



# The potential of crop models in simulation of barley quality traits under changing climates: A review

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## ABSTRACT

Most of the experimental and modeling studies that evaluate the impacts of climate change and variability on barley have been focused on grain yield. However, little is known on the effects of combined change in temperature, CO<sub>2</sub> concentration, and extreme events on barley grain quality and how capable are the current process-based crop models capture the signal of climate change on quality traits. Here in this review, we initially explored the response of quality traits of barley to heat, drought, and CO<sub>2</sub> concentration from experiential studies. Next, we reviewed the state of the art of some of the current modeling approaches to capture grain quality. Lastly, we suggested possible opportunities to improve current models for tracking the detailed quality traits of barley. Heat and drought stress increase the protein concentration which has a negative effect on malting quality. The rise of CO<sub>2</sub> concentration significantly reduces the grain protein, again resulting in a decline of the malting and brewing quality since the nitrogen concentration of grains needs to be kept at a specific level. The current crop models that simulate barley grain quality are limited to simulation of grain nitrogen concentration, size, and number in response to climate extremes and CO<sub>2</sub>. Nevertheless, crop models fail to account for the complex interactions between the conflicting effects of rising temperatures and droughts as well as increasing CO<sub>2</sub> concentrations on grain protein. They have mainly adapted wheat models that cannot capture barley's protein composition and whole grain malting quality. Implementation of experiments from gene to canopy scales which are explicitly designed to detect the interactions among environmental variables on detailed quality traits and couple the remote sensing plus data-driven approaches to crop models are possible opportunities to improve modeling of barley grain quality. The development of modeling routines can capture the detailed grain quality provide valuable tools for forming climate adaptive strategies. Equally important, they can guide breeding programs to develop climate-resilient but high-quality barley genotypes.

## 1. Introduction

Barley (*Hordeum vulgare* L.) is among the oldest cultivated global crops and, respect to other cereals, it is adapted to grow in many different environments spanning from the equator to the arctic circle and at many different latitudes (Newton et al., 2011; Dawson et al., 2015). Despite such potentially wide growing habitat barley is only the fourth most cultivated cereal (beyond wheat, maize and rice) and eleventh among the main cultivated crops (Newton et al., 2011; FAO-STAT, 2021). It is a crop that, depending of the socio-economic context, is used as animal feed and/or forage, food, and drink for humans (Newton et al., 2011). In general, barley grain yield is more stable

against seasonal variation and heat than wheat and most other small grains, so it is preferred by resource-poor farmers in order to reduce the risk of very low yield or crop failure (Akar et al., 1999). From 1961–2019 the mean harvested area was 64 million ha, ranging between 47 and 84 million ha (Fig. 1a). Since the 80 s the area harvested declined from 84 million ha to the actual 50 million ha recorded recently (Fig. 1a). The overall unit yield has increased, for the same period of about 2 t ha<sup>-1</sup> globally (Fig. 1b). For the period 2009–2019 the top 20 producers of barley, which produced about 84 % of the total world's barley, were reported in Fig. 1c, with Russia being the country that produced an average 17 million tons (± 3.4 million tons for the 2009–2019 period) of barley followed by France with 11.4 tons (± 1.4

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million tons for the 2009–2019 period; Fig. 1c).

Due to rising demands for crop production and a climate change threat, providing food for the ever-growing population to maintain food security has been a significant concern (Wheeler and Braun, 2013). Using process-based crop models, a wide set of studies have investigated the potential impacts of climate change (increased temperature, CO<sub>2</sub> concentrations, and weather extremes) on crop growth and productivity from local to global levels (Asseng et al., 2015; Liu et al., 2016; Jägermeyr et al., 2021). The yield stability of barley under climatic variabilities is frequently overestimated compared to wheat or maize, primarily due to their higher yield potential (Dawson et al., 2015). Future projections of climate trends indicate that most of the harvested barley areas will get warmer and drier, resulting in a global decline in barley yield and production (3–17 % depending on the environment) could lead to a more than 100 % increase in beer price (Xie et al., 2018; Cheng et al., 2019). However, that study only included barley yield ignoring the role of grain N % limits for brewing which is far more critical than yield (e.g., if grain N % is not in a given range, then a higher/lower yield is pointless). In addition, not all the countries will export/use the spring barley for beer production. A set of regional impact assessment studies in the Mediterranean basin (–25 % to –8 % depending on climate scenarios), Kazakhstan (–4.8 %), Czech Republic (–19 % to +5 %), Iran (–50 %) showed a relatively similar decline in barley yield under climate change conditions (Trnka et al., 2004; Cammarano et al., 2019; Mirgol et al., 2020; Schierhorn et al., 2020). The potential of rainfed farming of spring barley is languishing due to a

growing risk of severe droughts across western and central Europe due to climate change (Trnka et al., 2010). On the other hand, impact assessment studies in higher latitudes (e.g., Finland) demonstrated positive effects of temperature increase and elevated CO<sub>2</sub> on barley yield under optimistic climate scenarios (Rötter et al., 2012).

Beer and whisky production bring the highest added value of barley commercially. However, malting barley requires special qualitative features depending on malting, distilling or brewing industries. Quality traits of grains can be defined by physical and compositional properties, with thresholds based on end-use essentials (Nuttall et al., 2017). The crude protein content is the most crucial element specifying barley's quality for such industries as a function of grain nitrogen content (Prystupa et al., 2021). The high protein level in barley reduces the starch content leading to a lower alcohol level; nevertheless, yeast activity is restricted by nitrogen shortage under lower grain protein levels (Pettersson and Eckersten, 2007). Therefore, it is critical to keep the protein level of the barley grains in a particular range to ensure the malting quality (Luo et al., 2019). Such quality trait is controlled by the genotype, environmental characteristics and the processing (Slafer et al., 2002). Numerous studies have documented climate change's effects on crop yield, while the quality traits of crops is an essential aspect of food production, it has received considerably less attention (Asseng et al., 2019). An elevated CO<sub>2</sub> level under climate change would increase grain starch concentration, declining grain protein content, despite a higher magnitude of heat/drought stress reduced grain starch content (Erbs et al., 2010; Högy et al., 2013). The level of β-Glucan as an

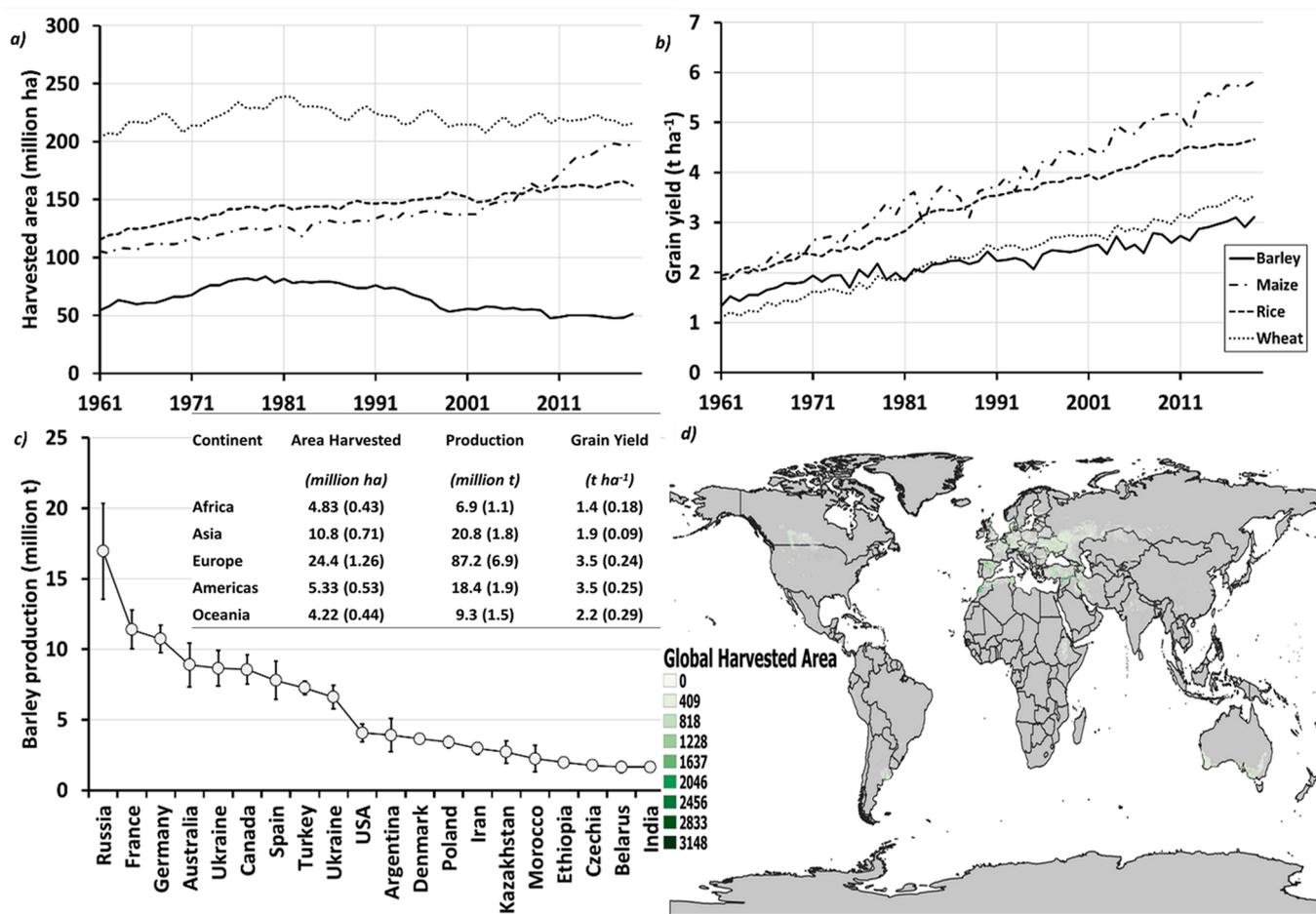


Fig. 1. Information of (a) the global harvested areas and (b) grain yield for barley (solid line), maize (dashed-dotted line), rice (dashed line), wheat (dotted line); and (c) barley production in million t for the 20 main producing countries in the world where the dots represent the mean of 10 years of data (2009–2019) and the error bars its standard deviation; Data for Fig. 1a-c are from FAOSTAT, 2021. The inset Table represents the statistical information for the 2009–2019 of area harvested, production and unit yield for each of the continents (FAOSTAT, 2021); (d) geographical distribution of the barley harvested area (from <http://mapspam.info/>).

essential indicator of digestibility and brewing quality in barley is significantly increased under high temperatures (Anker-Nilssen et al., 2008).

Wheat-specific crop models are commonly used to simulate barley yield and grain quality by changing crop parameters due to the similarities of physiological and morphological features (Rötter et al., 2012). A rare number of crop models simulate quality traits aside from grain nitrogen. Testing the performance of 18 crop models indicated that capturing the variability of wheat grain protein concentration is a major challenge under extreme temperatures (Asseng et al., 2019). SiriusQuality (Martre et al., 2006) and STICS (Brisson et al., 2003) are the crop models that simulate other grain quality (other than protein) aspects specifically for wheat. However, researchers and other stakeholders need to crop models addressing the grain nitrogen response to changing climate and management with remarkably higher accuracy and consider other barley specific quality traits. Two primary sources of uncertainty exist within the crop modelling process, including structure and parameter uncertainties (Wallach and Thorburn, 2017). Structure uncertainty is driven by the incompatibility of various equations that simulate different processes and values of the fixed model parameters in crop models (Wallach et al., 2017). The impacts of those sources of uncertainties need to be quantified on the results of quality traits simulations in a systemic approach.

This review aims to compile state of the art on (i) response of quality traits of barley to climate change (extreme temperature, drought, and CO<sub>2</sub> concentration), (ii) the capability and approaches of available process-based crop modeling platforms to simulate barley quality traits disentangling genotype, environment and management interactions, and (iii) potential opportunities to improve crop models grain quality estimations by coupling them into modern data-driven approaches (e.g. machine learning) and sensing technologies as future perspectives.

## 2. Impact of change in climatic variables and grain quality

There is little known regarding the impacts of climate change on brewing quality and supply of barley in the future since nearly all climate change impact assessments assess barley's yield and production response but not grain quality. The changes in climatic variables on quality traits of barley may be as equally significant as yield (Wardlaw et al., 2002). High temperature and lack of water availability can considerably change the grain quality throughout alteration in composition and concentration of starch and protein (Högy et al., 2013). Hence in this section, we focus on the effects of high temperature, heat episodes, water availability, and CO<sub>2</sub> on the grain quality of barley which is summarized in Fig. 2.

### 2.1. Increase in temperature and heat episodes

Most of the studies that evaluated the effects of high temperature stress on grain quality focused on changing the protein content as one of the most critical quality traits (Soares et al., 2019). The direct relationship between protein concentration and other grain quality measures of barley is well documented (Chen et al., 2012; Balyan et al., 2013). There is a robust negative correlation between high protein concentration due to high temperatures and malt extract in barley (Eagles et al., 1995). The starch accumulation in barley grains is negatively affected by heat stress (Savin and Nicolas, 1996). The protein content is a complex trait governed by interactions among genotype, soil conditions, agronomic management, and CO<sub>2</sub> concentration (Peña et al., 2002; Triboi et al., 2006; Wieser et al., 2008).

The increase in temperature and heat intensity leads to a significant increase in grain protein concentration as those stresses influence starch accumulation, and change the protein/starch balance (Spiertz et al., 2006; Triboi et al., 2006). Analysis of 160 barley malting genotypes in Australia showed that amplified rainfall between July and September was associated with declined grain protein. On the other hand, the

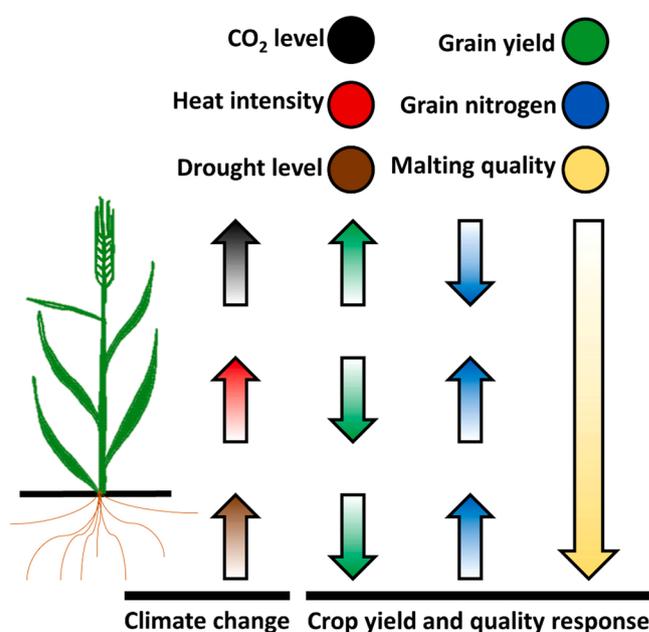


Fig. 2. Schematic illustration of crop yield and quality response to climate change including drought, heat intensity and CO<sub>2</sub> concentration. Light shades indicate less intense, and dark shades show more intense stress impacts.

number of days above 35 °C during grain filling was related to increased grain protein (Correll et al., 1994). Experimental evidence showed that the increase in protein concentration of spring barley under elevated temperatures is mainly driven by starch synthesis suppression instead of an increase in protein concentration per grain (Wallwork et al., 1998). The heating treatments significantly reduced the starch concentration by 5.0 % resulted in a remarkable decline in barley's malting quality (Barnabás et al., 2008).

### 2.2. Change in water availability

The malting quality and protein concentration of barley showed a relatively similar response to drought as high temperature (Mahalingam and Bregitzer, 2019). Drought stress generally occurred during the anthesis and grain filling period of barley; therefore, most of the studies targeted those stages as the most sensitive growth stages to abiotic stresses (Kalladan et al., 2013). Drought stress significantly reduced the starch assimilation and increased the grain nitrogen percentage (Savin and Nicolas, 1996). In addition, beta-glucan content is one of the critical malting quality factors of barley significantly reduced under drought stress (Macnicol et al., 1993). Heat and drought stress combined to reduce barley yields more severely than individual stress, but malting quality traits were unaffected compared to heat or drought stress alone (Mahalingam and Bregitzer, 2019).

Testing different barley genotypes indicated a remarkable decline in barley yield and malt extract by hampering the starch accumulation under drought stress (Wu et al., 2015). However, there was a significant variation in response of grain quality to drought stress among different genotypes (Wu et al., 2015). The drought-tolerant barley genotypes showed a larger re-mobilization capacity of the metabolites stored in the vegetative organs into the developing grains compared to sensitive genotypes (Hong et al., 2020).

### 2.3. Elevation in CO<sub>2</sub> concentration

One of the most significant consequences of climate change is the rapid rise in atmospheric CO<sub>2</sub> (Thrasher et al., 2013). The CO<sub>2</sub> concentration is projected to increase from 379 ppm to 538 ppm by 2100 (Meinshausen et al., 2011). The experimental evidence showed the

direct effects of CO<sub>2</sub> increase in enhancing photosynthesis and biomass accumulation, particularly for C3 crops such as barley (Torralbo et al., 2019). Significant changes in grain quality often accompany increases in biomass production under elevated CO<sub>2</sub> (Hampton et al., 2013). With an increase in CO<sub>2</sub> concentration, the chemical composition of crops will shift, resulting in a reduction in most elements, including nitrogen (Loladze, 2002). Doubling of CO<sub>2</sub> concentration can reduce barley grain protein concentration between 10 % and 15 % (Tabu et al., 2008). An excessive nitrogen application cannot fully compensate for such a reduction in protein concentration in cereals (Kimball et al., 2001).

The mechanisms involved in reducing nitrogen and protein concentration under elevated CO<sub>2</sub> are not well understood (Taub and Wang, 2008). CO<sub>2</sub> enrichment caused a significant increase in globulin and B-hordein proteins (Wroblewitz et al., 2014), which showed the most negative correlation with malt extract (Howard et al., 1996). The possibility of reducing nitrogen and protein concentration by increasing non-structural carbohydrates is one theory (Gifford et al., 2000). Other studies suggest that the decline in Rubisco levels in leaves and stems could explain the reduction in grain protein concentration (Ainsworth et al., 2002). A few studies have investigated how elevated CO<sub>2</sub> affects barley quality in field conditions using Free-Air Carbon dioxide Enrichment (FACE) systems. The CO<sub>2</sub> enrichment to 550 ppm declined the activity, and total and soluble β-amylase, single grain harvest, and the water extract's viscosity in barley (Erbs et al., 2010). The higher temperatures during the growth period were slightly compensated for reducing grain protein concentration under elevated CO<sub>2</sub> in wheat (Wang et al., 2019b). Another study on spring wheat showed that the total protein concentration increased under CO<sub>2</sub> and heat stress combined. Still, it resulted in a significant imbalance between structural and storage protein, leading to a remarkable decline in bread-making quality (Zhang et al., 2019). However, the quality of other crops such as rice declined further under a combined increase in heat stress and CO<sub>2</sub> concentration compared to sole elevation in CO<sub>2</sub> level (Chaturvedi et al., 2017). Therefore, we cannot generalize the quality response of different crops to combined heat and CO<sub>2</sub> elevation.

### 3. State of the art of current modeling approaches to capture grain quality

The available crop models simulating grain quality generally estimate grain N and protein content as the most representative quality measure interacting with water availability, temperature, and nutrients (Nuttall et al., 2017). Currently, models used for barley grain quality simulation can be divided into three types: (a) process-based models mainly developed based on wheat (Table 1) (b) empirical statistical regression models derived from experimental data and/or remote sensing, and (c) hybrid approach that integrates remote sensing data and process-based crop models via data assimilation. Process-based models simulate cropping systems' critical growth processes, capturing the complex interactions across genotype, management, and environment. However, those models are not suitable to employ when the specific processes not implemented in the model drive the variability of crop yield and quality traits (Rötter et al., 2018).

Statistical crop models are the second type that developed in a wide range of complexity (Yang et al., 2014). They are developed based on regression-based relationships that relate variation in observed crop yields and quality to changes in climate or other variables (Lobell and Asseng, 2017). Statistical models can partly capture the signal of pest and disease pressure (year and location-specific) which are not reflected in process-based models (Roberts et al., 2017b). However, the underlying mechanisms of the growth processes cannot be captured by them (Webber et al., 2020).

The process-based crop models commonly provide an abstraction of detailed crop processes. In addition, they poorly consider some of the fundamental factors such as pests and disease, which can significantly influence grain quality (Pirgozliev et al., 2003). Hybrid approach

integrates remote sensing/ground measured data and derived products with process models, which has been demonstrated to have an excellent potential for large-scale crop monitoring (Li et al., 2015b) to address processes ignored or poorly considered in crop models (Jin et al., 2018). Such hybrid approaches would also be employed to quantify individual physiological traits' contribution to grain yield and quality across the environments and range of management practices (Cammarano et al., 2021a; He et al., 2017a). Currently, data assimilation is commonly used to couple remote sensing information into crop models. Different types of state variables derived or retrieved from remote sensing and ground measurement can be merged into process models, including leaf area index, soil moisture content, canopy coverage, above-ground biomass, the fraction of absorbed photosynthetically active radiation, and evapotranspiration (de Wit and van Diepen, 2007). Data assimilation recalibrates and optimizes the simulation process of models, which is a practical approach to mitigate the controversy of observation and simulation errors to improve simulation accuracy (Jin et al., 2018). Remote sensing can also provide targeted phenotyping information to estimate crop model parameters which can be linked to loci or alleles embedded in pan-genomes to disentangle the complex interactions among environment, genotype, and management (Wang et al., 2019a). The coupling of crop models and machine learning would also improve the yield forecasts (Shahhosseini et al., 2021). In such coupling pipelines machine learning algorithms employ as external modifier of crop model results when the targeted outputs of the model used as predictors (Feng et al., 2019). They showed satisfactory performance in detecting long-term yield variability and extreme climate effects on yield, which the sole implementation of crop models cannot capture (Everingham et al., 2016; Feng et al., 2019). Under climate change, such potentials should be used to address the shortcomings of crop models for simulating barley-specific quality traits.

#### 3.1. Modeling of grain nitrogen and protein content

Process based crop models simulate the N uptake and its transfer to grain by two approaches; the simple one is the harvest index approach, in which N harvest index increases linearly with thermal time from zero at the start of grain growth to maximum N rate (e.g., 80 %) considering thermal accumulation (Jamieson et al., 1998). Another more complex approach is source-sink models (Jamieson and Semenov, 2000). The grain protein content is directly proportional to grain N content in the process-based modeling routines. Grain proteins are synthesized from the amino acids remobilized from the vegetative organs or the current N uptake. The growing conditions during the grain filling phase and the amount of N stored before anthesis determine the amount of N remobilized into the grain when the mechanism implemented (Barbottin et al., 2008).

Some process based models, see section below, consider the independent temperature function on N accumulation which can directly represent the impacts of temperature rise on grain quality (Ibrahim et al., 2019). The temperature rise indirectly resulted in a linear increase of grain N content in most crop modeling platforms which is limited by grain size and N concentration threshold (Alderman et al., 2014). However, there is no explicit routine in modeling platforms used for impact assessment studies to simulate the effects of extreme heat episodes on grain N accumulation (Osman et al., 2020). The models generally separate the dry matter and N accumulation for grains, and this can lead to failure in a simulation of grain protein under extreme drought and low N fertilizer application (Asseng et al., 2002). Linking of those two processes can significantly improve the simulation of grain nitrogen (Asseng et al., 2002). In general, the CO<sub>2</sub> fertilization effects on grain protein can be captured by crop models since dry matter accumulation increase by adjustment of radiation use efficiency or photosynthesis; however, the nitrogen concentration remains constant (Asseng et al., 2019).

The performance of a modeling routine in the simulation of specific

**Table 1**

A series of barley crop growth models, demonstrating their ability to simulate grain quality traits.

Model	ST scale	GN	GP	Other quality traits	Drivers of GN			Other drivers GN	Grain number	Grain size
					Temperature	Water	CO <sub>2</sub>			
APSIM	Daily/Point	Y	Y	N	Y	N	Y	–	Y	Y
CERES-Wheat	Daily/Point	Y	Y	N	Y	N	N	Development stage	Y	Y
CropSyst	Daily/Point	Y	N	N	N	N	N	Harvest index	N	N
DSSAT-CROPSIM	Daily/Point	Y	Y	N	Y	N	N	Development stage	Y	Y
FASSET	Daily/Point	Y	N	N	N	N	N	–	N	N
LINTUL3	Daily/Point	Y	N	N	N	N	N	–	N	N
MONICA	Daily/Point	Y	Y	N	N	N	N	Development stage	Y	Y
SiriusQuality	Daily/Point	Y	Y	Y	Y	N	N	Development stage	Y	Y
STICS	Daily/Point	Y	Y	Y	Y	N	N	Harvest index	Y	Y

ST: spatiotemporal, GN: grain nitrogen, GP: grain protein, Y: yes, N: no

growth processes (e.g. accumulation of grain nitrogen) depends on the balance of data availability, model complexity, spatial scale, and the environmental-management conditions that the model developed in the first place. For instance, the availability of the full spectrum of soil characteristics resulted in the best yield simulation for CERES-Wheat and CropSyst under semi-arid conditions. However, WOFOST indicated the best performance under the limitation of soil data (Castañeda-Vera et al., 2015). On the other hand, the availability of model parameters does not necessarily result in high accuracy of model outcomes (for spring barley) when implemented under low input cropping systems since study models (PSIM, CERES, CROPSYST, COUP, DAISY, EPIC, FASSET, HERMES, MONICA, STICS, and WOFOST) are developed under optimum management conditions (Salo et al., 2016). The complex crop models are generally developed for field conditions. Still, their application at a large scale may result in lower accuracy than simpler models due to a large number of parameters required for complex modeling routines, which are not generally available at large scales (Pasquel et al., 2022). Therefore, it is challenging to generalize which modeling approach provides the most satisfactory outcome for all conditions.

Statistical methods for grain N and protein content estimation can be performed by solely remote sensing indicator, remote sensing combined with crop physiological variables, and multiple measurement integration. Remote sensing captures reflectance of crops at leaf and canopy scales; as leaf N content is highly correlated to grain N/protein content (Hunt et al., 2005). Developing regression relationships between grain N/protein content and remote sensing spectral indices becomes a direct and rapid way for quantifying grain N and protein content (Liang et al., 2018). These spectral indices (e.g., GNDVI, NDRE) are mainly calculated using the green, red, red edge, and near-infrared bands. Other sources of remote sensing indicators such as thermal and narrow hyperspectral indices can be incorporated in the regression relationships for considering the effects of temperature, irrigation and fertilization management on grain features (Zhao et al., 2005). The second approach treated crop physiological variables that are more easily retrieved/estimated via remote sensing technology and highly related to protein and N content as a bridge to link remote sensing data and grain N/protein content. These physiological variables include canopy chlorophyll content, leaf carbon accumulation, leaf N content, and leaf N accumulation (Wang et al., 2021). The last approach is integrating remote sensing, soil conditions, sowing date, fertilization rate, climate conditions, and phenology in a complex empirical approach for estimation of grain N and protein content (Pettersson and Eckersten, 2007). Besides, coupling crop process model and remote sensing data is another effective way to assess grain N and protein content. For instance, a combination of DSSAT-CERES model and NDRE spectral indices resulted in better performance than the single spectral indices-based approach (Li et al., 2015b).

### 3.2. An overview on simulation functions of grain nitrogen, nitrogen stress, and other quality measures in current process-based models

**APSIM:** The grain N demand ( $N_{D,grain}$ ) begins at anthesis and is calculated using grain number ( $N_g$ ), thermal time, and potential grain N filling rate ( $h_{N,pot}$ :  $\text{g grain}^{-1} \text{ } ^\circ\text{Cd}^{-1}$ ) which is a model parameter and currently set at  $0.000055 \text{ g grain}^{-1} \text{ } ^\circ\text{Cd}^{-1}$  (Keating et al., 1999; Wang et al., 2002; Holzworth et al., 2018):

$$N_{D,grain} = N_g h_{N,pot} f_{N,grain} h_{grain}(T)$$

The  $h_{grain}(T)$  is a function of daily mean air temperature to impact grain filling ranging from 0 to 1, with 0 currently at  $0^\circ\text{C}$  and 1 at  $25^\circ\text{C}$ . While  $f_{N,grain}$  is the N factor for grain filling and calculated as follows:

$$f_{N,grain} = \frac{h_{N,pot} h_{N,grain}}{h_{N,min}} \sum_{stem,leaf} \frac{C_N - C_{N,min}}{C_{N,crit} \times f_{c,N-C_{N,min}}} \quad (0 \leq f_{N,fill} \leq 1)$$

where  $h_{N,min}$  is the minimum rate of grain filling and is a model's parameter set currently at  $0.000015 \text{ g grain}^{-1} \text{ } ^\circ\text{Cd}^{-1}$ ;  $h_{N,grain}$  is a multiplier for N deficit impact on grain, it is a model parameter and currently has a default value of 1;  $C_N$  is the N concentration of stem and/or leaves; the minimum N concentration ( $C_{N,min}$ ) is defined as the structural N required by the plant and cannot be re-translocated, the critical N concentration ( $C_{N,crit}$ ) is the minimum N concentration that plants will maintain and therefore drive the demand of N, and in this case they refer to stem and/or leaves; the  $f_{c,N}$  is a factor with value of 1 for stem meaning no impacts and if function of CO<sub>2</sub> concentration for leaves.

**CERES-Wheat and NWheat:** The CERES-Wheat model (Ritchie and Otter, 1984) simulates grain N using a simplified approach in which only the main processes are considered. Grain N is the direct result of dry matter and N accumulation in the grain. Both are accumulated independently and driven by potential accumulation per kernel (expressed as demand function) and actual supply. N accumulation in the grain is function of temperature.

The potential kernel N accumulation ( $\Delta KN_{pot}$  expressed in  $\mu\text{g N kernel}^{-1} \text{ day}^{-1}$ ) for a given kernel is calculated as:

$$\Delta KN_{pot} \left\{ \begin{array}{l} 0.49 \times T_{mean} \quad T_{max} \leq 10^\circ\text{C} \\ 4.83 + 1.06 \times T_{mean} + 0.25 \times (T_{max} - T_{min}) \quad T_{max} > 10^\circ\text{C} \end{array} \right\}$$

Where  $T_{mean}$  is the mean air temperature,  $T_{max}$  and  $T_{min}$  are the maximum and minimum air temperature, respectively. The CERES-Wheat did not consider genetics for N accumulation and also 4-fold increase of potential kernel N accumulation at  $10^\circ\text{C}$ .

Grain N accumulation demand per unit area ( $\Delta N_{pot}$ ;  $\text{g N m}^{-2} \text{ day}^{-1}$ ) is the product of  $\Delta KN_{pot}$  and number of kernels per unit area:

$$\Delta N_{pot} = \Delta KN_{pot} \times K \times 10^{-6}$$

Where  $K$  is the number of kernels per unit area. The grain N supply is obtained from different organs (such as stem, leaves, and roots) up to a point where the tissue N concentration is reduced to a minimum concentration that is function of the phenological stage. The tissue N crop is

the resultant of uptake before and during the grain filling period.

*Nwheat* (Asseng et al., 2002) changes: There have been three main changes to the *CERES-Wheat* routine:

- i. Upper boundary to limit N transfer to a maximum of 4 % of the daily dry matter transfer. The upper boundary considers that N transfer to grain requires some carbon;
- ii. The transfer of dry matter is limited so that accumulation is at least at 1.23 % N this daily transfer to ensures minimum grain N concentration observed in the field;
- iii. Initialization process at the beginning of grain filling period for kernel N with 3 %N. The N is received from the simulated aboveground tissue and below-ground if needed. This process reduces the above-ground tissue N to a level whose minimum limit is dependent on crop phenology; while the below ground tissue to a minimum limit of 0.45 % N. If the supply of N is not enough then the initial kernel N is reduced.

*CropSys*: In the model (Kemanian et al., 2007) the actual grain N concentration ( $N_g$ ) is dependent on the amount of N available for allocation ( $N_a$ ), and on the Harvest Index (HI) and calculated as follows:

$$N_g = N_{gn} + N_a \times P_g / HI$$

$$N_a = N_t - [HI \times N_{gn} + (1 - HI) \times N_{sn}]$$

Where  $N_{gn}$  is the minimum  $N_g$  that must be satisfied for growth to take place,  $N_t$  is the N concentration in the aboveground biomass at physiological maturity,  $N_{sn}$  is the minimum N concentration in straw that is needed for growth to take place.  $P_g$  is the grain partitioning factor and indicate the partitioning of  $N_a$  to the grain if both grain and straw have reached their maximum concentration, but it is modulated through the  $R$  parameter for accounting actual availability of N as explained below. The two parameters are calculated as follows:

$$P_g = [1 + (1 - HI) \times N_{sd} / (HI \times N_{gd})]^{-R}$$

$$R = \{N_a / [HI \times N_{gd} + (1 - HI) \times N_{sd}]\}^C$$

Where  $N_{gd}$  and  $N_{sd}$  are the grain N demand above the minimum concentration and are computed as:

$$N_{gd} = N_{gx} - N_{gn}$$

$$N_{sd} = N_{sx} - N_{sn}$$

The  $N_{gx}$  and  $N_{sx}$  are the maximum N concentration in grain (g) and straw (s) that cannot be exceeded. When  $N_a$  is multiplied by the aboveground biomass it expresses the N content (mass) that is available for grain and straw. The terms of the  $R$  factor represent the degree of saturation on N of the aboveground biomass. That means that it represents the fraction of N required to attain the maximum concentration in aboveground biomass as satisfied by  $N_a$ . For example, if the N in the aboveground biomass can only satisfy the minimum N concentration ( $N_{gn}$ ,  $N_{sn}$ )  $R$  will be 0 because there is no amount of N available for allocation ( $N_a = 0$ ). But, if there is enough N to satisfy the maximum concentration ( $N_{gx}$ ,  $N_{sx}$ ) then  $R = 1$ . The parameter  $C$  is dimensionless and is an empiric factor allowing adjustment of  $P_g$  for genotype effects. Higher  $C$  values indicate higher priority to the grain as sink in terms of  $N_a$ ,  $N_{gx}$ ,  $N_{sx}$ ,  $N_{gn}$ , and  $N_{sn}$  are constants and vary among species.

*DSSAT-CERES and DSSAT-CROPSIM*: The *CERES-Wheat/Barley* model in the *DSSAT* software package is a derivative of the original *CERES-Wheat* (Ritchie and Otter, 1984) and *CROPSIM-Wheat* (Hunt and Pararajasingham, 1995) models. The original *CERES* was changed both to allow it to fit within the structure of the overall CSM model (Hoogenboom et al., 2019), and to facilitate the removal of all parameters from that were in the code and placing them in external files. Grain N

concentration is the direct result of dry matter and N accumulation in the grain. Both are accumulated independently and driven by potential accumulations per kernel and actual supply; both are functions of temperature. The model considers the genetics of the particular cultivar being simulated, and calculates potential kernel N accumulation from an input parameter for the standard grain N concentration of the cultivar.

The N that needs to meet the potential demand is obtained from a reserve N pool, uptake from the soil, and withdrawal from the various vegetative organs, with the amount withdrawn each day from leaves, stems and roots being limited by input parameters. If the N supply is insufficient to meet the demand then the grain N concentration falls below the standard, but it is not allowed to fall below a lower threshold value that is set as an input parameter for the particular cultivar. Similarly, if the carbohydrates available for translocation to the grains are inadequate but N availability is good, the N concentration in the grain will increase, but only to a maximum value provided as an input parameter for the species. In *DSSAT-CERES* the grain N demand (*GNDEM*) is calculated as follow:

$$GNDEM = \min \left[ GROGRPA \times \left( \frac{GRNMX}{100} \right), LAGSTAGE \times TFGN \right. \\ \left. \times GRNUM \times G2 \times DU \times 0.001 \times \left( \frac{GRNS}{100} \right) \right]$$

where *GROGRPA* is the grain growth possible assimilation and is function of the potential grain growth (*GROGRPT*), the potential reserve growth and weight, and the grain growth from assimilates from stem; *GRNMX* is the grain N maximum concentration; *LAGSTAGE* is the lag phase of grain filling; *TFGN* is the temperature factor for N during grain filling; *GRNUM* is the grain per plant; *G2* is a user-defined coefficient and is the standard kernel size under optimum conditions (mg); *DU* is the developmental units; and *GRNS* is the grain N standard concentration.

The *DSSAT-CROPSIM* wheat (and barley) model in the *DSSAT* software package is a derivative of the standalone *CROPSIM* wheat model (Hunt and Pararajasingham, 1995). It was changed to allow it to fit within the structure of the overall CSM model (Hoogenboom et al., 2019), and so to make use of the soil and other modules standard to all models in the CSM package. The grain N was simulated in the same manner as described earlier for the *DSSAT-CERES* model. The grain N demand (*GRAINNDEM*) is then calculated from the grain growth rate a cultivar-specific grain N maximum concentration (*GNPCMX*) and impacted by temperature:

$$GRAINNDEM = \min \left[ GROGRPA \times \left( \frac{GNPCMX}{100} \right), TFGN \times GROGRP \right. \\ \left. \times \left( \frac{GNPCS}{100} \right) \right]$$

Where *GROGRPA* is the possible grain growth assimilation and is function of the potential grain growth (*GROGRP*), carbohydrates available in the aboveground biomass, current grain growth assimilation, and reserve weight; *TFGN* is the temperature factor for grain N (varies between 0 and 1); *GNPCS* is a cultivar coefficient for the grain standard N concentration.

*FASSET*: The N amount of grains in *FASSET* (Olesen et al., 2002) is simulated at maturity stage by assuming a linear relationships among N contents in the grains dry matter ( $N_g$ ), aboveground ( $N_v$ ) and below-ground ( $N_r$ ) biomass:

$$N_g = 0.74 + 1.86N_v$$

$$N_r = 0.75 + 1.00N_v$$

The sum of the N content in different organs used as total N content ( $U$ ) which is required for calculation of N nutrition index (*NNI*):

$$NNI = \frac{U}{U_x}$$

$$U_x = \left\{ \begin{array}{l} 0.069(W_v + W_g) + 0.0175W_r, \quad W_v + W_g < 150 \\ 0.083\left(\frac{W_v + W_g}{100}\right)^{0.56} + 0.0175W_r, \quad W_v + W_g \geq 150 \end{array} \right\}$$

Where  $U_x$  is maximum crop N content.  $W_v$ ,  $W_g$  and  $W_r$  are dry matter of aboveground, belowground and grains, respectively.

**LINTUL3:** The absorbed N is distributed proportionally among the plant organs according to their share in the total N demand at each day. The N demand of plant organs (except grains) calculated based on desirable maximum concentration in specific organ and current amount of N in organ. The N uptake from soil is ceased at anthesis and the N demand of grains in LINTUL3 (Shibu et al., 2010) meet by N translocation from leaves, stems and roots. The grains N demand is calculated by maximum and actual N content which is limited by amount of translocatable N from other organs. The N nutrition index (NNI) defined as condition that actual N content drops below the critical threshold:

$$NNI = \frac{\text{actual crop } [N] - \text{residual } [N]}{\text{critical } [N] - \text{residual } [N]}$$

Residual N referred to non-transferable N content which store in cell structure.

**MONICA:** The crude protein content ( $P_{FM}$ ) of grains in MONICA (Nendel et al., 2011) is calculated from the ratio between N concentration in aboveground dry matter ( $N_A$ ) and a series of crop-specific parameter:

$$P_{FM} = \frac{N_A}{W_S + (p_N \times W_R)} \times \frac{1}{0.16}$$

Where  $W_S$  and  $W_R$  are grain and aboveground dry matter, respectively.  $p_N$  is N distribution coefficient which determine as ratio between mean N concentration in biomass and mean N concentration in grain yield. The N stress factor ( $\delta_N$ ) is calculated based on minimal ( $N_m$ ), critical ( $N_{crit}$ ) and actual ( $N_{act}$ ) concentration of the N in biomass:

$$\delta_N = 1 - e^{-\left(5 \times \frac{N_{act} - N_m}{N_{crit} - N_m}\right)}$$

$$N_{crit} = a \times (1 + b \times e^{-5.26 \times D_{rel}})$$

Where  $a$  and  $b$  are plant specific parameters.  $D_{rel}$  is the ratio between current temperature sum and the temperature sum of the development stage.

**SiriusQuality:** A sink priority rule in SiriusQuality (Martre et al., 2006) determines how N is allocated and mobilized among different organs. All non-structural aboveground N ( $N^{supply}$ ) transfer to grains (as daily N flux) during the grain filling period as function of mean temperature ( $\Delta T$ ) and duration of the grain filling period:

$$N^{supply}(T) = (N_{ns}^{stem}(T) + N_{ns}^{leaf}(T)) \times \frac{\Delta T}{D_{gf} - D_{cd}}, \quad T > D_{cd}$$

Where  $N_{ns}^{stem}$  and  $N_{ns}^{leaf}$  are non-structural N concentration of stems and leaves, respectively.  $D_{gf}$  and  $D_{cd}$  are duration of grain filling and cell division phase, respectively. The structural or metabolic grain N ( $N_{stru}^{grain}$ ) is a function of N/carbon ratio and structural carbon of the grains. Finally, the daily N storage of the grains ( $N_{sto}^{grain}$ ) is calculated based on the difference between the daily potential rate of supply and the daily rate of accumulation of structural N, by implementing the grain number ( $G_{num}$ ) into the equation:

$$N_{sto}^{grain}(T) = \frac{N^{supply}(T)}{G_{num}} - \Delta N_{stru}^{grain}(T), \quad T > D_{cd}$$

The grain protein composition (mainly developed for wheat) is simulated by dividing the structural N into albumin-globulin ( $N_{alb-glo}$ ) and amphiphilic ( $N_{amp}$ ). The storage N is also divide into gliadin ( $N_{gli}$ )

and glutenin ( $N_{glu}$ ) proteins:

$$\left\{ \begin{array}{l} N_{alb-glo}(T) = \alpha_{alb-glo} \times (N_{stru}^{grain}(T))^{\beta_{alb-glo}} \\ N_{amp}(T) = N_{stru}^{grain}(T) - N_{alb-glo}(T) \end{array} \right\}$$

and

$$\left\{ \begin{array}{l} N_{glu}(T) = \alpha_{glu} \times (N_{sto}^{grain}(T))^{\beta_{glu}} \\ N_{gli}(T) = N_{sto}^{grain}(T) - N_{glu}(T) \end{array} \right\}$$

Where  $\alpha_{alb-glo}$  and  $\alpha_{glu}$  are dimensionless adjusting parameters.  $\beta_{alb-glo}$  and  $\beta_{glu}$  indicate the concentration of defined portions in mg N of the grains. The N stress ( $F_N$ ) calculated based on the minimum ( $[N]_{min}$ ), maximum ( $[N]_{max}$ ) and actual ( $[N]$ ) N concentration:

$$FACN = \frac{2([N] - [N]_{min})}{[N]_{max} - [N]_{min}}$$

Factor 2 allows the N concentration to pass the N amount required for unrestricted growth under luxury N application.

**STICS:** The crop N content simulated in STICS (Brisson et al., 2003) depends on carbon accumulation and available N in the rootable zone. In grains, N quantities increase as a fraction of the N stored in the biomass. The daily increase in grain N concentration (DLTAGN) calculates based on N harvest index (IRAZO) and amount of the N in biomass (QNPLANTE) which is adjusted by a temperature-dependent factor (FTEMPREMP):

$$DLTAGN(I+1) = [IRAZO(I+1) \cdot QNPLANTE(I+1) - IRAZO(I) \cdot QNPLANTE(I)] \cdot FTEMPREMP(I)$$

The N harvest index calculates by an increasing rate which is modified by the carbon harvest index. To simulate the concentration of N in each organ, the model used dilution curves. The crop is at risk of N deficiency if the N concentration falls below the critical point. Using the curve, N nutrition index (INN) can be defined as the ratio of actual N concentrations (CNPLANTE) to critical concentrations (NC) corresponding to total biomass which determined N stress index (INNS):

$$INN = \frac{CNPLANTE}{NC} \text{ and } INNS = \min(1, INN)$$

STICS simulates separately the moisture content of grains (TEAUGRAIN), which is an important variable that determines barley malting quality. That is a function of difference between canopy (TCULT) and air temperature (TAIR). Prior to the onset of grain filling, the water content of harvested organs is constant:

$$TEAUGRAIN(I) = H2OFRVERT_p - DESHYDBASE_p(I - IDEBDES + 1) - \sum_{J=IDEBDES}^I TEMPDESHYD_p(TCULT(J) - TAIR(J))$$

Where H2OFRVERT<sub>p</sub> is water content of grains at start of grain filling, DESHYDBASE<sub>p</sub> is dehydration parameter, IDEBDES is onset of water dynamics of grains, and TEMPDESHYD<sub>p</sub> is Proportionality coefficient based on the difference between canopy and air temperature.

#### 4. Shortcomings of current crop models and future perspectives

In order to better understand how changes in climate affect the functional properties and end-use value of barley, it is crucial to improve crop models' predictive capability for grain quality. Nearly all of the crop models used for simulation of grain yield and quality of barley were initially developed for wheat. Users of the crop models change the specific growth parameters of those wheat models to simulate barley growth. However, there is a substantial difference between fundamental quality measures of wheat and barley. Current crop models generally fail to predict detailed whole-grain characteristics, grain protein compositions, or functional properties by simulating only average grain size and N concentration or protein content (Fig. 3). The temperature is the only variable that directly affects grain nitrogen accumulation in most crop models (Table 1). However, experimental results indicated that drought

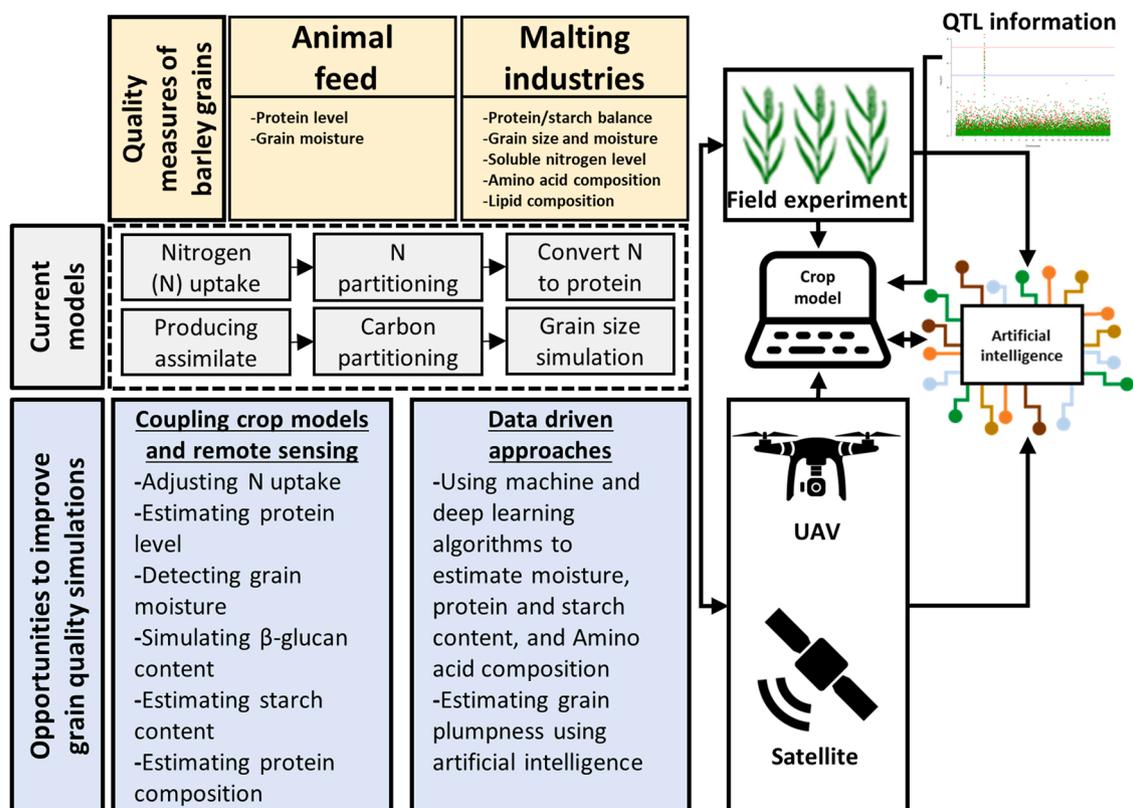


Fig. 3. The state of the art of current crop models and possible options using new technologies to improve the simulation of grain quality in barley.

and CO<sub>2</sub> could also significantly change the grain nitrogen concentration. The interactions among temperature, water, and CO<sub>2</sub> on grain nitrogen accumulation need to be thoroughly explored for mechanism understanding and implemented in new crop modeling routines.

A few crop models such as SiriusQuality (Martre et al., 2006) partly account for protein composition using empirical functions but do not particularly simulate the quality measures of barley for malting, brewing, and distilling. On the other hand, a set of statistical models were also developed to simulate specific quality measures of barley in response to the environment, management, and genotype (Fox et al., 2006; Matthies et al., 2014; Nielsen et al., 2016). However, those empirical functions can only capture the variation in quality measures (within the environments that the models developed). Despite this, they cannot provide any information regarding the underlying mechanisms explaining observed responses (Roberts et al., 2017a). Coupling the statistical models to available process-based crop modeling platforms would be an immediate option to partly cover the mechanistic overview of barley grain quality driving variables required in impact assessment studies. Coupled models can also reflect the grain quality response to interactions between management and genotype which are not included in statistical models across the environments.

The crop models were generally calibrated using empirically estimated genotype-specific parameters for phenology, plant structure, and biomass accumulation processes obtained from field experiments (Di He et al., 2017b). However, most of the quality simulation modules developed for crop modeling platforms do not consider the variability of genotypes in quality traits using fixed parameters due to the lack of data and knowledge on complex interactions among different drivers of grain quality (Bertin et al., 2010). One possibility of estimating a suitable parameter range for grain quality traits simulations is linking them to QTLs or genes (Barrasso et al., 2019). Such gene base modules coupled to crop models can also translate gene-by-gene (epistatic) and gene-by-environment interactions on grain quality under different climate change and adaptation scenarios. The potential of QTL (in the

absence of information on specific genes or loci) and gene base information was employed to capture traits to improve the yield under extreme conditions for cereals (Guitton et al., 2018; Kadam et al., 2019; Cooper et al., 2021). Nevertheless, only a few efforts have been conducted to use such potential for improving the grain quality simulation modules (Quilot et al., 2005). To date, the greatest challenge facing the development of gene-based models for complex traits is the lack of information on responsible genes and their interactions (Baldazzi et al., 2016).

Remotely sensed (RS) information provided by UAV and satellite sensors would give a real-time estimation of the spatial pattern of the grain protein content of malting barley (Söderström et al., 2010) to adjust model outcomes from field to regional scale. The accuracy of the crop quality traits estimations of cereals using RS information depends on the phenological phase (Wang et al., 2014), which RS can also track. Using vehicle-based high-throughput spectral proximal sensing can provide an estimation of the protein content of spring barley genotypes at mid-season (Barmeier et al., 2017) adjust the model outcomes. The grain moisture at harvest as one of the quality measures of malting barley can also be detected by remotely sensed canopy chlorophyll content (Xu et al., 2019) inform crop models on the timing of the harvest for specific purposes, particularly for large scale applications. Coupling DSSAT-CERES and hyperspectral data (red-edge bands) resulted in the simulation of gluten content as a fundamental quality measure in wheat (Li et al., 2015a). RS information also can be used to estimate the other nutrient concentration such as potassium and calcium in barley (Holland et al., 2019), which crop models do not commonly simulate. The more detailed quality measures, including starch content, hardness, and barley hot water extract, which can be estimated using near-infrared reflectance (Fox et al., 2011), can also be included in crop models to simulate targeted quality measures of barley. The remote sensing data can be integrated with crop models either by pre-assimilated then calibration of the model or forcing the crop model to adjust the growth processes such as N accumulation to grains by RS driven estimations

(Kasampalis et al., 2018). However, technical issues need to be considered incorporating sensing information with crop models, such as frequency/resolution of observations and identifying symptoms from images under multiple stresses (Ozdogan et al., 2010; Huang et al., 2018).

Combining big data platforms and high-performance computing technologies with artificial intelligence (machine and deep learning) makes it possible to better understand the relationship between genotypes, environment, and management on barley quality measures (Mohr and Kühn, 2021). Machine and deep learning algorithms provide a practical tool to analyze the sensing information detecting the hidden relationships between canopy reflectance and crop quality measures (Jung et al., 2021). Support vector machines and random forest algorithms showed a significant performance in the detection of different elements (cadmium and magnesium) of rice cultivars using plasma mass spectrometry (Maione et al., 2016). Truncated Gaussian radial basis function and multilayer perceptron algorithms also indicate a remarkable predictive power in estimating the protein content of barley obtained from hyperspectral imagery from different environments (Wiegmann et al., 2019). Gaussian mixture algorithm detected the malting barley N concentration under various N management schemes based on multispectral imagery (Nelsen and Lundy, 2020).

## 5. Conclusion

The current process-based crop models used in climate change impact assessments to test the potential of adaptation strategies on barley growth and development can also capture the interactions among environments, genotype, and management on grain N as a quality trait. Nevertheless, nearly all crop model developers have limited the simulation of quality measures into grain number, size, and N content. Further, a few models such as *SiriusQuality* that simulate grain protein composition are basically wheat models and would not provide a piece of beneficial information on changes in malting or brewing quality of barley under climate change. Therefore, the development of barley-specific modeling routines to assess the impacts of climate change and variability on grain quality (based on stakeholder's essentials) is fundamental to design effective adaptation plans. The efforts to develop such routines should focus on two parallel directions. First, designing and implementing FACE and temperature free-air controlled enhancement (T-FACE) experiments that explicitly explore the effects of combined change in temperature, CO<sub>2</sub>, water and nutrient availability on detailed grain quality measures of barley to improve the process understanding. Since most of the previous FACE and T-FACE experiments focused on growth processes and grain quantity but not quality. Second, coupling the information obtained from sensing technologies and data-driven approach into current modeling routines. It can improve the accuracy of simulations by considering that the effects of variables and processes are not simulated in crop models. In addition, predicting quality traits based on complex relationships would be better explained by data-driven approaches (e.g., machine learning) in high spatiotemporal resolutions. In conclusion, a comprehensive barley quality model contributes developing adaptation strategies that compensate for the adverse impacts of climate change and provide an influential tool for leading and accelerating barley breeding efforts.

## Declaration of Competing Interest

We declare no competing interest.

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