

Adapting to changes in climate and in consumer demand for commodities will force us to diversify land uses from the current status. Livestock grazing systems are dominant agricultural practices in the western regions of the British Isles. It has been suggested that grasslands in the region could be converted to other land uses, e.g. growing of cereal crops. We hypothesized that soil workability and trafficability would be important factors determining the feasibility and environmental impact of such conversion.

OBJECTIVE

Objectives were 1) to investigate the impacts of weather conditions under the current (baseline) climate on agronomic management and crop yield of winter wheat using the SPACSYS model; and 2) to assess potential impacts of the land use conversion (grassland converted into arable land) on the environment under soil conditions representative of the region under baseline and future climatic conditions.

METHODS

Using simulation modelling we investigated the impacts of baseline and future climates under the Representative Concentration Pathways (RCP2.6, 4.5 and RCP8.5) on soil workability and trafficability at sowing and harvest respectively of winter wheat and its consequences for crop productivity and key indices of environmental sustainability for three major soil types of the region.

RESULTS AND CONCLUSIONS

Under baseline and future projections, the probability of successfully sowing winter wheat on these soils was between 38 and 76%. Simulations showed that grassland conversion to arable in the region would not be sustainable in terms of carbon sequestration with a decline in soil carbon stock of 165 – 280 kg C ha^{-1} yr^{-1} on average over the simulation period. Rates of decline were greater when soil workability was taken into consideration. Although CO_2eq emissions from silage–based grassland soil were higher than those from the converted arable land, these were offset by the greater net productivity of grassland making it a larger net sink for carbon. When soil workability at sowing was considered, the NUE_{crop} (crop N content/N fertilizer applied) for winter wheat was lower than that for perennial ryegrass on all soil types under the baseline climate and RCP2.6, but comparable or greater under RCP4.5 and RCP8.5. In terms of C sequestration, grassland conversion for production of winter wheat is unsustainable under these soil–climatic conditions.

SIGNIFICANCE

Our results demonstrated that soil workability is a major factor influencing the potential impact of land-use conversion in clay soils and a wetter climate.

Projected climate effects on soil workability and trafficability determine the feasibility of converting permanent grassland to arable land

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Key words: modelling; SPACSYS; land–use conversion; soil workability; winter wheat

1 Introduction

Changes in climate and in consumer demand for commodities such as meat versus plant–based food, low environmental footprint goods and other ecosystem services are likely to drive changes in agricultural land use over the next few decades. Research has suggested that, if unabated, future climate change could push arable cropping in the UK further north and west, with the east and southeast unable to support crop production by the end of the century (Godfray et al., 2018; Ritchie et al., 2019).

Not only would agricultural practice be expected to respond to the changing climate, it may also contribute to strategies for mitigating against global warming. The UK government has pledged to achieve net zero carbon (C) emissions by 2050 (UK Committee on Climate Change, 2019) and one of the actions to be taken is to reduce greenhouse gas (GHG) emissions, especially methane from ruminant animals and N_2O from added nitrogen (N) fertilisers and by encouraging farmers voluntarily to improve practices in soil and land management. One option is to free up grassland (and also arable land producing livestock feed) for other purposes. In England, the area of arable land has been increasing and that of permanent grassland decreasing over recent years (Tomlinson et al., 2018), indicating the conversion of grassland to other land uses. Winter wheat is the highest yielding cereal crop in the UK with average farm yields ranging from 7.0 to 9.0 Mg ha^{-1} over last five years (Defra, 2021). From a productivity point of view, therefore, it is an attractive arable crop to grow for those considering conversion of land use. However, wet conditions affect soil workability and reduce the number of machinery work-days, potentially impeding a shift to arable cropping systems (Olesen and Bindi, 2002).

Livestock grazing systems are the dominant agricultural practices in the SW of the UK. To date, the opportunities for, and limitations to, converting permanent grassland to arable production in this region have not been explored to any great extent. The characteristics of the main agriculturally managed soils in the region do not inherently exclude production of arable crops. However, the production of high yields of arable crops hinges on the ability to establish the crop successfully and to conduct management operations such as the application of inputs (fertilisers and crop protection treatments) and harvesting in a timely manner. As such, an important step in evaluating the potential for converting permanent grassland to arable production is the assessment of the land's suitability for field management activities. Trafficability is the capability of the soil to support operations of agricultural machinery without causing significant structural damage or compaction. Workability is the ability of the soil to support tillage operations. Soil physical properties, especially topsoil and subsoil textures, weather conditions, prior soil water content and ground pressure from machinery (Bibby et al., 1982; Müller et al., 2011), largely determine the limits to workability and trafficability. In arable land, unsuitable soil conditions during the sowing or harvest periods might decrease grain yield if sowing or harvest are delayed or cause complete crop failure if they are prevented entirely. Various indicators have been proposed in previous studies to predict trafficability and workability, including soil moisture deficit and soil moisture content (Obour et al., 2017) alone or in combination with amount of recent precipitation (Kolberg et al., 2019). Although workability by tillage is affected by soil being too dry or too wet, excess water is the main reason in the context of the UK climate and is the major factor limiting trafficability (Armstrong, 1986). In the IPCC sixth report, it was concluded that changes in the climate system will become more extreme including heavy precipitation events (IPCC, 2021), which could further reduce opportunities for working soil. However, using land capability assessments based on soil wetness risks to workability and trafficability it was concluded that areas of SW Scotland, currently unsuitable for arable cropping, may become suitable in the future (Brown, 2017). Brignall and Rounsevell (1995) investigated the effects of step changes in temperature and rainfall on land suitability for wheat production in England and Wales using indices of drought and soil moisture limitations on trafficability. Their findings suggested that suitability for wheat production in the SW of England will depend more on the effects of climate change on rainfall than temperature. However, neither of these studies involved the use of process-based models of crop growth and resource capture and thus do not account for the possible effects of a changing climate on crop growth and phenology, nor on the effects of land use change on indices of environmental sustainability such as soil C stocks and GHG emissions.

Modelling is an effective tool to assess whether proposed land–use changes/conversions are sustainable in the long–term. The SPACSYS (Soil–Plant–Atmosphere Continuum SYStem) model, a weather–driven and process–based agricultural model with various time steps (up to daily) (Wu et al., 2007; Wu et al., 2015; Wu et al., 2019), is able to simulate arable and grassland production systems. The model has been calibrated and validated for winter wheat under UK regional climates and soil types (Bingham and Wu, 2011; Wu et al., 2019) and other locations (Liang et al., 2018; Liu et al., 2020; Zhang et al., 2016) and proved to be effective in simulating crop growth and the dynamics of soil water fluxes, C and N stocks, and N_2O emissions (Wang et al., 2019). In addition, all components of the model have previously been calibrated and validated for grassland production systems in SW England (Carswell et al., 2019; Li et al., 2017; Liu et al., 2018; Wu et al., 2016).

The aim of the current study was to determine the feasibility of converting permanent grassland to winter wheat production on contrasting soil types in the SW of the UK and to investigate the consequences of restrictions imposed by soil workability and trafficability on the environmental sustainability of such a conversion in land use. To use the SPACSYS model for this, we first needed to calibrate and validate it for wheat production in SW

England. Specific objectives then were: 1) to investigate the impacts of weather conditions under the current (baseline) climate on agronomic management and crop yield of winter wheat using the SPACSYS model; and 2) to assess potential impacts of the land use conversion (grassland converted into arable land) on the environment in terms of the GHG emissions, N leaching and soil C sequestration under soil conditions representative of the region under baseline and future climatic conditions.

2 Materials and methods

2.1 The SPACSYS model

The SPACSYS model has been described elsewhere (Wu et al., 2007; Wu et al., 2015; Wu et al., 2019) so here the main characteristics are summarised. The model includes a plant growth component, N and P cycling components coupled with a C cycling component, a water component, which includes the representation of water fluxes downwards through the soil layers, surface runoff loss and evapotranspiration, and an energy transformation component. In the plant component, the following processes are included: plant phenology, assimilation, respiration, and partitioning of photosynthate and mineral nutrients from uptake, N fixation for legume plants, and root growth and development. In addition, the impacts of the atmospheric CO_2 concentration on photosynthesis and transpiration are implemented (Yin, 2013). Soil N and C cycling covers organic matter decomposition, N mineralization, nitrification and denitrification, including estimation of gaseous N (NO, N_2O and N_2) emissions based on substrate content in the soil, environmental conditions (especially soil water content), transformation processes from ammonium to N_2O, and gas diffusion (Wu et al., 2015). A component to estimate rates of production, oxidation, diffusion, plant transport and ebullition of methane (CH_4) is also included in the model for soil CH_4 emissions. The Richards equation for water potential and Fourier's equation for temperature are used to simulate water and heat fluxes, which are inherited from the SOIL model (Jansson, 1991) in which the Hooghoudt drainage flow equation with modification is adopted for the subsurface drainage flow.

2.2 Model calibration and validation

All components of the model have previously been calibrated and validated for grassland production systems in SW England. Specific parameters relating to soil C and N cycling (Table A.1.) and parameters relating to ryegrass growth (Table A.2.) were adopted from previous studies at the investigated site.

The data used for model calibration and validation for wheat production were from an experiment carried out in 2016–17 (Sánchez-Rodríguez et al., 2018) on a free–draining Dystric Cambisol of the Crediton series (Avery, 1980) with a clay loam texture (FAO classification) at Rothamsted Research–North Wyke (50°79′40′′N, 3°95′25′′E, e.a.s.l. 180 m), southwest of England, with a temperate climate. The average annual temperature is 10.1℃ and annual precipitation 1033 mm, with a minimum of 705 mm and a maximum of 1361 mm between 1982 and 2016. Over 60% of the average annual precipitation falls in the winter period (October – March). Specifically, the relevant soil, plant and gaseous emission data from the zero-N control and the N fertiliser response treatment (ammonium nitrate fertiliser applied at 150 kg N ha^{-1} split into 3 applications between March and April) were used for model calibration and the digestate application treatment (anaerobic digestate from food waste supplying 150 kg ha^{-1} of available N) for model validation. Model calibration focused on the dates of phenological stage (emergence, anthesis and physiological maturity), partitioning of photosynthates and plant N uptake, soil moisture (at three depths), and dry matter and N content for different plant organs. In addition to these variables, N_2O emissions were used for model validation. Monitored dates on emergence, anthesis and physiological maturity of winter wheat were used to adjust the required accumulated temperatures between critical stages, using the error–prone method. Numerous simulations were run, changing the parameters that control the phenological development of winter wheat (requirement for accumulated temperatures) until the differences between the simulated and observed dates were within three days, which was considered as acceptable. The procedure adjusted the date of seedling emergence first, then the date of anthesis and finally that of physiological maturity. Other parameters were optimised by the Shuffled Complex Evolution Metropolis global optimization algorithm that has been implemented in the model package (Vrugt et al., 2003). After calibration, the model was run for the digestate application treatment from Sánchez-Rodríguez et al. (2018) with the calibrated parameters and the simulation results were used for validation against the experimental observations.

2.3 Simulation scenarios

Workability and trafficability were assessed based on the water content of the topsoil in soils typical of the SW of the UK. Following Dexter and Bird (2001), the upper wet tillage limit (θ_{crit}, kg kg^{-1}) was defined as:

$$\theta_{crit} = \theta_{infl} + 0.4 \times \left(\theta_s - \theta_{infl}\right) \quad (1)$$

where θ_s is the saturated soil water content (kg kg^{-1}) and θ_{infl} is the water content (kg kg^{-1}) at the point of inflection of the van Genuchten equation (van Genuchten, 1980) and calculated by:

$$\theta_{infl} = (\theta_s - \theta_{res})\left(1 + \frac{1}{m}\right)^{-m} + \theta_{res} \quad (2)$$

where m is a parameter that governs the shape of the pF curve with the van Genuchten equation and is derived from the pore size distribution index estimated based on soil texture with the pedotransfer functions of (Saxton et al., 1986) and θ_s is the residual water content (kg kg^{-1}).

To predict the impacts of climate change on winter wheat and ryegrass, the daily bias-corrected weather data for three future (2021 – 2100) climate scenarios and the baseline climate (1921 – 2000) based on the HadGEM2-ES model (Collins et al., 2011; Jones et al., 2011) were downloaded from the Inter-Sectoral Impact Model Intercomparison Project (www.isimip.org, Arneth et al., 2017). As the focus of this study was to investigate the feasibility of land use conversion, we only used data generated by the first realization, initialization, and physics (r1i1pi) of the climate model without considering its uncertainty. The future climate scenarios were Representative Concentration Pathway (RCP) 2.6 (very low emissions, RCP26 thereafter), 4.5 (an intermediate scenario, RCP45) and 8.5 (high–emissions, RCP85) (van Vuuren et al., 2011). The downloaded data were then downscaled to the site based on geolocational information using the R 'ncdf4' package (R Core Team, 2021). The atmospheric CO_2 concentration was kept at a constant 400 ppm under the baseline scenario (1921–2000) but was set to 402 ppm initially in 2020 and increased progressively to 454, 548 and 924 ppm for RCP26, RCP45 and RCP85 in 2100, respectively. A summary of the precipitation and temperature over the period for each climate scenario and the baseline climate is given in Table 1. The climate data showed greater precipitation and more heavy rain (daily precipitation > 20 mm) days per year in the future scenarios than those under the baseline.

To assess the suitability of the land–use conversion under the baseline and future climatic scenarios, we designed five simulations to compare permanent ryegrass with continuous wheat production where there were no soil moisture restrictions on workability and trafficability at sowing and harvest, where there were restrictions at just sowing, just harvest, or both sowing and harvest. The simulations were as follows:

1) permanent ryegrass in the field (S0 thereafter), with the assumption that grass is cut for silage three times in a year (normal grass management in the research region): mid–May, mid–July, and the end of September (we assumed that soil moisture conditions would not affect the harvesting dates as trafficability is not normally restricted in the summer months);
2) winter wheat as a continuous cropping system following the initial ploughing out of grassland, assuming the same agronomic management strategies as for the ammonium nitrate treatment (150 kg N ha^{-1}) of the field experiment (Sánchez-Rodríguez et al., 2018) but harvesting when physiological maturity is reached; no soil moisture restrictions (S_{con} thereafter);
3) as for S_{con}, but with the sowing date varied each year according to soil moisture conditions (sowing only permitted when soil moisture content is lower than θ_{crit}); no restrictions on harvest (S_{sow} thereafter);
4) as for S_{con}, but with the harvest date each year determined by soil moisture content at physiological maturity of the winter wheat (harvesting only permitted when soil moisture content is lower than θ_{crit}); no restrictions on sowing (S_{harv} thereafter);
5) as for S_{con}, but with both sowing and harvest dates each season set according to soil moisture conditions ($S_{sowharv}$ thereafter).

Most commercial cultivars of winter wheat currently available are sown in October in England. Considering the requirement for vernalisation and a high yield potential, sowing should not be after December. We assumed that planned field management (sowing or harvesting) has to be postponed until soil water content is less than the upper wet tillage limit (θ_{crit}) for more than three consecutive days. If there is no suitable date for sowing by the end of December, then there will be no winter wheat grown in the season. If there is no suitable date for harvesting by the end of October, then it was assumed there is no grain yield for the season.

For all scenarios, initial soil conditions were set to the same values as the measured data in the field experiment (Sánchez-Rodríguez et al., 2018) and the same wheat cultivar was assumed. The field was ploughed before the sowing season in the first year of conversion to arable land for simulations 2–5, while ryegrass was grown continuously for simulation 1. Ploughing was assumed to occur a week earlier than the planned sowing date and no earlier than 1st of October each year, based on weather conditions. The sowing date referred to in this paper, therefore, is the date at which ploughing and seedbed preparation for sowing occurred. The harvesting date each year was determined by the simulated grain maturity date. For S_{harv} and $S_{sowharv}$, however, the latest permissible harvesting date was the end of October in the growing year. If no winter wheat was sown in a growing season, then neither ploughing occurred nor fertiliser was applied over the season and the soil remained bare. The simulations were run with ammonium nitrate fertiliser applications. Fertiliser application rates and timings were identical to those in the field experiment. In order to compare the change in land-use independently of N fertiliser application rate, the total N fertiliser application rate for the grassland was the same as that for the converted arable land but the application timings followed local practice (early March, May, June and July with 35, 20, 20 and 25% of the total annual application, respectively). This represents a moderate to relatively low N input for each system (AHDB, 2020). Finally, as equal application rates for grass and wheat may be considered an unusual practice, additional simulations were run under the baseline climate condition with the full recommended application rate (300 kg N ha^{-1}) and timings (monthly between March and August) for grass silage (AHDB, 2020).This was to evaluate the sensitivity of sustainability indices (below|) to N applications over the range moderate (150 kg N ha^{-1}) to high (300 kg N ha^{-1}).

To investigate the influence of soil type on workability, soil C sequestration capacity, GHG emissions and yield under different weather conditions, three soil types were selected: a free–draining Eutric chromic endoleptic cambisol of the Crediton series, the soil type in which the field experiment was carried out; a well–drained Stagni–eutric cambisol of the Hallsworth series; and slowly permeable Stagni–vertic cambisol of the Denbigh series (Avery, 1980). The Hallsworth and Denbigh series account for 11 and 1.5% of grassland in England and Wales, respectively (Cranfield University, 2022). Given the information in Table A.3, θ_{crit} was set to 0.28, 0.30 and 0.30 m^3 m^{-3} in the top 15 cm soil layer for the Crediton, Hallsworth and Denbigh soil types, respectively. All other inputs and management practices described above were set the same for the different soil types. A total of 60 simulations were run across the combinations of climate, soil type and land use, and each simulation ran 80 years (2021 – 2100 for the future scenarios or 1921 – 2000 for the baseline) continuously.

2.4 Indicators for sustainability

We considered sustainability in agriculture to be the development of technologies and practices that lead to improvement in food productivity but do not adversely affect environmental functionalities (Pretty, 2008). There are numerous indictors under the envelope of sustainability. In this study, we used crop yield and its annual variability as an indicator for production sustainability and the following three indicators for environmental sustainability: i) Nitrogen use efficiency (NUE_{crop}; Congreves et al., 2021) defined as harvested N in above–ground biomass as a percentage of total N–fertiliser input in a growing year, ii) the rate of change in soil C stock, iii) annual gross primary productivity (GPP) from plants, and iv) annual total soil GHG emissions, expressed as CO_2 equivalent (100 years)

(CO_2eq) to compare the two systems (i.e. permanent ryegrass vs. any one of the continuous winter wheat scenarios). CO_2eq was calculated as:

$$CO_2eq = CO_2 + 273 \times N_2O + 27 \times CH_4 \quad (3)$$

where CO_2, N_2O, and CH_4 are annual emissions from a soil, and 265 and 28 are the 100–year global warming potential for N_2O, and CH_4-non fossil from the sixth assessment report of the International Panel on Climate Change (Forster et al., 2021), respectively.

Average annual GPP was derived from the average annual C fixation over the simulation period for each climatic scenario. The average grain yield of winter wheat and NUE_{crop} over the simulation period were calculated over all years. When soil conditions prevented a crop being sown or harvested, the yield for that year was recorded as zero and included in the average.

2.5 Statistical analysis

Two groups of diagnostics for evaluating process–based models described by Smith et al. (1997) were used for statistical analysis of model validation: the goodness–of–fit and the bias. To assess the goodness–of–fit between simulated and observed data, the lack of fit (LOFIT) F–test was used for the variables with measurement replicates (dry matter and N content of wheat aboveground organs) or the normalised root mean square error (nRMSE, %) together with the modelling efficiency (EF, optimum value equal to 1) and the coefficient of determination (CD , $0 \leq CD < +\infty$) that was defined by Loague and Green (1991) for those without replicates (soil moisture, gas emissions in this study). CD values can be greater than 1, which indicates that the model describes the measured data better than the mean of the samples. The bias in the total difference between simulations and measurements was expressed by the relative error (RE) and the correlation coefficient (r, $-1 \leq r \leq 1$) was used to demonstrate how well the shape of the simulation matches the shape of the measured data. The diagnostics of the first group are calculated as:

$$\mathrm{nRMSE} = \frac{100}{\overline{O}}\sqrt{\frac{\sum_{i=1}^{n}(S_i - O_i)^2}{n}} \tag{4}$$

$$\mathrm{EF} = \frac{\sum_{i=1}^{n}\left(O_i - \overline{O}\right)^2 - \sum_{i=1}^{n}(S_i - O_i)^2}{\sum_{i=1}^{n}\left(S_i - \overline{O}\right)^2} \tag{5}$$

$$\mathrm{CD} = \frac{\sum_{i=1}^{n}\left(O_i - \overline{O}\right)^2}{\sum_{i=1}^{n}\left(S_i - \overline{O}\right)^2} \tag{6}$$

where O_i are the observed data, S_i are the simulated values, $\bar{O}$ is the mean of the observed data and n is the number of samples.

3 Results

3.1 Model calibration and validation

Statistical indicators for model performance for the winter wheat at both the calibration and validation stages are shown in Table 2. Simulated soil water content agreed well with measured values for both calibration and validation, with relative errors < 10% and the correlation coefficients > 0.73. Goodness–of–fit indicators suggest that the simulated values better describe the trend in the measured data (EF>0) and the model slightly over–estimated soil water content (CD < 1.0) at the calibration stage whilst under–estimating at the validation stage (CD > 1.0).

Similarly, there was good agreement between simulated and measured values of accumulated dry matter and N content in various wheat organs. The exception was the simulated N content in stems at the validation stage, where F values for the lack of fit F–test were lower than the critical value at P=0.05, indicating that it did not simulate well. A comparison of the dynamics of the simulated and measured aboveground dry matter and N content is shown in Fig. A.1.

Of all checked variables, simulation of the N_2O emission rate was the least satisfactory (Table 2). However, the dynamics of the simulated emission rate follow the trend of the measured rate (Fig. A.2) and the simulated and observed cumulative N_2O emissions over the measured period compared well (481 vs. 431 g N ha^{-1}).

3.2 Workability and trafficability

Workability and trafficability under the various climatic conditions for the different soils is presented in Table 3. Under the baseline climate conditions, seeding (by the end of December; S_{sow}) succeeded in just 62% of the growing seasons for the Denbigh soil which was the highest success rate among the soil types. The lowest seeding success rate for all soil types was under the RCP26 scenario, with only a 38% success rate for the Hallsworth soil. Without soil restrictions on sowing (S_{harv}), harvesting success was greater than 94% in all scenarios (Table 3). When both sowing and harvest restrictions were included ($S_{sowharv}$), the success rate mirrored that of the sowing restriction only (S_{sow}) in 9 of the 12 soil–climate scenarios. However, on the Denbigh soil under the RCP85 scenario, the success rate fell to 28% when soil wetness restricted both harvesting and seeding compared to 71% when only seeding was restricted.

3.3 Sustainability indicators

Average grain yields of winter wheat for each soil type under different climatic scenarios varied (Fig. 1). When soil workability was not considered, the highest (14.2 Mg ha^{-1}) average grain yield for the Denbigh soil occurred under the RCP85 scenario and the lowest (10.2 Mg ha^{-1}) for the Crediton soil under the baseline climate. However, when considering soil condition impacts on both sowing and harvest dates, the average grain yield for the Denbigh soil under the RCP85 scenario was only 2.6 Mg ha^{-1}. For a given climatic scenario, annual variability in grain yields under S_{sow} (sowing dates determined by workability) was larger than that under S_{cow}. As there was a certain proportion of simulated years without winter wheat growth and where yield was recorded as zero, the standard deviations under $\mathrm{S_{sow}}$ and $\mathrm{S_{sowharv}}$ were larger than those under $\mathrm{S_{con}}$ and $\mathrm{S_{harv}}$.

Simulated $\mathrm{NUE_{crop}}$ under different climatic scenarios and land uses on various soil types are presented in Fig. 2. Ryegrass (S0) had a high $\mathrm{NUE_{crop}}$ (~ 98%) on all soil types and was relatively consistent across the different climatic scenarios and individual years within a simulation (as shown by the small standard deviation). For wheat, failure to establish a crop would have no effect on $\mathrm{NUE_{crop}}$, because no fertiliser was applied when a crop was not sown. When soil workability at sowing was not considered ($\mathrm{S_{con}}$ and $\mathrm{S_{harv}}$), $\mathrm{NUE_{crop}}$ for winter wheat was greater than that for ryegrass apart from under the baseline conditions. Unlike ryegrass, $\mathrm{NUE_{crop}}$ of wheat increased progressively with changing climatic conditions from ~95% under the baseline to ~115% under the RCP85 projection. However, when soil workability at sowing was considered ($\mathrm{S_{sow}}$ and $\mathrm{Ss_{owharv}}$), average $\mathrm{NUE_{crop}}$ for wheat differed widely between soil types and climate projections and the variability between individual years increased considerably (large increase in standard deviation). Thus, under the baseline climate and RCP26, average $\mathrm{NUE_{crop}}$ was reduced compared to ryegrass, with the greatest reduction occurring on the Hallsworth soil, but under RCP45 and RCP85 it was generally comparable to, or greater than ryegrass, depending on the soil type. The lowest NUE_{crop} (~40%) occurred on Denbigh soil under RCP85 (Ss_{owharv}), which is the result of the high failure to harvest in this scenario as applied fertiliser was not recovered in the crop at harvest. As for grain yield, the standard deviations for NUE_{crop} at S_{sow} and $S_{sowharv}$ were larger than those at S_{con} and S_{harv}.

Simulated annual rates of change in soil C over the simulation period under different climatic scenarios and land uses on different soil types are shown in Fig. 3. Under grassland, SOC declined slightly with time under each of the climatic scenarios because added soil C from dead materials was less than soil respiration. When grassland was converted into wheat production, however, all soils lost organic C at a greater rate, the size of the decrease differing between soil type, climate and soil workability scenario. In any given soil and climate combination, the rate of decline was greater when soil workability at sowing was accounted for (S_{sow}) than when it was not (S_{con}).

Averaged annual GPP over the simulation period under the different climatic scenarios and land uses for the different soil types is shown in Fig. 4. Ryegrass (S0) had a high capacity to fix atmospheric CO_2 (24.15 – 45.36 Mg C ha^{-1} yr^{-1}) and GPP was greater than that of winter wheat (S_{con}) on all types and under all climate projections. GPP increased with the temperature trajectory in S0, S_{sow} and $S_{sowharv}$. It is unsurprising that GPP of wheat was lower for S_{sow} and $S_{sowharv}$ compared to S_{con} and S_{harv}, because not all years were suitable for establishing wheat crops.

Averaged soil GHG emissions (expressed as CO_2eq) over the simulation period were greater for grassland (7.71 – 12.50 Mg CO_2eq ha^{-1} yr^{-1}) (S0) than for grassland converted to arable land (Fig. 5) by 1.7 to 2.2 times without considering workability (S_{con} and S_{harv}), and by 1.9 to

4.2 times when considering workability (S_{sow} and $S_{sowharv}$). Among the soil types, the smallest difference in average annual CO_2eq was found for the Crediton soil under the RCP85 projection with or without considering workability for sowing (S_{sow} and S_{con}), and under any of the future climatic scenarios. For S0, CO_2eq was higher for the Hallsworth and Denbigh soils than Crediton under all climatic scenarios. The potentials were generally lower for S_{sow} and $S_{sowharv}$ than for S_{con} and S_{harv} because of the lack of agronomic inputs in some years (i.e. when crops could not be established). Although soil CO_2eq emissions were higher when growing ryegrass compared to wheat, they were offset by the greater photosynthetic CO_2 fixation of grassland, for example, net primary production (NPP, the net C gain by plants) of ryegrass was between 1.2 and 2.3 times that of wheat without considering soil workability and trafficability under various climate scenarios (Table A.4).

A comparison of the indicators between two rates of N fertiliser application on grassland under the baseline climate conditions is shown in Table 4. With the higher application rate, GPP increased and the changes in SOC stocks were marginally closer to neutral, but NUE_{crop} was slightly lower and there were greater CO_2eq emissions from all the soils. The changes associated with the increase in fertiliser N rate were in general much smaller than those associated with a change in cropping under equivalent rates of N.

4 Discussion

4.1 Model performance

Statistical indicators for grain yield, dry matter accumulation of different organs of winter wheat and soil water content suggested the SPACSYS model simulated these variables well (Table 2), which is consistent with previous studies under different soil types and climatic conditions (Liang et al., 2019; Liu et al., 2020; Wu et al., 2019; Zhang et al., 2016). The poorer agreement for N_2O emissions (although cumulative emissions were in good agreement) could be due to error propagation in the modelling but also to uncertainties in the field observations, where high spatial and temporal variation in emissions is commonly observed. The model does not necessarily represent the complexity of the underlying microbial production and consumption processes, which are still not all well understood and characterised (Butterbach-Bahl et al., 2013). Apart from the pathways included in the model, there are other pathways that can be occasionally dominant for soil N_2O production, e.g. dissimilatory nitrate reduction to ammonium and anaerobic ammonium oxidation (Hu et al., 2015), which should be further exploited in the future.

4.2 Suitability of converted grassland for winter wheat cropping

The model simulations suggest that, for the southwest of England and regions under a similar combination of soil types and climates, planting winter wheat between October and December would not be possible in all years because of constraints on soil workability (Table 3). Our finding is supported by a previous study that suggested the region would be only marginally suitable or unsuitable for winter wheat with future increase in both temperature and rainfall (Brignall and Rounsevell, 1995). This also can be extended to other regions with a wet climate in north Europe (Rounsevell et al., 1999). Our results also show that the predicted success rate of crop establishment differed with soil type and future climate scenario and that it increased to a small extent under projection RCP85 in spite the greater autumn rainfall compared with the baseline climate. In contrast to sowing, harvest operations appeared to be at lower risk of failure. The difference in risk of failure of harvest and sowing can be explained by the time period between the two operations and the rate at which the soil moisture content is restored to values above the upper wet tillage limit. This will be influenced by both the amount of rain falling between harvest and sowing and the soil moisture deficit at harvest as soils with a lower moisture content require a greater input of water to bring them up to the upper tillage limit. We assumed that harvest date was only affected by soil wetness. Although harvesting may be delayed or interrupted by rainfall after the grain has reached harvest maturity, providing the soil remains trafficable, complete harvest failure is unlikely as combine harvesting can be undertaken between rainfall events once the crop has dried. When soil workability at sowing and trafficability at harvest were considered, the success rate of cropping fell below that predicted from workability at sowing alone, but only on the Denbigh soil under projection RCP85. Delayed sowing under a warming climate reduces the chance of the crop meeting its vernalisation requirement, thus delaying the date of crop maturity to a point when trafficability may be prohibitive. Our predictions suggest that the consequences of this for a successful harvest are dependent on the soil type.

4.3 Yield and nitrogen use efficiency of winter wheat

Under each soil type and climate projection, simulated grain yields were greatest under S_{con} and S_{harv} and least under S_{sow} and $S_{sowharv}$. A delay in sowing beyond the optimum date may reduce yield (Ortiz-Monasterio et al., 1994; Spink et al., 2000) by reducing the amount of solar radiation intercepted over the season (Hay and Porter, 2006). Yield reductions in our simulations, however, were dominated by instances where crops could not be sown by the cut–off date of 31st December, because in these seasons the yield of winter wheat was recorded as zero. In practice, long delays to harvest can result in the pre–harvest shedding and sprouting of grain and other forms of grain deterioration. However, our simulations indicated that the average delay to harvesting in S_{harv} compared to S_{con} ranged from 0.0 to 1.0 day with a standard deviation of 0.3 to 3.9 depending on the soil type and RCP projection. We conclude that delays to harvest would have had minimal effects on the average yield.

Our results showed that NUE_{crop} of wheat was greater than 100% when effects of soil wetness on sowing or harvesting dates were not considered in the future climate scenarios. As NUE_{crop} is defined at the N content of the crop per unit of fertiliser N applied, it does not account for N that may have come from sources other than fertiliser. Thus, values greater than 100% suggests a significant contribution of N mineralised from soil organic matter to N uptake in addition to that from fertiliser (Bingham et al., 2012; King et al., 2001). The greater NUE_{crop} of wheat under those scenarios compared to ryegrass may reflect greater mineralisation of organic matter following soil disturbance during seed bed preparation as well as differences in root length and distribution between the two plants which could influence the efficiency of N capture (King et al., 2003). However, our simulations also show that NUE_{crop} is strongly dependent on sowing date in autumn and its interactions with soil type and climate. Delayed seed bed preparation and sowing into cooler soils will reduce rates of autumn root growth and the size of the root system in spring and increase the risk of overwinter N losses, all of which would be expected to reduce N uptake and NUE_{crop} (Barraclough and Leigh, 1984).

In common with many agricultural models we did not explicitly consider any potential impact of disease on crop growth. However, in view of the warmer temperatures and greater precipitation predicted under each of the RCP projections we might expect an increase in disease pressure placing further restrictions on the suitability of the region for wheat production (Figueroa et al., 2018; Juroszek and von Tiedemann, 2013; Lynch et al., 2017). High levels of disease control are required to minimise the CO_2eq costs of production (Berry et al., 2008).

4.4 Soil C Carbon sequestration and GHG emissions under different land uses

Grassland conversion in the region would not be sustainable in terms of C sequestration although applications of livestock manure or other organic materials could mitigate soil C losses to some extent. It is evident that SOC declines when intensive permanent grassland is converted to arable land under any climatic scenario and soil type (Fig. 3), as supported by many published studies (Deng et al., 2016; Kämpf et al., 2016; Li et al., 2020; Potter et al., 1999; Spohn and Giani, 2011). On the other hand, grassland can maintain or increase SOC stocks, which again is in agreement with previous studies (Mayel et al., 2021; Soussana et al., 2004). Under the baseline climate scenario, however, SOC in grassland was simulated to decrease in the present study, with the rate depending on soil type. This contrasts with the conclusion by Conant et al. (2001) that grassland fertilisation increased forage production and SOC; this may be a result of the lower fertiliser application rate assumed in our study. However, Eze et al. (2018) suggested that the effect of fertiliser N application on SOC stock is insignificant. Indeed in our study, the rate of change of SOC stocks under two fertiliser application rates were similar (Table 4), with only a small reduction in C loss at the higher fertiliser rate. Under the projected climate scenarios, conversion of grassland to arable reduced SOC by between 165 and 280 kg C ha^{-1} yr^{-1}. The loss rate may depend on the initial C stock in the different soils. Although an average rate of decline in SOC over the simulation period is presented in Fig. 3, the rate of decline is initially high and diminishes with time until it reaches an equilibrium level, taking the dynamics in Hallsworth as an example (Fig. A.3).

The simulated soil GHG emission (as CO_2eq) from grassland was higher than that from the land converted to arable (Fig. 5), as supported by previous studies (Kandel et al., 2018; Oertel et al., 2016). Although these values cannot be validated with the limited field observations in this study, the simulated CO_2eq emission under the baseline climatic scenario for grassland is close to the value reported from an experiment carried out in Scotland (Jones et al., 2005). Despite a higher rate of soil CO_2eq emissions from grassland, the simulations showed permanent ryegrass can add more C to soils through dead materials than wheat. Hence, soil C stocks decline more slowly in grassland. A reported soil sink of 2020 ± 760 kg C ha^{-1} yr^{-1} derived from eight experiments in managed grasslands across Europe (Soussana et al., 2007) is supportive of this. It is difficult to compare observed or calculated CO_2eq between different studies because N_2O and CH_4 emissions are extremely sensitive to management practices, soil nutrient substrates and environmental conditions, as well as the chosen parameter value for the global warming potential of each of these gases.

Our simulation results are affected by our assumptions: 1) a single climatic model was used to generate data for the projected climate scenarios, as mentioned earlier in the discussion; 2) winter wheat is the only crop grown in the converted grassland; and 3) soil erosion was not included in the model. We assumed that no cropping occurred if winter wheat could not be sown in a given year. In reality, farmers would find an alternative, e.g. spring or catch crops to fill the gap rather than leaving soil bare for the whole year. In this case, the values of the sustainability indicators could change accordingly. For permanent grassland, we assumed that harvesting dates of ryegrass would not be affected by soil moisture conditions. This might not always be true under different climatic scenarios. In some years, soils might be too wet in the autumn for the last cut in a year and a delayed cutting can reduce forage quality substantially. The effect of soil moisture on ryegrass cutting dates, which in turn influence forage quality, is worthy of further investigation in the future.

It should be noted that we only chose limited indicators to investigate suitability for the land conversion and did not quantify biodiversity, nutrient leaching losses and soil erosion. For example, soil erosion from arable land is generally greater than from permanent grassland

(Cerdan et al., 2010). Therefore, there is also a high risk of soil erosion as a result of grassland conversion to arable. Our ongoing monitoring programme on the North Wyke Farm Platform has shown severe erosion from recently converted fields compared with that from permanent grassland nearby (http://resources.rothamsted.ac.uk/farmplatform, accessed on 10 April, 2021).

5 Conclusions

The calibrated SPACSYS model successfully simulated the dry matter accumulation and grain yield of winter wheat and the soil water content. Our simulations highlight the importance of soil workability at sowing in determining the agronomic success and environmental sustainability of a change in cropping practice. Under baseline and future climate projections, the probability of success in sowing winter wheat in the main grassland climatic/soil regions in a given year was estimated to be between 38 and 76%. Although the grain yield could reach 9 to 16 Mg ha^{-1} in successful years, delays to sowing and the failure to establish and harvest a crop in some years had a significant negative effect on average on yield and mixed effects on indices of environmental sustainability. Compared to perennial ryegrass, winter wheat had a lower NUE_{crop} on all soil types under the baseline climate and RCP26 projections when soil workability at sowing was accounted for, but a comparable or greater NUE_{crop} under RCP45 and RCP85. Wheat fixed less atmospheric CO_2 because of the shorter growing season and time to establish a full canopy. Although average annual soil GHG emissions from silage–based permanent grassland were higher than from land converted to arable, this was compensated by the higher C fixation rate of the ryegrass. Under the baseline climatic condition, soil C stocks were predicted to be maintained or marginally decline in permanent grassland. However, the predicted rate of decline was much greater under all climatic scenarios when grassland was converted to arable land. We conclude that in terms of C sequestration, conversion of grassland to winter wheat cropping is unsustainable in soil/climatic zones such as those in much of the southwest of England.

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Figure captions

Figure 1. Average grain yield of winter wheat over the simulation period under different climatic scenarios on various soils (Crediton, Denbigh and Hallsworth). Error bars show the standard deviation. (Characters after the soil name in the x–axis indicate climatic scenarios: B – baseline; 26 – RCP26 (very low emissions); 45 – RCP45 (an intermediate scenario) and 85 – RCP85 (high–emissions)).

Figure 2. Simulated annual agronomic efficiency of nitrogen (NUE_{crop}, %) under different climatic scenarios and land uses on various soil types. Error bars show the standard deviation. (Characters after the soil name in the x–axis indicate climatic scenarios: B – baseline; 26 – RCP26 (very low emissions); 45 – RCP45 (an intermediate scenario) and 85 – RCP85 (high–emissions)).

Figure 3. Simulated annual rate of change in soil carbon under different climatic scenarios and land uses on various soils (Crediton, Denbigh and Hallsworth). (Baseline – baseline climate; RCP26 – future climate with a very low emissions scenario; RCP45 – future climate with an intermediate scenario and RCP85– future climate with a high emissions scenario. S0, permanent ryegrass; S_{con}, keeping the sowing date as the plot experiment was applied but harvesting when simulated physiological maturity is reached; S_{sow}, as for S_{con} but with the sowing date varied each year according to soil moisture conditions; S_{harv}, as for S_{con} but with the harvest date each year determined by soil moisture after physiological maturity of the winter wheat; and $S_{sowharv}$, as for S_{con} but with both sowing and harvest dates each season set according to soil moisture conditions)

Figure 4. Simulated average annual gross primary productivity (Mg C ha^{-1}) over the simulation period under different climatic scenarios and land uses on various soil types (Crediton, Denbigh and Hallsworth). Points for $S_{sowharv}$ and S_{harv} are masked by those for S_{sow}

and S_{con} respectively. (Baseline – baseline climate; RCP26 – future climate with a very low emissions scenario; RCP45 – future climate with an intermediate scenario and RCP85– future climate with a high emissions scenario. S0, permanent ryegrass; S_{con}, keeping the sowing date as the plot experiment was applied but harvesting when simulated physiological maturity is reached; S_{sow}, as for S_{con} but with the sowing date varied each year according to soil moisture conditions; S_{harv}, as for S_{con} but with the harvest date each year determined by soil moisture after physiological maturity of the winter wheat; and $S_{sowharv}$, as for S_{con} but with both sowing and harvest dates each season set according to soil moisture conditions)

Figure 5. Simulated average annual soil CO_2eq emissions (Mg CO_2eq ha^{-1}) over the simulation period under different climatic scenarios and land uses on various soil types (Crediton, Denbigh and Hallsworth). (Baseline – baseline climate; RCP26 – future climate with a very low emissions scenario; RCP45 – future climate with an intermediate scenario and RCP85– future climate with a high emissions scenario. S0, permanent ryegrass; S_{con}, keeping the sowing date as the plot experiment was applied but harvesting when simulated physiological maturity is reached; S_{sow}, as for S_{con} but with the sowing date varied each year according to soil moisture conditions; S_{harv}, as for S_{con} but with the harvest date each year determined by soil moisture after physiological maturity of the winter wheat; and $S_{sowharv}$, as for S_{con} but with both sowing and harvest dates each season set according to soil moisture conditions)

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Table 1. Characteristics of baseline and scenario climates for the site. Numbers in parentheses are standard deviation.

	Precipitation (mm)			heavy rain[1] days in a year (d)	Annual temperature (°C)	Annual global radiation (MJ)	CO_2 concentration range (ppm)
	Annual	Aug – Oct	Oct – Dec				
Baseline	986.2 (156.6)	275.8 (99.5)	347.7 (100.0)	5.6 (2.9)	9.9 (0.5)	3772 (152)	400
RCP26	1513.2 (227.9)	426.3 (146.6)	600.4 (150.4)	17.1 (4.4)	11.5 (0.6)	4159 (150)	402 – 454
RCP45	1428.3 (228.9)	333.2 (138.8)	544.1 (154.7)	16.4 (5.0)	12.1 (0.8)	4148 (166)	402 – 548
RCP85	1389.7 (238.6)	331.2 (115.6)	551.1 (160.8)	16.0 (4.8)	12.9 (1.3)	4232 (149)	402 – 924

[1] Defined as days where daily precipitation is greater than 20 mm.

Table 2. Statistical summary for model calibration and validation for dry matter (DM) and nitrogen (N) content of different wheat aboveground organs, soil volumetric water content and gas emissions with under different treatments

Statistics†	number	r	LOFIT F value	nRMSE (%)	EF	CD	relative error (%)	ME
Calibration								
soil water	496	0.7369*	N/A	18	0.18	0.74	8.5	2.16
leaf DM	12	0.8853*	0.36*	25	0.75	0.87	–1.7	–2.62
stem DM	12	0.9699*	0.13*	19	0.92	1.39	2.7	11.66
grain DM	6	0.9124*	0.65*	33	0.10	0.39	–16.9	–94.74
leaf N content	12	0.9912*	0.05*	11	0.98	1.06	–4.2	–0.15
stem N content	12	0.9368*	0.59*	32	0.81	1.97	8.4	0.30
grain N content	6	0.9331*	0.15*	18	0.78	0.69	5.1	0.49
Validation								
soil water	160	0.8505*	N/A	15	0.68	1.07	4.6	1.15
leaf DM	6	0.8382*	1.38*	28	0.64	0.87	3.8	6.35
stem DM	6	0.9462*	1.25*	30	0.81	1.83	13.9	71.08
grain DM††	3	0.9975*	0.27*	14	0.90	1.19	13.2	105.36
leaf N content	6	0.9327*	1.78*	25	0.86	1.27	5.0	0.20
stem N content	6	0.7426	3.49	42	0.55	1.50	1.7	0.06
grain N content‡	3	0.9934*	1.38*	33	0.39	3.12	27.3	3.53
N_2O emissions	60	0.1982	N/A	132	–0.26	4.43	55.6	0.00

* indicates statistically significant ($p < 0.05$)

† If all predicted and observed values were the same, then r (correlation coefficient) = 1, ME (mean difference) = 0.0, RMSE (root mean square error) = 0.0, CD (coefficient of determination) = 1.0 and EF (modelling efficiency) = 1.0.

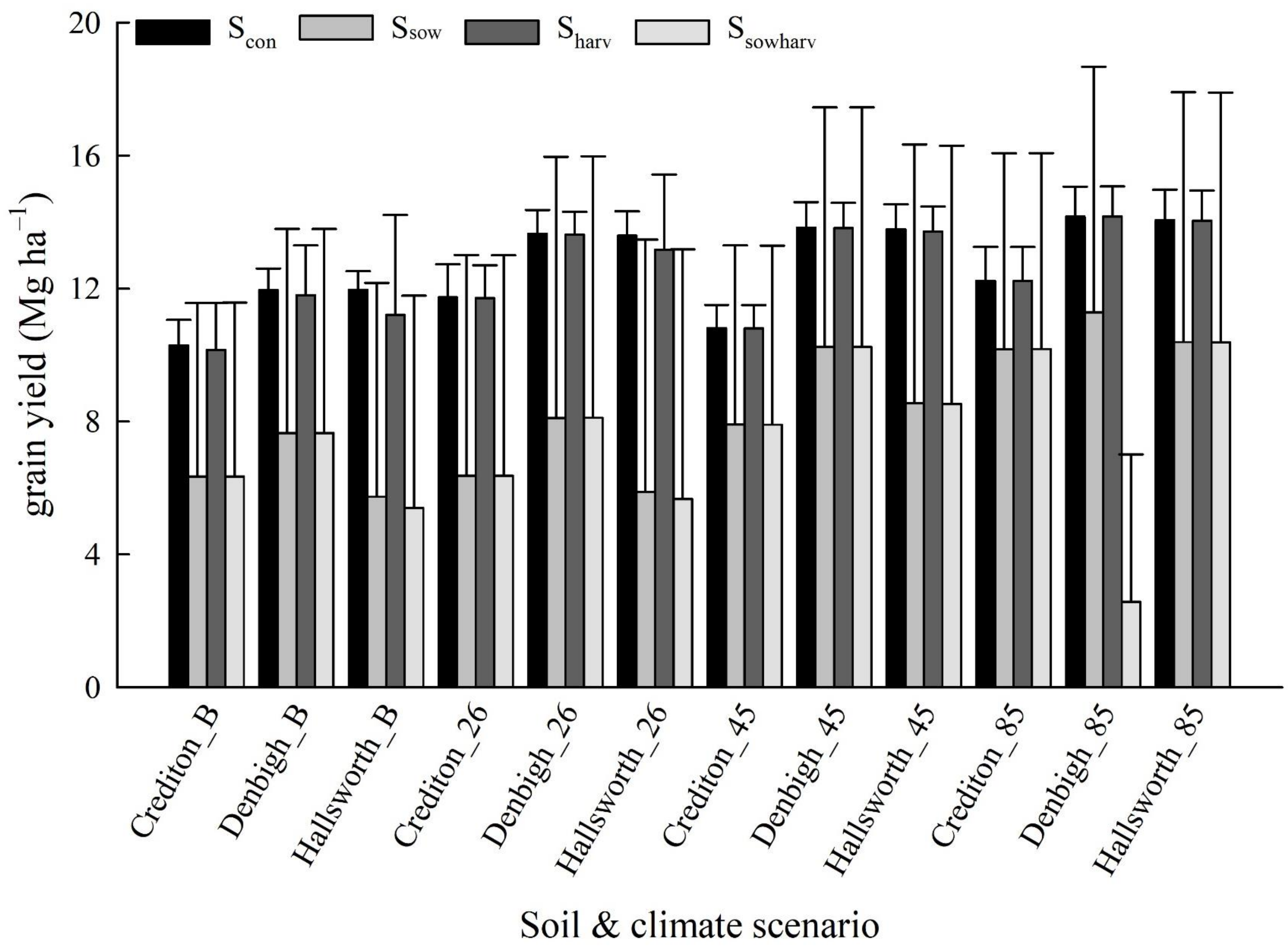
‡ Statistical analysis is only considered as a reference because of limited sampling number.

Table 3. Predicted success frequency (%) of establishing and harvesting winter wheat under various climatic conditions for different soils based on workability of soil at sowing (S_{sow}), harvest (S_{harv}) and both seeding and harvest ($S_{sowharv}$). Success is expressed as a % of values for scenario S_{con}.

Soil type	Climatic scenario	Workability		
		Sowing	Harvesting	Both
Crediton	Baseline	60	99	60
	RCP26	49	100	49
	RCP45	69	100	69
	RCP85	76	100	76
Denbigh	Baseline	62	99	62
	RCP26	53	100	53
	RCP45	68	100	68
	RCP85	71	100	28
Hallsworth	Baseline	45	94	42
	RCP26	38	97	37
	RCP45	55	100	55
	RCP85	67	100	67

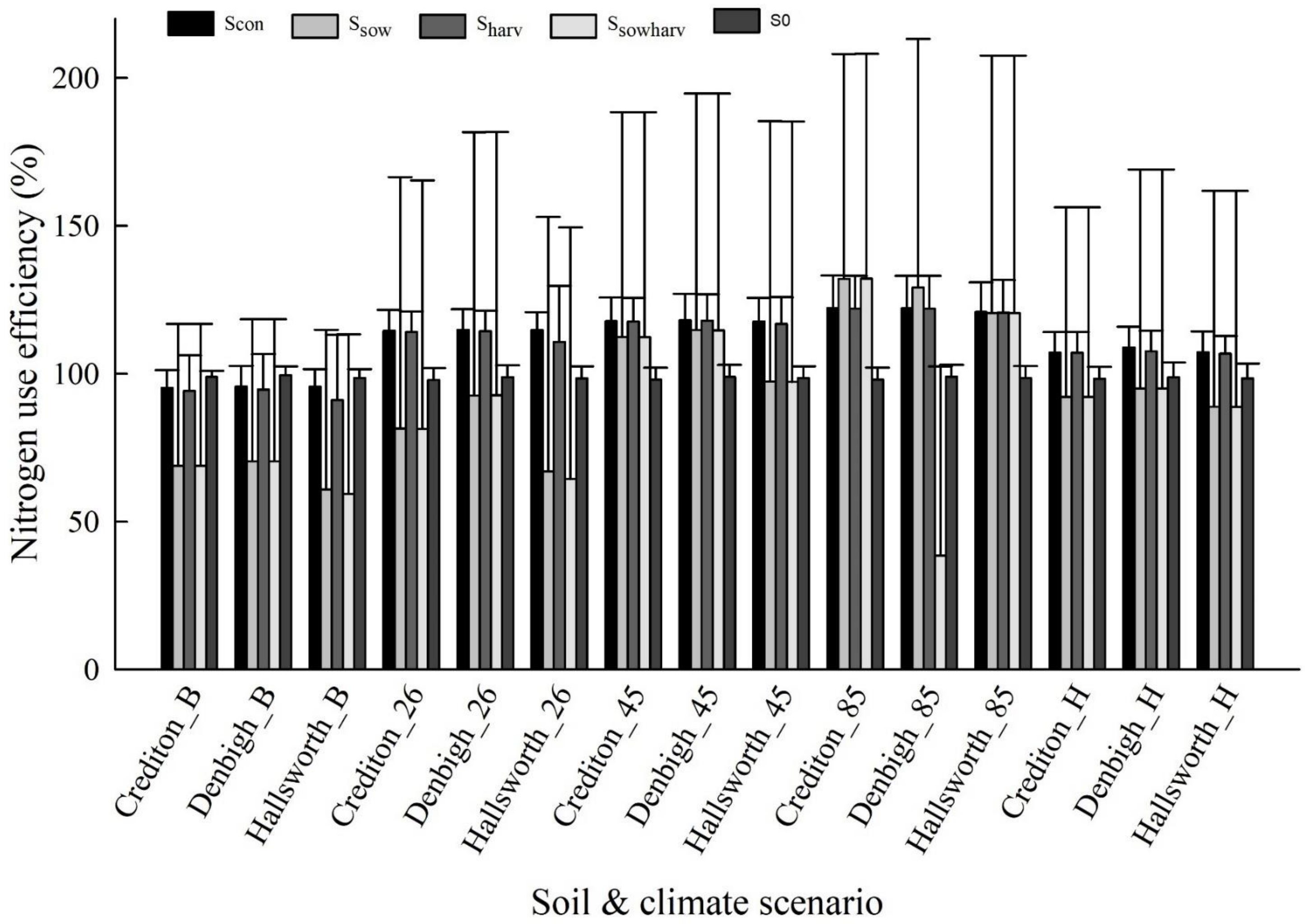
Table 4. Simulated sustainability indicators for grass grown on different soil types under the baseline climate condition with different chemical fertiliser application rates and timings. Numbers in parentheses are standard deviation. GPP, gross primary productivity; CO_2eq, soil greenhouse gas emissions expressed in CO_2 equivalents; SOC, soil organic carbon; NUE_{crop}, N use efficiency.

Indicator	Soil	Application rate (kg N ha^{-1} yr^{-1})	
		150	300
GPP (Mg C ha^{-1} yr^{-1})	Crediton	24.1 (1.2)	25.5 (1.4)
	Denbigh	28.4 (0.7)	30.4 (0.8)
	Hallsworth	29.0 (0.7)	31.2 (0.8)
NUE_{crop} (%)	Crediton	99.0 (2)	96.3 (4)
	Denbigh	99.5 (3)	95.1 (4)
	Hallsworth	98.6 (3)	94.4 (4)
CO_2eq (Mg CO_2eq ha^{-1} yr^{-1})	Crediton	7.7 (0.5)	8.1 (0.5)
	Denbigh	9.7 (0.7)	10.3 (0.8)
	Hallsworth	9.5 (0.9)	10.1 (1.0)
SOC change rate (kg C ha^{-1} yr^{-1})	Crediton	–39	–37
	Denbigh	–19	–15
	Hallsworth	–26	–11



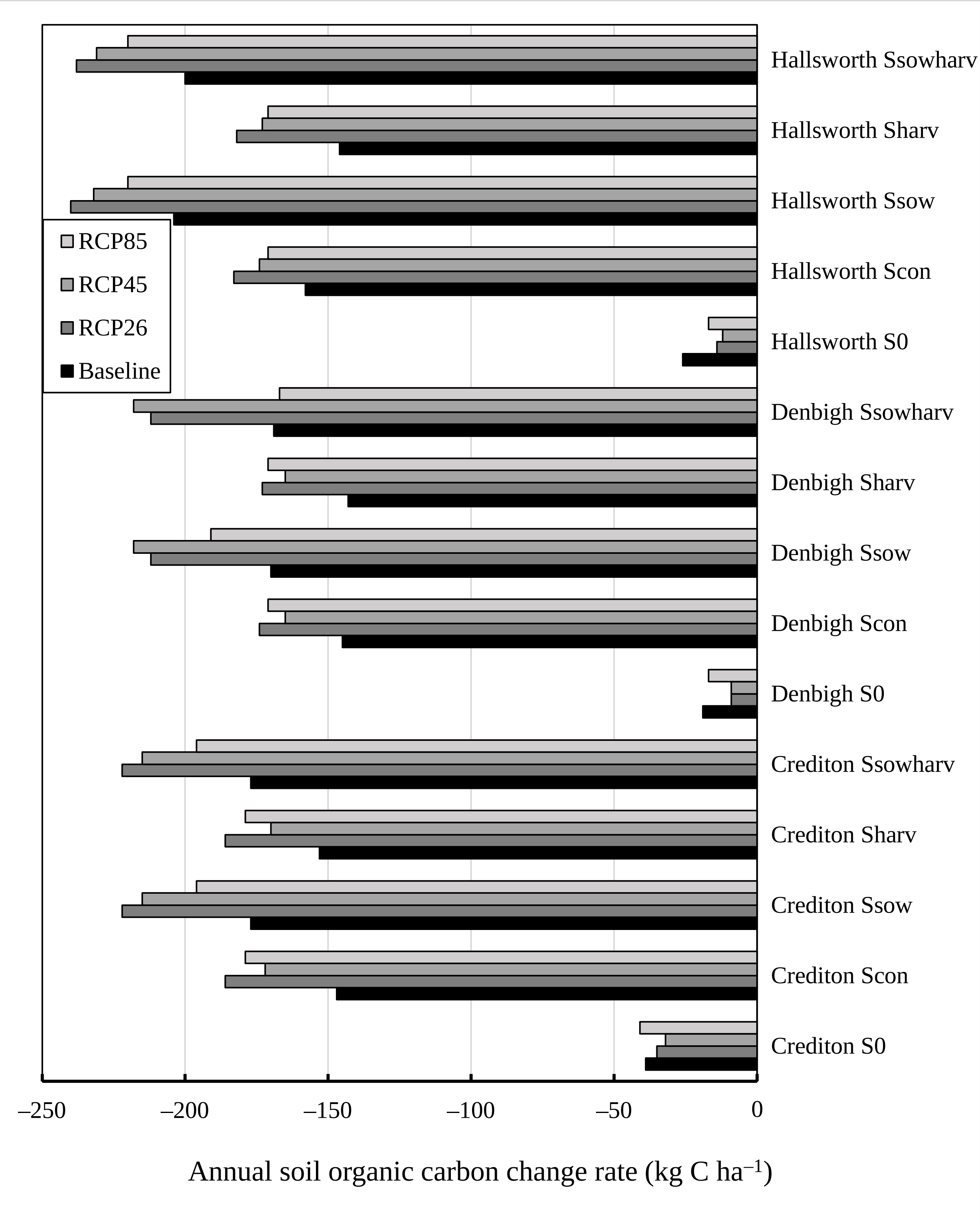
20
16
12
8
4
0
grain yield (Mg ha^{-1})
S_{con}
S_{sow}
S_{harv}
$S_{sowharv}$
Crediton_B
Denbigh_B
Hallsworth_B
Crediton_26
Denbigh_26
Hallsworth_26
Crediton_45
Denbigh_45
Hallsworth_45
Crediton_85
Denbigh_85
Hallsworth_85
Soil & climate scenario

Figure 1



Scon
Ssow
Sharv
Ssowharv
S0
Nitrogen use efficiency (%)
200
150
100
50
0
Crediton_B
Denbigh_B
Hallsworth_B
Crediton_26
Denbigh_26
Hallsworth_26
Crediton_45
Denbigh_45
Hallsworth_45
Crediton_85
Denbigh_85
Hallsworth_85
Crediton_H
Denbigh_H
Hallsworth_H
Soil & climate scenario

Figure 2



Hallsworth Ssowharv
Hallsworth Sharv
Hallsworth Ssow
Hallsworth Scon
Hallsworth S0
Denbigh Ssowharv
Denbigh Sharv
Denbigh Ssow
Denbigh Scon
Denbigh S0
Crediton Ssowharv
Crediton Sharv
Crediton Ssow
Crediton Scon
Crediton S0
RCP85
RCP45
RCP26
Baseline
–250
–200
–150
–100
–50
0
Annual soil organic carbon change rate (kg C ha–1)

Figure 3

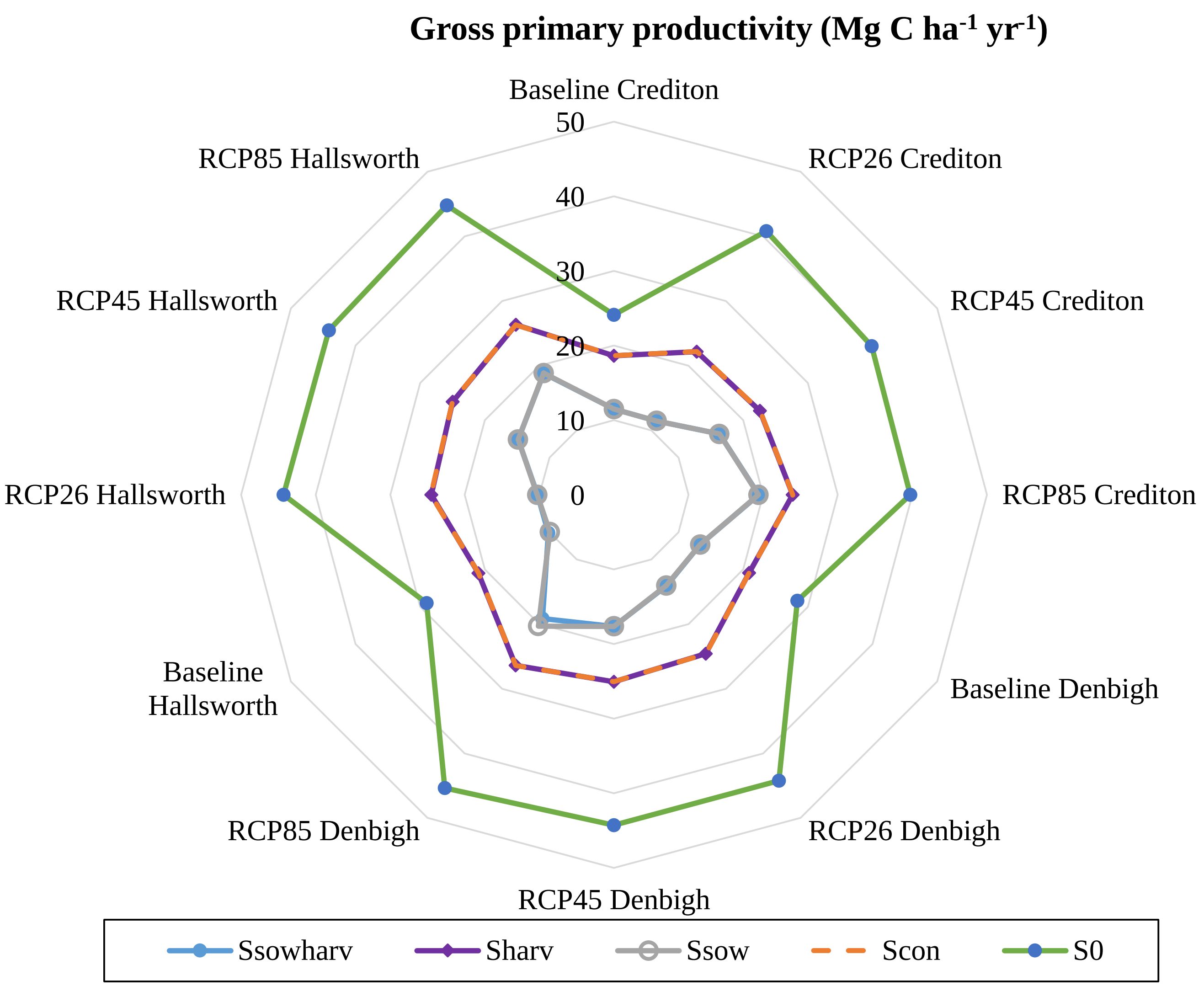
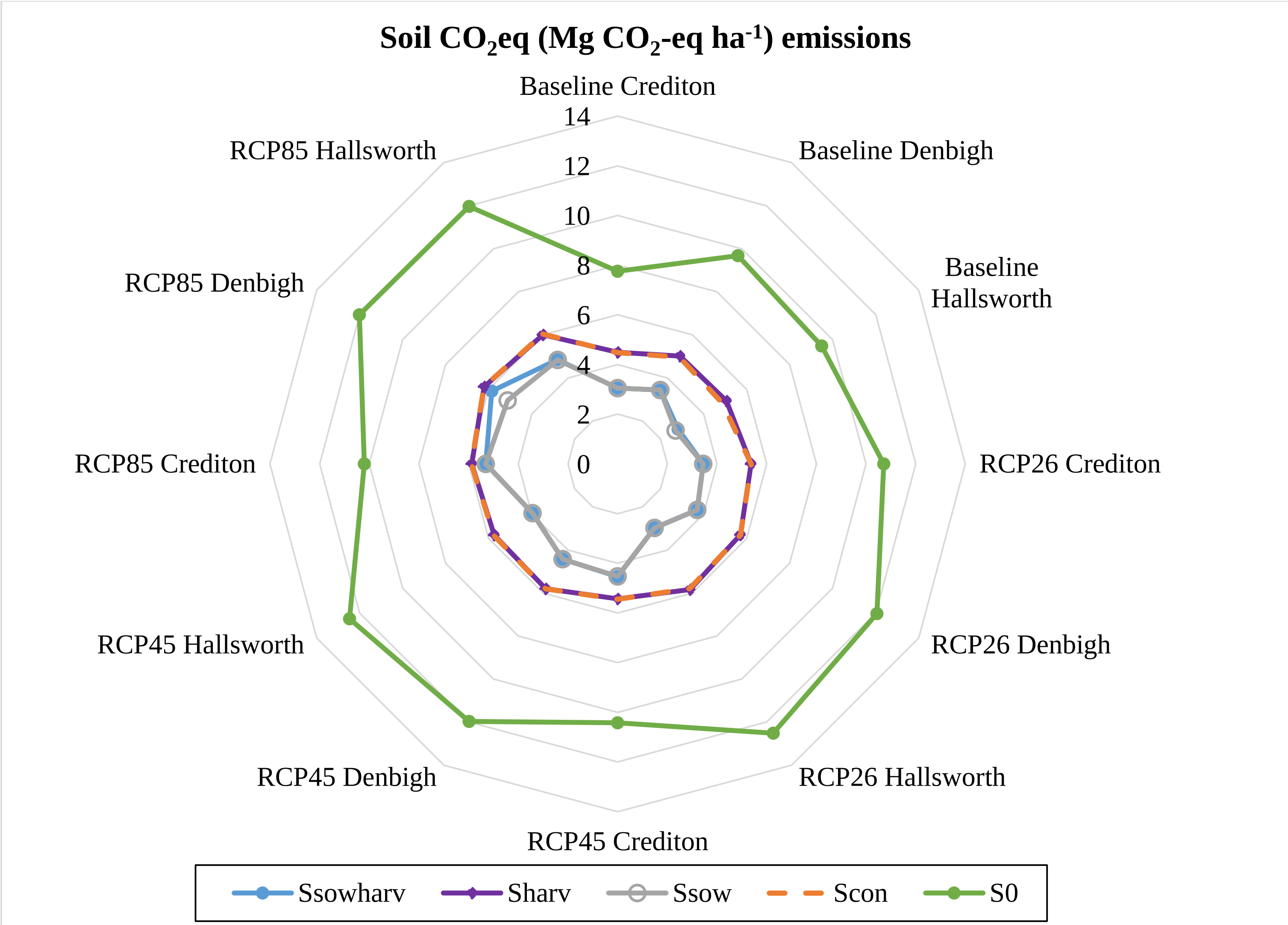

Gross primary productivity (Mg C ha-1 yr-1)
Baseline Crediton
RCP26 Crediton
RCP45 Crediton
RCP85 Crediton
Baseline Denbigh
RCP26 Denbigh
RCP45 Denbigh
RCP85 Denbigh
Baseline Hallsworth
RCP26 Hallsworth
RCP45 Hallsworth
RCP85 Hallsworth
50
40
30
20
10
0
Ssowharv
Sharv
Ssow
Scon
S0

Figure 4



Soil CO_2eq (Mg CO_2-eq ha^{-1}) emissions
Baseline Crediton
Baseline Denbigh
Baseline Hallsworth
RCP26 Crediton
RCP26 Denbigh
RCP26 Hallsworth
RCP45 Crediton
RCP45 Denbigh
RCP45 Hallsworth
RCP85 Crediton
RCP85 Denbigh
RCP85 Hallsworth
14
12
10
8
6
4
2
0
Ssowharv
Sharv
Ssow
Scon
S0

Figure 5