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Rainfall and temperature impacts on barley (*Hordeum vulgare* L.) yield and malting quality in Scotland

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ABSTRACT

Barley is one of the most important cereals worldwide and is a key crop for Scotland's agriculture due to its use in distilleries to produce whisky. Climatic variability, especially significant changes in rainfall patterns are a present challenge for barley production. Thus, the objectives of this study were: i) to evaluate the performance of a crop model to simulate water and N stresses in spring barley in the east of Scotland; ii) to quantify the impacts of rainfall and temperature on barley grain yield and quality; and iii) to understand how grain nitrogen concentration varies in relation to climate variability. Three field experiments were undertaken at the James Hutton Institute near Dundee, UK. The 2018 experiment consisted of two levels of N (0 N and 120 N) and two levels of water (rainfed and irrigated). Data from two experiments were used as additional evaluation. The Decision Support System for Agrotechnology Transfer (DSSAT v4.7) model was used to evaluate the crop performance. The evaluation of the crop model using the different years, locations and water by nitrogen stress levels, using the same cultivar (Concerto), showed that the cultivar parameters were well calibrated. There was a weak negative and non-significant ($p = 0.14$) relationship between air temperature and simulated yield, but a strong ($p < 0.05$) positive relationship between growing season rainfall and simulated yield. During the spring barley growing season (Apr-Aug), the last two decades were drier than the long-term average, with May (time of expansive growth) having about 25 mm less rainfall than the long-term average. The results of this study highlight how rainfall is more important than the temperature for the production of spring barley in Scotland. Our simulated results showed that the premium grain for distilling is reached 41 out of 45 years investigated in this study.

1. Introduction

Barley (*Hordeum vulgare* L.) is among the oldest cultivated crops in the world, grown at different latitudes, from close to the equator up to 70 °North, under low and high-input cropping systems (Newton et al., 2011; Dawson et al., 2015). Its use includes human and animal feed and the production of alcoholic drinks (Newton et al., 2011). Barley production has a particular importance in Scottish agriculture due to its use in distilleries for the production of whisky. Given that in Scotland winter sown barley does not satisfy malting requirements and it is more expensive to grow, spring sown barley is used for distilling. Spring barley is cultivated over 245,000 ha in Scotland, with an average grain yield of 5.9 t ha^{-1} (RESAS, 2017). The importance of barley production in the Scottish alcohol industry is represented by the revenue generated by the industry. The average turnover across all Scottish business is about €779,700; using this average across businesses as "baseline", the distilling of whisky has a turnover of about €6.1 million and brewing is €315,500 (O'Connor, 2018). Given the importance of this industry to the Scottish economy, spring barley yield and quality in regions close to the distilleries have important economic consequences.

Management factors, such as sowing dates, fertilizer rates and amount, and plant density can be manipulated to optimize barley production and quality. For spring barley, early sowing might be beneficial in terms of increasing the length of the growing season, but could

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incur into a penalty, due to late frosts and might be impractical due to poor soil conditions for tillage and sowing in early spring. The application of nitrogen (N) fertilizer in spring barley is often lower than for winter-sown barley, reflecting the lower yield potential. In addition, the lower N amount is also justified because barley for malting requires a grain N of less than 1.85% (HGCA, 2001; UK Malt, 2019). However, even where these agronomic variables are optimized to aim for the maximum potential yield, environmental conditions can still have a major impact on the outcome in terms of yield and product quality at the end of the season (Newton et al., 2011).

Scotland has an average annual rainfall of about 1000 mm, but with a high spatial variability. While the Western parts of Scotland can receive more than 1600 mm, the eastern part receives between 700 and 800 mm (SEPA, 2019). The spring barley growing season includes the months from April to August and the growing season rainfall ranges from 180 to over 400 mm depending on the geographical location (Cammarano et al., 2016a). The general perception is that spring barley would not be limited by water stress and that its productivity is mostly influenced by the length of the growing season. However, in the last decade, especially during early summer, the east of Scotland has experienced a series of drought events which had negative consequences on spring barley productivity. In 2018, most of the east of Scotland experienced low rainfall from April to August; for example, some locations experienced only 100 to 170 mm of growing season rainfall, with only 60 to 80 mm between sowing and flowering. Daily maximum temperatures did not reach values that could negatively affect crop development (the maximum recorded for one day was about 28 °C, with a growing season average of 18 °C). In addition, due to the high latitude, the days are long and, with no clouds for longer period and high solar radiation, the crops could experience periods of drought stress. A better understanding of the impact of rainfall on spring barley production at high latitudes is therefore needed before addressing proper agronomic and breeding efforts towards adapting to climate change.

To assess the impacts of climatic conditions on grain yield and quality, long-term weather records are necessary because they contain years with contrasting patterns of rainfall and temperature that can occur in the short term (e.g. within a growing season) and can be a proxy for describing, in a probabilistic manner, the likely impacts of climate on spring barley (Cammarano et al., 2016b). The "*in-silico*" assessment of climate impact is generally done using crop simulation models (Cammarano et al., 2012). These are tools that simulate crop growth and development and the temporal effects of water and nutrient stresses on phenological and physiological crop responses (Jones et al., 2003; van Ittersum et al., 2003). This approach generally requires daily weather data, soil and management information, initial conditions (e.g. soil water and mineral nitrogen contents), and crop species as input variables, although the amount of detailed input data varies between models.

The aim of this work was to study the rainfall patterns in a long-term series of weather data and to integrate field experimentation with crop modelling to get a better understanding of the water stress impacts on spring barley in Scotland. Thus, the objectives of this study were: i) to evaluate the performance of a crop model to simulate water and N stresses in spring barley in the east of Scotland; ii) to quantify the impacts of rainfall and temperature on barley grain yield and quality; and iii) to understand how grain nitrogen concentration varies in relation to climate variability.

2. Materials and methods

2.1. Experimental site and description

2.1.1. Experiment 1

The experimental site was located at the James Hutton Institute experimental farm (Invergowrie, Dundee, 56° 27′ N 03° 04′ W, 27 m a.s.l.). The soil was classified as Brown Forest Soil – Carpow Association according to Bell and Hipkin (1988). The soil texture was loam according to the USDA soil survey (2019). Weather records were available on-site from a local weather station, providing information on daily solar radiation, air minimum and maximum temperature, and rainfall from 1974 to 2018.

The crop used for the experiment was spring barley cultivar Concerto and was planted on the 4th of May 2018 at 360 seeds m^{-2} in 12, 2 m x 12 m plots. The experiment consisted of 3 replicates of 2 levels of N (0 N and 120 N) and 2 levels of water (rainfed and irrigated) in the following treatment combinations: N-Fertilization and Irrigation (+N-IRR); N-Fertilization and no Irrigation (+N-RF); no Fertilization and Irrigation (0 N-IRR); no Fertilization and no Irrigation (0 N-RF). A 6 m buffer strip was planted with spring barley between irrigated and rainfed plots to avoid confounding effects between treatments (Fig. S1). In the fertilized plots 550 kg ha^{-1} NPK fertilizer (YaraMila SULPHUR CUT, 22-4-14 + 7.5 SO_3), consisting of 120 kg N ha^{-1} (120 N), was applied at sowing. The N fertilizer was applied in a single dose due to the late sowing date. Irrigated plots received about 800 L min^{-1} through sprinklers with a coverage of 5 mm of water per h^{-1} set for 3 days *per* week for a total of 45 min per day, corresponding to about 11 mm per week.

The field was sampled one day before sowing (3rd May 2018) for soil texture, organic carbon, soil water content, mineral N (NH_4 and NO_3). Six soil samples were taken to a depth of 60 cm *per* plot on the day before sowing and analyzed at the Yara analytical service laboratory for soil texture, organic carbon, and mineral N (NH_4 and NO_3). Gravimetric soil water from each plot was also determined by weighing 40 g of 24 field soil samples oven dried at 105 °C for 48 h (McKenzie et al., 2002). Additional sampling dates were the 7th June, 2nd July and 17th August 2018, when both soil and plant samples were collected. At each date, gravimetric soil water content and soil mineral N were determined. In addition, three replicates *per* treatment of plant biomass and plant N% were sampled at the same time as the soil sampling on one square meter. The plant N% was determined at the Yara analytical service laboratory. Plant biomass was oven-dried at 105 °C until constant weight and weighted. At harvest (17th August) straw biomass, grain biomass, grain protein, grain N%, seed number, seed weight, and thousand grain weight were determined. Anthesis and maturity dates were also recorded.

2.1.2. Experiments 2 and 3

Two additional experiments were used for a further evaluation of the crop model used. These experiments were carried out at the Balruddery experimental farm, Dundee (56° 28′ N, 03° 03′ W, 132 m a.s.l.) during the growing season 2011, 2012 (Experiment#2), and 2017 (Experiment#3). The Balruddery farm is 170 ha and data were gathered from a range of different fields. The soil was classified as Brown Earth (Bell et al., 2009). The 2011 and 2012 data were from a whole field experiment, where barley was in rotation with other spring/winter cereals under conventional management practices. The 2017 data were from a plot-scale N response trial. The spring barley was planted on 04-Apr-2011, 22-Mar-2012, and 13-Apr-2017 with 360 seeds m^{-2}, using cultivar Concerto. Fertilizer was applied at sowing at a rate of 285 kg ha^{-1} (30-0-0 + 19% SO_3) in 2011, and at a rate of 280 kg ha^{-1} (30-0-0 + 19% SO_3) in 2012. The 2017 experiment consisted in fertilized and non-fertilized treatments. The fertilized treatment received a total of 500 kg ha^{-1} YaraMila SULPHUR CUT, 22-4-14 + 7.5% SO_3. The N application was split, with 77 kg N ha^{-1} applied at sowing and 33 kg N ha^{-1} applied on the 5th of June 2017 for a total of 110 kg N ha^{-1} applied during the whole growing season. For the experiments 2 and 3, anthesis dates, maturity, and grain yield were available. In addition, for the 2017 experiment, crop biomass and plant nitrogen content were available. Soil information for both experiments were reported in Table S1. Hydraulic limits were not available at all the sites and they were estimated using the DSSAT internal pedo-transfer function (Tab. S2). All the observed values were reported in Tables S3 and S4. Biomass values were reported as dry matter (DM) and grain yield was reported as dry weight.

2.2. Crop modelling

The Decision Support System for Agrotechnology Transfer (DSSAT v4.7) model was used for this study. In particular the CSM-Barley was utilized to simulate the experimental data (Jones et al., 2003). The input data used were daily weather data, soil data, management data (timing and inputs), and initial conditions of volumetric soil water content and soil mineral N content. Both soil water and soil N prior sowing were measured at all sites.

The crop model was calibrated using the 2018 +N-IRR for phenology (anthesis and maturity), crop biomass and grain yield by modifying the crop parameters of the model, such as vernalization and photoperiod sensitivity, phyllochron, kernel number *per* unit canopy weight at anthesis, and standard kernel size under optimum conditions. Firstly, the phenology was calibrated until the simulated and observed dates for anthesis and maturity were close by adjusting the parameters of vernalization and photoperiod sensitivity. Next, the biomass accumulation was calibrated by adjusting the phyllochron parameter, and finally grain yield was calibrated. All the parameters were adjusted by trial and error. The model was evaluated on soil water, soil N, plant biomass, plant N%, grain yield, and grain protein for Experiment 1. The Balruddery 2011 and 2012 data (Experiment 2) were used for the evaluation of phenology and grain yield simulation, while the 2017 (Experiment 3) was used for the evaluation of phenology, biomass and grain yield.

The daily weather data (1974–2018) from the Invergowrie site (Experiment 1) were used as input to the crop model for the long-term simulation runs. In order to capture the impacts of climate variability on crop growth, development and yield, the crop management was kept the same every year, with the weather being the only variable factor. The initial conditions of soil water and N were re-set every year to optimal conditions. The amount of N applied to the simulation was 120 kg N ha^{-1}.

The information about the end-use of barley, the requested quality and the market share were obtained from The Maltsters' Association of Great Britain (UK Malt, 2019). These data were used to compare the observed data from Experiment#1 and the simulated data using long-term weather data (45 years) to quantify the number of years in which the grain N% was not suitable for distilling/brewing purposes (Table 1).

2.3. Statistical analysis

The goodness of fit of the simulated vs. observed data for calibration and evaluation was calculated using the Root Mean Square Error (RMSE) as follows:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}(y_i - \hat{y}_i)^2} \qquad (1)$$

Table 1
End-use of barley, amount of grain N requested for each use and the relative amount of market share. The number of years occurring represents the number of years that the simulated values of grain N reached the requested grain N%.

End use	Grain N requested	Market Share	Years occurring
–	*(%)*	*(%)*	*(#)*
Cask-conditioned ale	up to 1.55	5	11
Distilling	up to 1.65	30	17
Most UK & EU brew	1.55-1.75	40	11
Third countries brewers	1.70-1.85	20	23
Other use	N.A.	5	–
Malting premium paid to Scottish barley producers	Up to 1.85%	–	41

where y_i are the observations, $\hat{y}_i$ the simulations, and n is the number of comparisons. In addition, the Wilmott index of agreement (D-Index) was calculated (Wilmott, 1982). The index ranges from 0 (poor model fit) to 1 (good model fit). The index is a descriptive measure and can be widely applied to make cross-comparison between models (Wilmott, 1982). It is calculated as follows:

$$D - Index = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(|y_i - \bar{y}| + |\hat{y}_i - \bar{y}|)^2} \qquad (2)$$

where $\bar{y}$ is the mean of the observed values.

The long-term weather data was analyzed for patterns of daily minimum and maximum temperature changes using a regression analysis. In addition, for each month, the long-term trends of daily minimum and maximum temperature were analyzed. The monthly rainfall was analyzed as absolute changes between the long-term average for that month and the monthly rainfall. The monthly maximum and minimum temperatures were also analyzed by decomposing the time-series into three components: the overall trend component, the seasonal component and the irregular (noise) component. The time-series analysis was done using R statistical software and the TTR package (Ulrich, 2018). The main time-series trend was presented in the main manuscript while the decomposed variability was available in the Supplemental Material.

3. Results

3.1. Calibration and evaluation

The simulation of barley phenology for the + N-IRR calibration dataset is shown in Fig. 1a. After calibration a very good simulation of phenology was obtained. The simulated days after planting for anthesis was only one day different from the observed one. The simulated days after planting for maturity was the same as the observed one. The observed grain yield was 3500 kg of dry matter (DM) ha^{-1}. Simulated grain yield was 240 kg DM ha^{-1} greater than the observed one; however, the standard deviation of observed yield was 500 kg DM ha^{-1} (Fig. 1b). With the independent evaluation set, simulation of anthesis dates across the different treatments and for different years showed a RMSE of 3.5 and a D-index of 0.97 (Fig. 1c), while simulated maturity dates had a RMSE of 1.2 d and a D-index of 0.99 (Fig. 1d). The simulated barley yield had a RMSE of 471 kg DM ha^{-1} and a D-index of 0.99. The standard deviation of the observed yield ranged from 174 kg DM ha^{-1} for the 0 N-RF treatment to 840 kg DM ha^{-1} for the 2011 field experiment (Fig. 1e). The simulated grain N% showed an RMSE of 0.13% with the simulated values over-grain N% (Fig. S2). The crop coefficient parameters used in the model after calibration are reported in Table S5.

The simulated and measured above ground biomass is shown in Fig. 2 for all the 4 treatments of the Experiment#1. Overall, the patterns of simulated biomass were able to capture the biomass changes in the observed data, despite a general tendency to overestimate measured values. The RMSE was 701, 475, 852, 416 kg DM ha^{-1} for the + N-IRR, +N-RF, 0 N-IRR, 0 N-RF, respectively (Tab. S6). The observed relative changes in biomass respect to the + N-IRR was also evaluated between observed and simulated data. The + N-RF had 49% less biomass at harvest than the + N-IRR, while the 0 N-IRR and the 0 N-RF had -48% and -63%, respectively (Tab. S7). The simulated changes of biomass, respect to the + N-IRR, were -50%, -40%, and -62% for the + N-RF, 0 N-IRR, and 0 N-RF, respectively (Tab. S7).

The simulated volumetric soil water content at each soil depth is shown in Fig. 3 for all the treatments of the 2018 experiment. Overall, the rainfed treatments showed lower observed soil water content for the first sampling; but the differences were less marked for the remaining points over time and among different depths (Fig. 3). The RMSE and D-Index for all the treatments are shown in Table S6. The values or RMSE

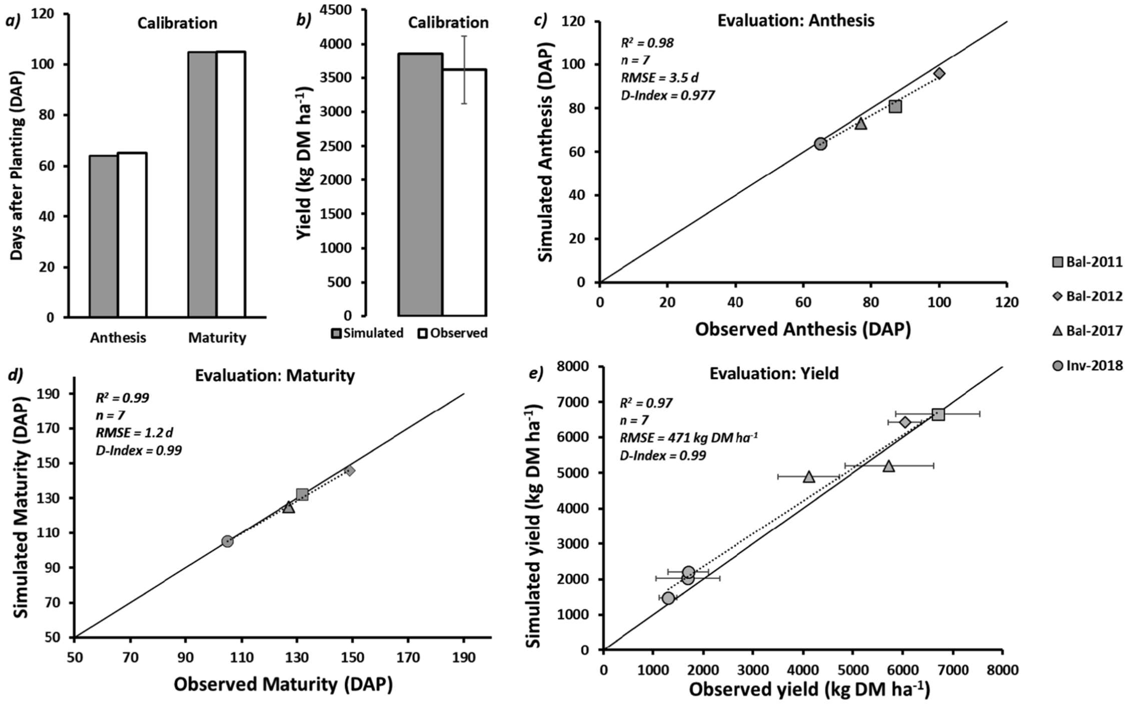

Fig. 1. The use of DSSAT software to simulate spring barley with a: (a) calibration for anthesis, maturity and (b) grain yield; (c) evaluation of flowering dates (DAP = Days after planting); (d) maturity dates; and (e) grain yield for all the other treatments and experiments. The circles represent the Invergowrie 2018 treatments (+N-RF; 0 N-IRR; 0 N-RF; Experiment#1), the square and diamond represent the Balruddery 2011 and 2012 experiments (Experiment#2), the triangle the Balruddery 2017 fertilizer experiment (+N and 0 N; Experiment#3), respectively.

ranged from 0.03 to 0.06 across the treatments, with D-Index for the 0 N-IRR showed the lowest value of 0.50 (Tab. S6).

The simulated soil N content and plant N% showed good agreement vs. observed + N treatments, irrespective of the irrigation levels, whilst the 0 N treatments showed lower RMSEs and D-Index values than + N treatments (Figs. S3-4 and Tab. S6).

3.2. Climate trends

The historical patterns of daily maximum temperature showed a

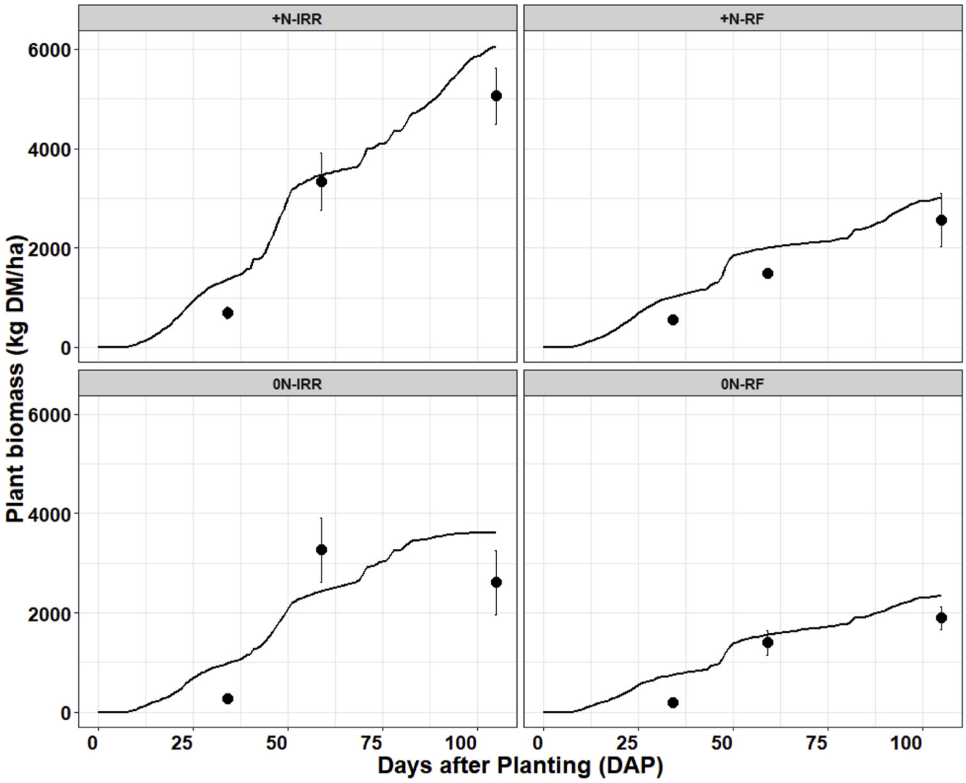

Fig. 2. Simulated (full line) and observed (dots) crop dry biomass at Experiment#1 for the fully irrigated and fertilized (+N-IRR), fertilized and rainfed (+N-RF), non-fertilized and irrigated (0 N-IRR), and non-fertilized and rainfed (0 N-RF) treatments. The vertical lines on the observed values of biomass represent the standard deviation of the average (n = 3).

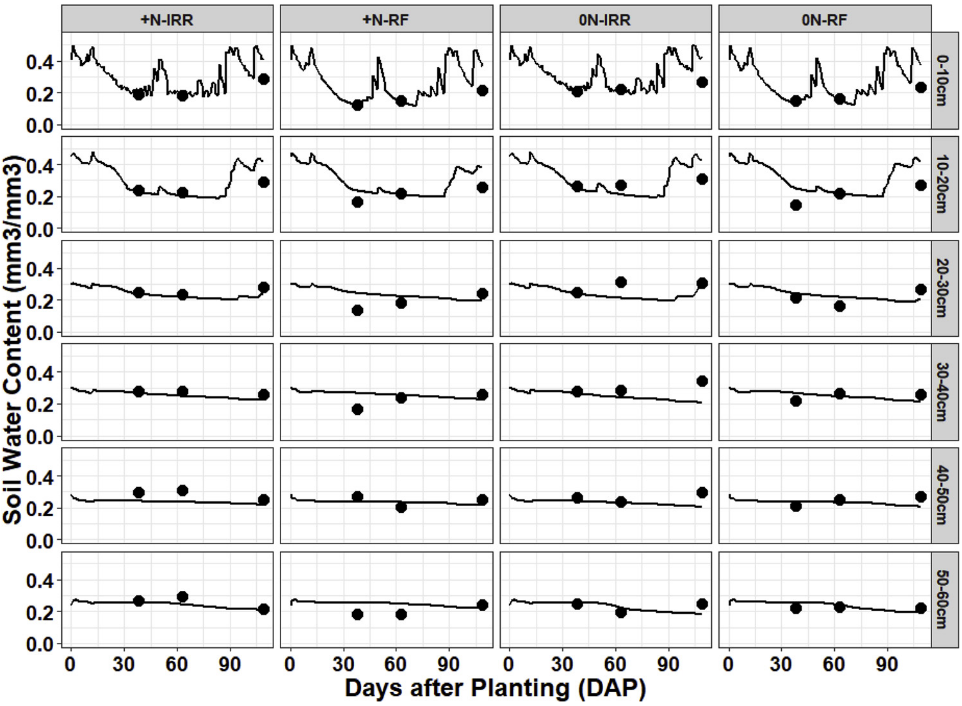

Fig. 3. Simulated (full line) and observed (dots) volumetric soil water content at six depths (0–10, 10–20, 20–30, 30–40, 40–50, 50–60 cm) for Experiment#1 for four treatments: the fully irrigated and fertilized (+ N-IRR), fertilized and rainfed (+ N-RF), non-fertilized and irrigated (0 N-IRR), and non-fertilizer and rainfed (0 N-RF).

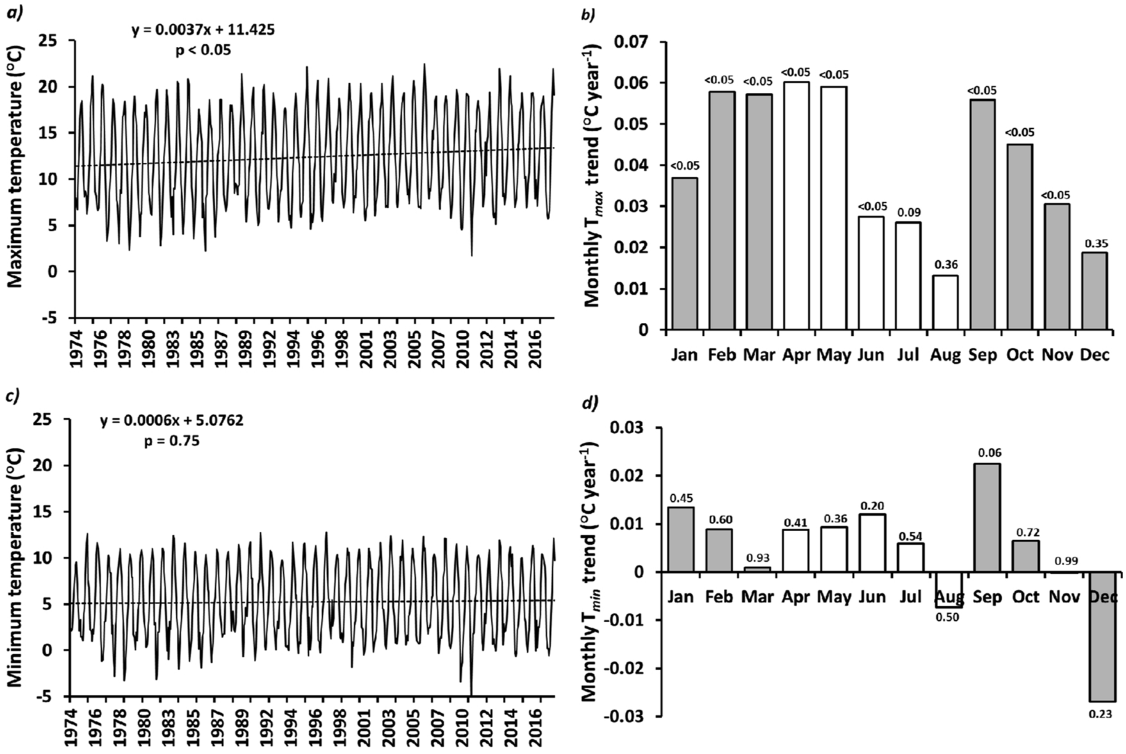

Fig. 4. (a) Monthly air temperature patterns for maximum temperature (°C); (b) monthly maximum temperature (°C) changes over 45 years, the numbers on top of the bars represent the p values of the slope of the changes, the white bars represent the usual spring barley growing season; (c) patterns for minimum temperature (°C); (d) monthly minimum temperature (°C) changes over 45 years, the numbers on top of the bars represent the p values of the slope of the changes, the white bars represent the usual spring barley growing season.

slight but statistically significant ($p < 0.05$) increase over the 45 years (Fig. 4a and Fig. S5) with Feb, Mar, Apr, May showing about 0.06 °C year^{-1} increase in daily maximum temperature (T*max*), while Jun, Jul, Aug and Dec showed the lowest T_{max} increase (Fig. 4b). On the other hand, the daily minimum temperature (T*min*) was stable over the 45 years with no-significant changes of the slope ($p = 0.75$; Fig. 4c and Fig. S6), with some months, like Aug and Dec showing a decrease of -0.001 and -0.0025 °C year^{-1} T*min*, respectively (Fig. 4d). Therefore, for some months (e.g. Aug), the amplitude between maximum and minimum temperature diverged (Fig. 4).

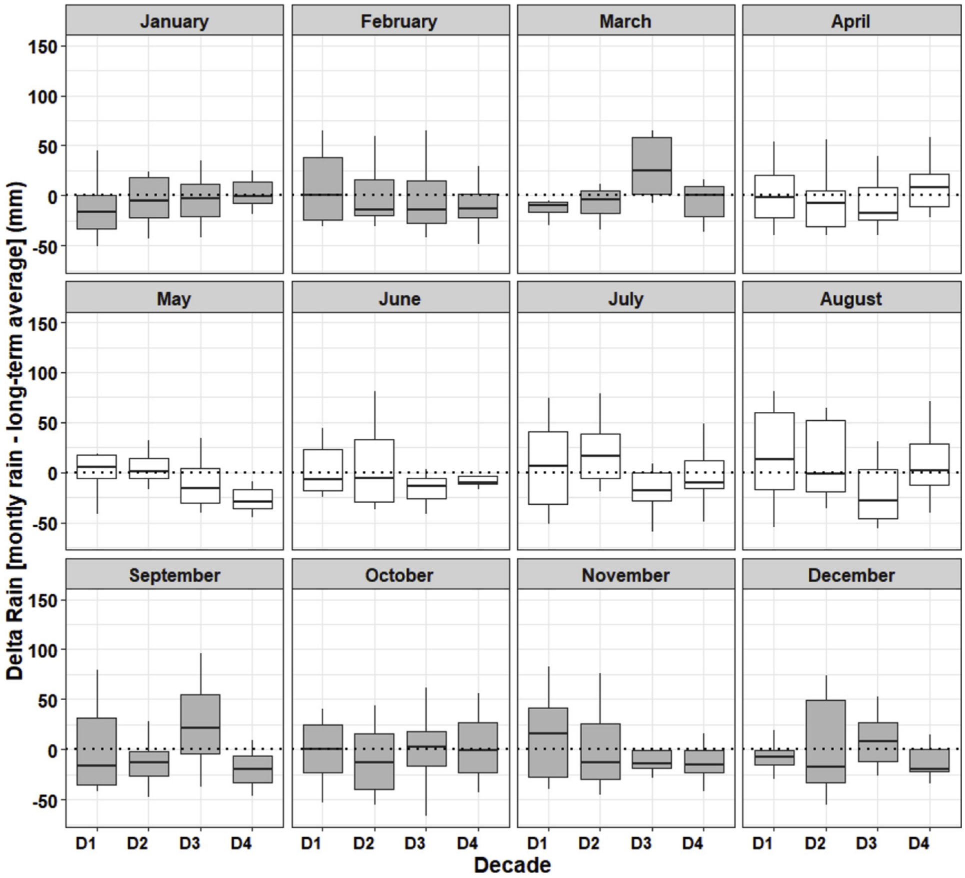

Fig. 5. Boxplots of delta monthly rainfall (mm) (monthly rainfall minus long-term average) for the months where spring barley grows (white boxplots) and for the remaining months (grey boxplots). Long-term weather data from weather station of Experiment#1. For each boxplot, the end of the vertical line represents, from top to the bottom, the 10th percentile and the 90th percentile. The horizontal line of the box, from the top to the bottom represents the 25th, median, and 75th percentile, respectively.

The long-term rainfall was disaggregated into months. The months when spring barley is grown (from April to August) were considered as the growing season rainfall. Fig. 5 showed the box plots of the difference between monthly rain and long-term averages for each of the 4 decades (1974–1983; 1984–1993; 1994–2003; 2004–2013) of recorded daily rainfall. Overall, the mean delta rainfall for months when barley does not grow ranged between 50 and 80 mm, with March (when soil is normally cultivated for planting) showing little change across decades, except for the third decade (1994–2003) that had about 55 mm more rainfall than the long-term average (Fig. 5). On the other hand, during the growing season months, the last two decades of May were drier than the long-term average with -25 mm rainfall compared to the long-term average (Fig. 5). The average long-term growing season rainfall was 215 mm and the 2018 growing season rainfall (140 mm) was well below that average as well as growing seasons 1982, 1984, 1989 and 1975 (Fig. S7).

3.3. Long-term crop modelling simulations

The simulated grain yield for the 45 years corresponded with the patterns of growing season rainfall for each year (Fig. 6a). In contrast, there was no relationship between mean air temperature and simulated grain yield (Fig. 6b). The patterns of simulated anthesis dates and mean air temperature is shown in Fig. 6c. There was a decrease in anthesis date between 1974 to 2018 of about 6 days, while at the same time the daily mean growing season temperature increased (Fig. 6c). Similar patterns were observed for the simulated maturity dates (Fig. 6d).

The simulated biomass growth patterns were highly related to the timing and amount of water stress (Fig. 7). The extent and severity of the water stress, which, in the model impacts on expansive growth processes and therefore biomass and yield, was related to the timing and amount of rainfall events. The blue line in the Fig. 7 represents the Water Stress Index, which in DSSAT is calculated from the ratio between water supply to water demand of the crop and ranges between 0 (no stress) to 1 (maximum stress). For example, in 2016 there was a moderate to severe early water stress which impacted biomass in a similar manner to the water stress in 2005. Severe water stress in 1984, 2003, 2018 also negatively affected biomass (Fig. 7). In years when there was no or little water stress (e.g. 2004, 2012) there was high above-ground biomass. From a year like 2012 to a dry year like 2018 there was about 50% difference in biomass accumulation and consequently in grain yield (Fig. 7). The daily simulated soil water content for each year (Fig. S8) showed that soil water content was usually being depleted from sowing to harvest, except the wetter years, in which the residual soil water content at harvest was greater than at the beginning of the growing season (Fig. S8). The patterns of water stress impacted the simulated partitioning of soil evaporation and plant transpiration during each growing season, with dry years showing a greater cumulated soil evaporation relative to plant transpiration (Fig. S9). The year 2018 was dryer and warmer than average and the observed delta soil water content (final minus initial values) was about −20 mm (Fig. S10a). The delta soil water content calculated on the simulated data over 45 years ranged from -60 to 25 mm with an average delta of −38 mm (Fig. S10a). This meant that for every growing season there was, on average, less water at harvest than at the beginning of the season.

3.4. Grain nitrogen

The relationship between observed grain N% and grain yield for each treatment of Experiment 1 is shown in Fig. 8. Overall, additional N tended to increase grain N% while additional water caused higher yield. From the experiment 1, 0 N-RF showed on average 1.48% grain N and 1300 kg DM ha^{-1} yield, whereas the irrigated treatment (0 N-IRR)

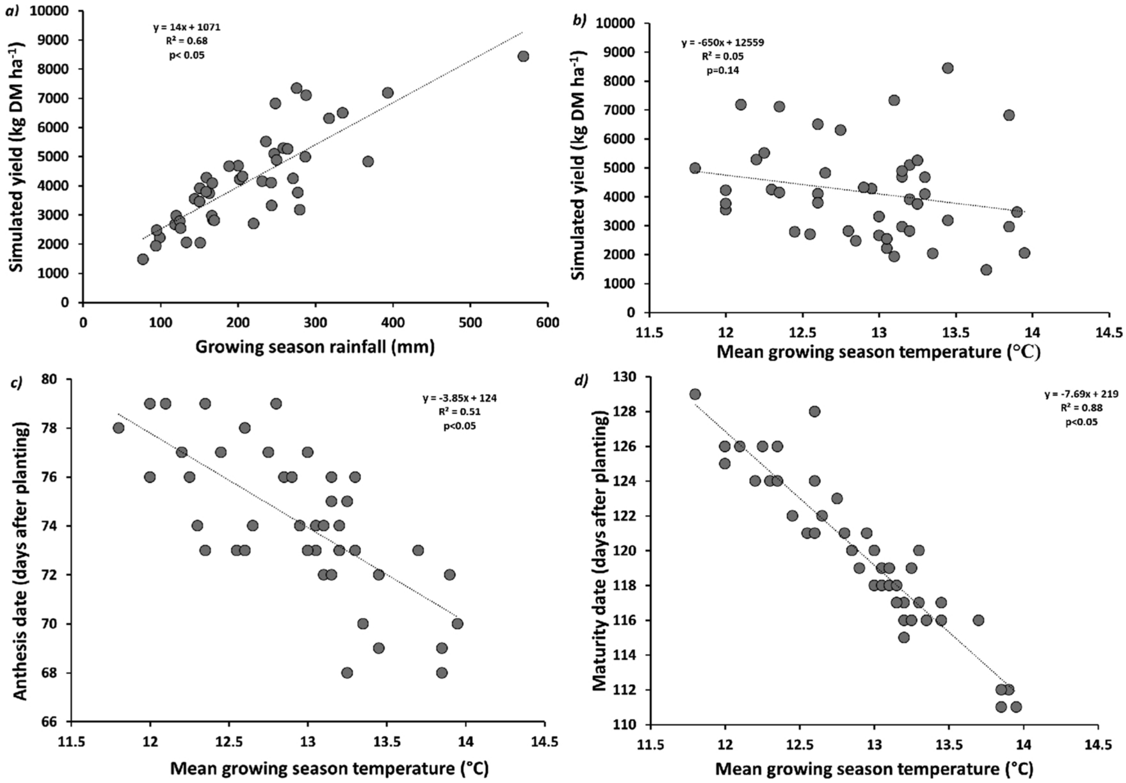

Fig. 6. Relationship of long-term simulations between (a) simulated grain yield (kg DM ha^{-1}) and growing season rainfall (mm); (b) simulated grain yield (kg DM ha^{-1}) and mean growing season temperature (°C); (c) simulated anthesis dates (days after planting) and mean growing season temperature (°C), and (d) simulated maturity dates (days after planting) and mean growing season temperature(°C).

showed 1.52% of grain N and 1700 kg DM ha^{-1} yield (Fig. 8). The addition of fertilizer with no irrigation (+N-RF) resulted in harvested yield values of 1700 kg DM ha^{-1} and 1.65% grain N, and for the irrigated and fertilized plot there was the greatest yield of 3600 kg DM ha^{-1} and 1.57% grain N (Fig. 8). The simulated dataset using long-term weather data showed values of yield and grain N% that fell within the range of the observed ones (Fig. 8).

The different requirements for grain N% was a function of the use of barley for either malting or distilling (Table 1). For cask-conditioned ale the requirements in the UK were to have a grain N% up to 1.55% while for distilling was up to 1.65%. However, the premium paid to Scottish barley producers included grain N up to 1.85%. 40% of the market shares for barley production was represented by UK and EU brewers which required a grain N% between 1.55–1.75%. The simulated results showed that these conditions in our study area were not always met. The requirements for UK-EU brewers for cask-conditioned ale were met only 11 out of 45 years (Table 1).

Simulated crop N uptake was correlated with the amount of rainfall through the growing season up to a certain level, in fact, above 300 mm of rainfall there was no additional N uptake (Fig. 9a). The residual soil N amount at harvest ranged from 9 to 215 kg N ha^{-1} and showed a negative relationship with rainfall (Fig. 9b). The grain N content showed similar patterns as the crop N uptake showing no additional grain N above growing season rainfall of 300 mm (Fig. 9c). The extractable soil water content at harvest ranged from 2 to 30 mm for years with a growing season rainfall up to 200 mm, while in years with above 300 mm of rainfall there was no increase in extractable soil water content which levelled off at 63 mm (Fig. 9d).

4. Discussion

4.1. Experimental data – experiment 1

The 2018 growing season was particularly dry, with about 140 mm of rainfall during the growing season. All the treatments started with the same soil water content, but the irrigated treatments (-IRR) kept a soil water content around 80–90 mm for the whole growing season while the rainfed ones dropped one month after sowing to values of 20–30 mm (Fig. 3). Thus, the grain yield of + N-IRR treatment (3500 kg DM ha^{-1}) produced greater yield, while for the other treatments (0 N-IRR and + N-RF) there was no yield effect (1700 kg DM ha^{-1}) (Fig. 8). The effects of nitrogen deficiency on barley growth are well known (Chapin et al., 1988) and were similar to those associated to water stress with N under rainfed conditions: the N applied to the soil is not taken up by the water stressed crop resulting in similar impact on photosynthesis and plant growth associated to N deficiency confirming the results reported by Garstang and Vaughan (1992). In addition, the sowing date was particularly late for a typical spring barley and that was another factor that negatively impacted on the yield level of the experiment.

4.2. Calibration and evaluation

The evaluation of the crop model using different stress levels (from the Experiment#1) and experiments that were made in different years and different locations, using the same cultivar (Concerto), showed that the cultivar was well calibrated. A previous multi-modelling comparison study of spring barley in northern Europe showed higher degrees of variability between observed and simulated results (Rötter et al., 2012). However, in the study of Rötter et al. (2012) the amount of data provided for model calibration and evaluation was less than that used for the current study. In addition, the focus here is on the application of a

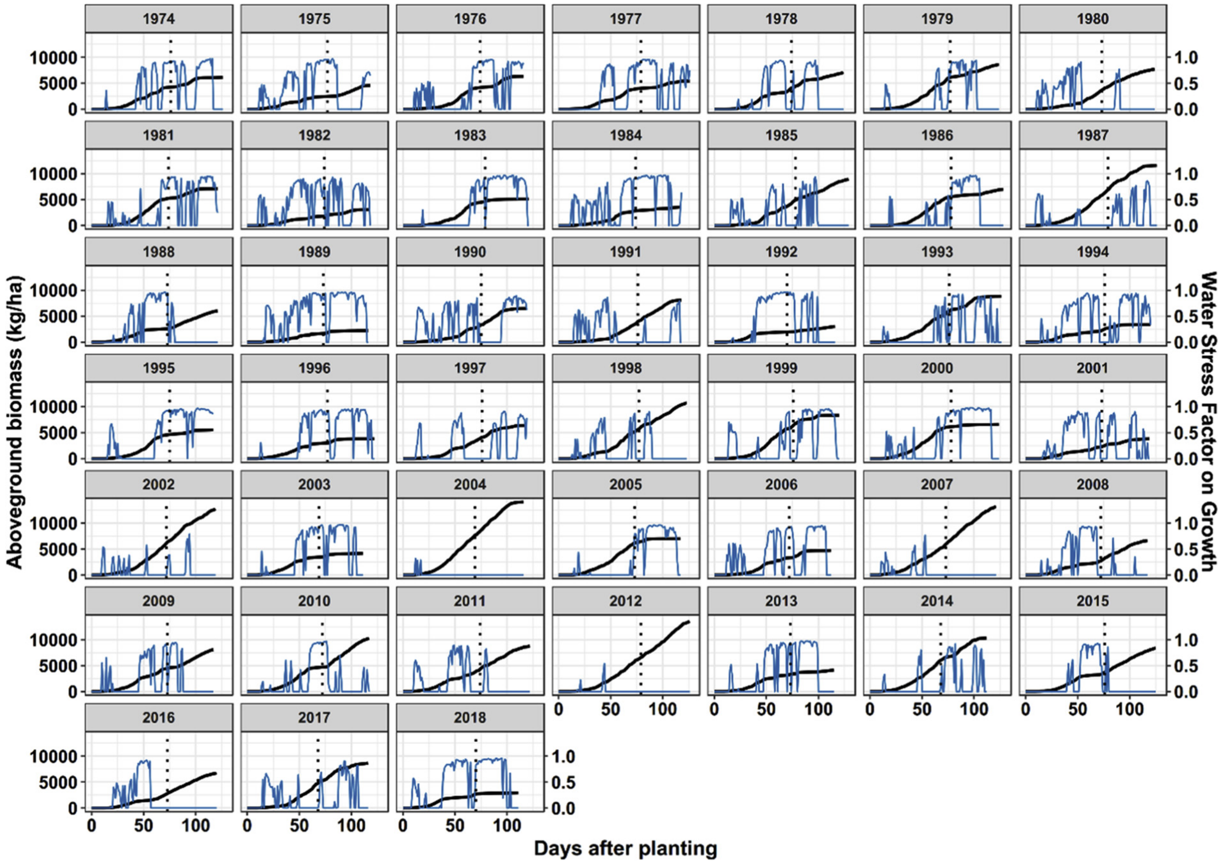

Fig. 7. Simulated patterns of daily biomass growth (kg ha^{-1}) (black line) and the simulated water stress factor (0 = no stress; 1 = max stress) that affects expansive growth processes in the crop model (blue line). The vertical dotted line represents the simulated anthesis date for each year. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

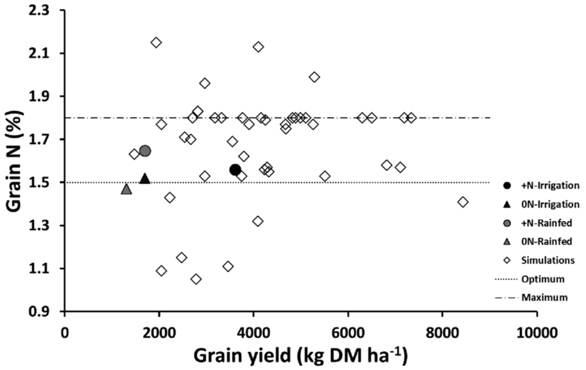

Fig. 8. Observed values of grain N (%) and grain dry yield (kg DM ha^{-1}) for the irrigated and fertilized treatment (+N-IRR black dot), the non-fertilized and irrigated treatment (0 N-IRR black triangle), the fertilized and rainfed treatment (+N-RF grey dot), and the non-fertilized and rainfed treatment (0 N-RF grey triangle) for Experiment 1 and from the 45 years of simulated data (open diamond). The dotted line represents the optimum N% amount needed by distilling and the dash-dot line the maximum N% amount above which there is no premium paid according to The Maltsters' Association of Great Britain (UK Malt, 2019).

crop model for extrapolating additional information on the soil-plant-atmosphere interactions. Given that the initial conditions of soil water and nitrogen were provided, the model, after the calibration, showed good fit with the independent datasets used for comparison. For all the 2018 treatments the simulated biomass was higher than the observed values, but the changes relative to the + N-IRR showed similar values for the observation and the simulations (Tab. S7). This means that even if model simulations overestimate plant N% and yield values, changes resulting from stressed conditions tend to be closer to the observed values. Such behaviour has been reported elsewhere using different crop models and different combinations of stresses (Asseng et al., 2004; O'Leary et al., 2015).

4.3. Climate trends

The daily maximum and minimum temperatures were analyzed in three different ways, as a yearly trend and as a monthly change (Fig. 4) and as a growing season change (Fig. 6). Fig. 4 showed that during the barley growing season there was a trend towards increasing mean air temperature, but such a trend was not too evident in the yearly changes (Fig. 4 a and c). The monthly temperature patterns indicated that during the months of maximum spring barley growth (Apr to Jun) there was an increased trend of maximum and minimum temperature associated with a decrease in monthly rainfall, especially in the last decade (Figs. 4 and 5). The weak relationship between yield and mean air temperature (Fig. 6b) is expected because in Scotland the daily maximum air temperature rarely reaches the optimal cardinal temperature threshold, above which there would be negative consequences for phenology and growth of barley (Luo, 2011). There was the expected negative relationship between increase in mean temperature and trends of anthesis and maturity dates (Fig. 6c and d). But this did not cause yield reductions because the environments are not radiation limited and a small acceleration in crop development did not cause a shortening of biomass accumulation. Therefore, while the analyses of Fig. 6 and the relationship between weather impacts on yield and phenology were based using long-term observed data and simulated yields, they still provide valid information on patterns for typical for the east of Scotland

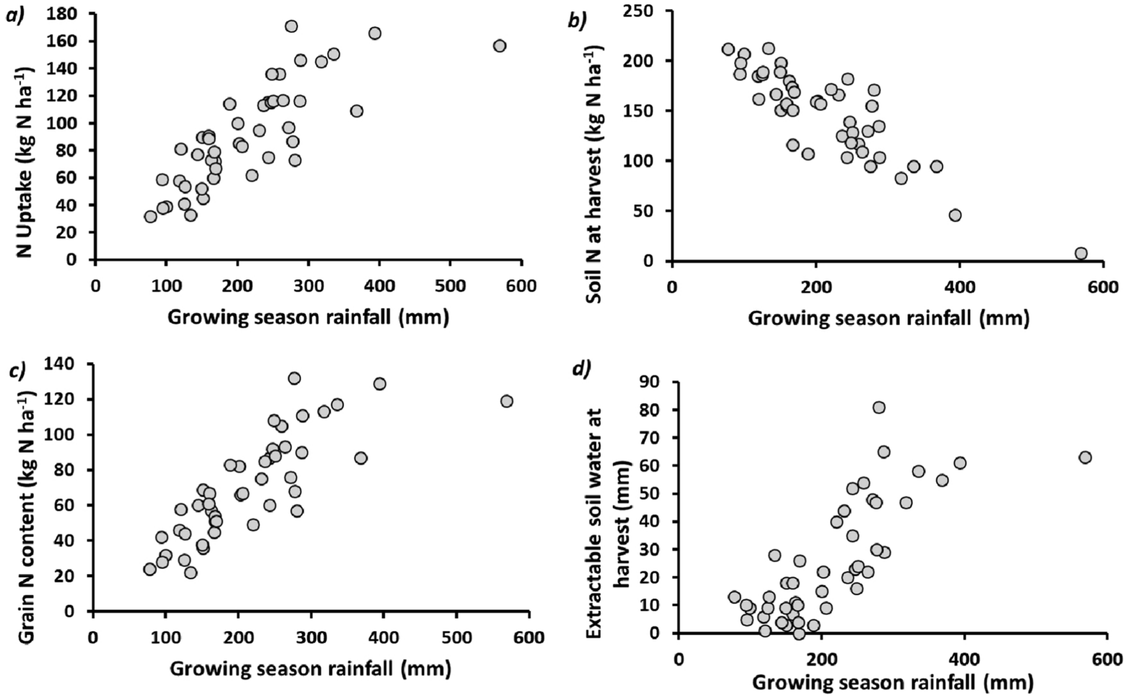

Fig. 9. Relationships between growing season rainfall and simulated values of (a) crop N uptake (kg N ha^{-1}); (b) soil N content at harvest (kg N ha^{-1}); (c) grain N content (kg N ha^{-1}); (d) extractable soil water (mm) at harvest for the simulations using long-term weather data.

environment.

The amount of the growing season rainfall impacted the timing and severity of the water stress and this was observed in the biomass reduction (Fig. 7). From anthesis (vertical dotted line of Fig. 7) to maturity there was often some water stress experienced by the crop. The dotted line (anthesis) represents also the subdivision of barley growth into two phases. In the first phase, from sowing to anthesis, barley captures and assimilates resources (canopy and root system) and establishes potential grain sites. In the second phase, from anthesis to maturity, grains develop and fill (Samarah, 2005). When mild water stress was experienced during vegetative stages, the crop recovered to produce high biomass values, like for example in 2007 and 2012. There was a positive relationship between growing season rainfall and N uptake, grain N content and the extracted soil water content at harvest (Fig. 9 a, c, d).

Scotland is a country with high annual rainfall, but there is a high spatial variability in its annual distribution, e.g. 1100 mm for Glasgow, West Scotland vs. 700 mm for Dundee, Scotland (Cammarano et al., 2016a). In a recent study Cammarano et al. (2016a) showed how the spatial distribution of rainfall for the spring barley growing season ranged from an average of 160 to 400 mm with high values on the west and inland and low values on the east coast. The results of the present study highlight how rainfall is more important than temperature for production of spring barley. In a different study Werritty (2002) using long-term precipitation data showed that the east of Scotland was becoming drier resulting in less water runoff. Martin et al. (2017) found that, in the North Atlantic regions, including Scotland, the long-term climate patterns meant better opportunities for expanding barley production, but the high rainfall at maritime sites, and low rainfall at continental sites, will limit the ability of growers to benefit from the warming trend.

In drier years there is a co-limitation effect of water and nitrogen for plants; in such years, water stress can impair the capability of plants to uptake nutrients. Passioura (2006) discussed how the evaporative loss of water from the soil was being influenced by the nitrogen status because of its impacts on leaf area growth. Sadras (2004) using a combination of observed and modelled data, concluded that in systems with both nitrogen and water limitations, yield and water-use efficiency of water- and nitrogen-stressed crops increase with increasing degree of co-limitation. Francia et al. (2011) found that in Mediterranean environments barley production can be negatively impacted by terminal drought events.

The overall yield results of the experimental year (2018) agreed with the finding of Sadras (2004) where the rainfed treatment with the addition of N (+N-RF) showed higher yields than the unfertilized one (0 N-RF). The subsequent modelling approach showed that in drier years when both water and N stresses were present (Fig. 7 and S11) the cumulative amount of soil evaporation was higher than the simulated plant transpiration (Fig. S9). In such years there was low crop N uptake and high residual N in the soil left at harvest (Fig. 9 and S12).

A combination of better agronomic practices such as shifting sowing dates (Al-Ajlouni et al., 2016; Cammarano et al., 2019) (which can be beneficial in the short-term) and breeding for better rooting traits (beneficial in the long-term) can help to offset such rainfall trends in the mid-long term.

4.4. Grain nitrogen

Most of the market share reported by UK Malt (2019) showed how spring barley is preferentially used by UK and EU brewers with a requirement of grain N of ˜ 1.55–1.75%. In recent years, the expansion of the distilling industry for whisky production in Scotland meant that most of the spring barley produced is used locally. In this case, the malting premium is paid to Scottish spring barley producers only for grain N up to 1.85% (Table 1). Our simulated results showed that the premium for distilling is reached in 41 out of 45 years (> 90%) investigated in this study. But if quality parameters are restricted according to the values indicated Table 1 then such occurrence would change. The impacts of environmental factors, such as water and temperature, and management practices like seeding rates and cultivar choice influences the malting quality of barley more than the N fertilization rates (Sainju et al., 2013). In addition, McTaggart and Smith (1995) reported that fertilizer form (such as calcium nitrate, ammonium nitrate and ammonium sulphate) did not influence grain N content. The same authors also showed that dry soil conditions can reduce grain yield, increasing grain N content like also observed in the present study (Fig. 8).

The different requirements for grain N% was a function of the use of barley for either malting or distilling (Table 1). For cask-conditioned ale the requirements in the UK are to have a grain N% up to 1.55% and for distilling was up to 1.65%. However, 40% of the market shares for barley production are represented by UK and EU brewers which require a grain N% between 1.55–1.75%. The simulated results showed that these conditions in our study area were not always met. The requirements for UK-EU brewers for cask-conditioned ale were met only 11 out of 45 years (Table 1). On the other hand, if the requirements for premium paid to Scottish farmers (grain N up to 1.85%) were being analyzed the conditions occurred 41 out of 45 years (Table 1). Other malting quality parameters are important as well, such as the 1000 grain weight, viscosity, calibre of the seeds and hot water extract. The calibre along with the 1000 seeds weight indicates the degree of grain filling, and to produce malt classified as good quality grains with calibre of 2.5 mm or higher are used. The hot water extract indicates the extracted material used during the alcoholic fermentation and it is an important parameter for quality purposes. However, if these measurements were determined on the experimental site, they could have not been simulated using the modelling approach because most of the crop simulation models only simulate grain N%. Therefore, it was considered, among the indicators of grain quality, the parameter that could be directly compared to what the industry uses as benchmark (UK Malt, 2019). Martre et al. (2006) developed a specific model for grain quality on wheat and future work is needed to adapt that model to barley.

5. Conclusions

In conclusion, the east of Scotland, where most of the spring barley grows is prone to spring droughts, and this can have an impact on crop expansive growth and grain yield production. However, the grain N% needed for distilling quality is not affected and crops will be within the specifications required for premium in 41 out of 45 years. If the water stress impact is minimized the spring barley yields could be further increased without causing a decrease in grain quality, which will represent an economic advantage to farmers. Future work should consider other management factors (e. g. seeding rates, N fertilizer rates and cultivar choice) impacting grain quality and the interaction with water stress.

A combination of shifting sowing dates and breeding for better rooting traits can help to offset the effects of spring rainfall trends observed in eastern Scotland on barley yield. The impacts of projected climate on grain quality and water stress should also be considered. Soil health and biodiversity will become more important in offsetting the impacts of climate variability. Practices, such as increasing soil carbon, direct drilling, under-sowing with clover, and intercropping are worth to be explored to test their effectiveness in providing more resilience to the system and therefore reduce climatic risks in barley production. Crop traits such as root traits can help offsetting the risk of yield penalties as well as breeding for low input conditions.

Results of this study are limited to a typical climate zone of Scotland and further work would also require the scaling up of such kind of analysis at the whole barley growing area of Scotland.

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