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Improved Prediction of Leaf Emergence for Efficacious Crop Protection: Assessing Field Variability in Phyllotherms for Upper Leaves in Winter Wheat and Winter Barley

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Abstract: The choice of the phyllotherm value for predicting leaf emergence under field conditions is pivotal to the success of fungicide-based disease risk management in temperate cereals. In this study, we investigated phyllotherm variability for predicting the emergence of the three uppermost leaves (i.e., three last leaves to emerge) in winter wheat and winter barley fields. Data from four sites representative of wheat and barley growing regions in Luxembourg were used within the PROCULTURE model to predict the emergence of F-2, F-1 and F (F being the flag leaf) during the 2014–2019 cropping seasons. The phyllotherms tested ranged between 100 °Cd and 160 °Cd, in 15 °Cd steps, including the current default value of 130 °Cd. The comparisons between the observed and predicted emerged leaf area were qualitatively evaluated using the mean absolute error (MAE), the root mean square error (RMSE) and Willmott's index (WI). A phyllotherm of 100 °Cd accurately and reliably predicted the emergence of all three upper leaves under the various environmental conditions and crop cultivars of winter wheat and winter barley over the study period. MAE and RMSE were generally <5% and the WI values were most often ≥ 0.90 for F-1 and F. For phyllotherm values \geq 115 °Cd, the prediction errors generally increased for F-1 and F, with MAE and RMSE exceeding 20% in most cases. F-2 agreement between observed and predicted values was generally similar when using 100 °Cd or 115 °Cd. These results tie in valuable, complementary information regarding the variability of phyllotherms within leaf layers in winter wheat and winter barley in Luxembourg. Accurate and reliable leaf emergence prediction from F-2 to F allows for timely fungicide application, which ensures lasting protection against infections by foliar fungal disease pathogens. Hence, understanding phyllotherms can help ensure timely, environmentally sound, and efficacious fungicide application while increasing the likelihood of improved yields of winter wheat and winter barley.

Keywords: phenology; leaf emergence; crop protection; fungal disease risk

1. Introduction

The upper three leaves (the flag leaf 'F', and the two leaves below F, F-1 and F-2) of wheat (*Triticum aestivum* L.), and the F-1 and F-2 leaves and the ear of barley (*Hordeum vulgare* L.) contribute



most to yield, respectively (in barley, the contribution from the flag leaf is minimal due to its small size) [1–3]. The reliable prediction of the emergence of the upper leaves (i.e., last leaves to emerge) in wheat and barley is thus pivotal to the fungicides applied to control fungal diseases and ensure a satisfactory yield. In the absence of fungicides, several diseases are particularly limiting to the yield of both crops [2,4–7]. On the upper leaves, infections by fungal pathogens must occur early in development if the disease is to become severe, assuming favorable environmental conditions are met and that the leaves are left unprotected. In Luxembourg, foliar fungal diseases including Septoria tritici blotch (STB, caused by Zymoseptoria tritici (Desm.) Quaedvlieg & Crous), brown (Puccinia triticina Roberge ex Desmaz.) and stripe (P. striiformis Westend) rusts, as well as powdery mildew (Blumeria graminis DC. f. sp. tritici em. Marchal), are among the major threats which can cause grain yield losses, which, in turn, result in economic losses [6,8]. To safeguard crops against economic losses from diseases, Luxembourgish farmers typically apply two to three preventive foliar fungicide treatments, in conjunction with suitable management practices (e.g., use of disease-resistant cultivars, crop rotation, etc.). Crop management advice for fungicide applications is provided by the Luxembourgish Chamber of Agriculture. Depending on the fungicide's persistence and prevailing weather conditions, a foliar fungicide applied between growth stage (GS) 37–39 (flag leaf just visible to flag leaf blade all visible) up to GS59 (ear emergence) [9] increases the chances of all three upper leaves being protected against infection from fungal foliar pathogens [6]. Additional fungicide applications may be required to fully protect all three leaves if there were earlier applications (i.e., before GS37) of fungicide. Likewise, applications at GS59 may result in yield losses due to disease as the upper leaves F to F-2 were left unprotected during their emergence and expansion. Consequently, yield losses may occur, providing favorable weather conditions for a disease epidemic are met. Hence, there is a need for reliable leaf emergence prediction within an integrated decision support system (DSS) that can be used to guide optimum fungicide application timing [6].

A number of models with varying levels of complexity and data requirements have been evaluated for simulating winter wheat and winter barley crop phenology: from relatively simple equations based on cultivar thermo-photoperiodic response (e.g., [10–12]) to complex algorithms that describe variations in the rate of development in response to environmental factors including temperature, vernalization and photoperiod (e.g., [13–16]). Under conditions of constant diurnal day length and temperature, and in the absence of severe stress, it is assumed that the phyllochron remains generally constant across all leaf layers [16–18]. A phyllochron is defined as the time duration (usually given in days) that separates the appearance of two successive leaves; the corresponding degree-day sum is termed the phyllotherm ([19,20]). Phyllotherms for wheat and barley can be as low as 52 °Cd [20,21] or as high as 160 °Cd [22] depending on the genotype, growth stage and environmental conditions (i.e., field or growth chamber conditions).

Changes in leaf appearance rate in winter wheat and winter barley as a function of leaf number or as a chronology factor have been considered (e.g., [23–26]). For example, Miglietta [23] assumed an exponential decrease in the rate of leaf appearance with the number of emerged leaves in wheat. Jamieson et al. [24] considered an increase in phyllotherm throughout the growing season in winter wheat, which ranged from 75 °Cd (base temperature = 0 °C) for the two lowest leaf positions to 100 °Cd for leaf positions 2 to 8, to 130 °Cd for leaf positions > 8. Decreasing leaf appearance rates are expected as the number of emerged leaves increases [25,27,28]; that is, the duration between the appearance of two successive upper leaves is longer compared to the duration between the lower leaves. Within a DSS for managing fungal disease risks in cereals in Belgium and Luxembourg (i.e., the PROCULTURE model [6,29,30]), a constant phyllotherm value of 130 °Cd (base temperature = 0 °C) is commonly used for predicting the emergence of all five upper leaves (F-4 to F) [29,31]. However, the simultaneous and continuous variations in temperature and photoperiod under field conditions can affect the rate of leaf emergence in different leaf layers. Exploring the use of leaf-specific phyllotherms between the lower (F-4 and F-3) and upper (F-2 to F) leaves within the DSS requires further research to ensure the reliable prediction of the emergence of leaves F-4 to F. In particular, improved prediction of the emergence of leaves F-2 to F in winter wheat and winter barley will help ensure timely, environmentally friendly and efficacious fungicide applications to help maximize yields.

The main objective of this study was to investigate the variability in phyllotherm for predicting the emergence of the three upper leaves, F-2 to F, in winter wheat and winter barley in the field. The overarching objective was to improve the performance of the DSS used for managing foliar fungal disease risk in the Grand-Duchy of Luxembourg (GDL). Specifically, five phyllotherms (i.e., 100 °Cd to 160 °Cd, in 15 °Cd steps) were assessed for predicting the emergence of leaves F-2 to F for both winter wheat and winter barley using the PROCULTURE model [29]. The predicted values were compared to field data collected during the 2014–2019 cropping seasons at four sites representative of the Luxembourgish wheat- and barley-growing regions. The emergence of F-2 to F, which correspond generally to the period spanning GS31 (first node detectable) to GS37 in winter wheat and winter barley in the GDL, is a critical period for efficacious fungicide-based fungal disease management [6]. Thus, accurate and reliable leaf emergence prediction for F-2 to F will allow for timely fungicide application to ensure lasting protection against infections by foliar fungal disease pathogens and to maximize disease control.

2. Materials and Methods

2.1. Study Areas

Data from fields of winter wheat and winter barley located at Bettendorf (6.19 E, 49.87 N), Burmerange (6.28 E, 49.52 N), Everlange (5.95 E, 49.78 N), and Reuler (6.04 E, 50.06 N) in the GDL were used in the study. The experimental sites were selected across commercial winter wheat and winter barley fields during the 2014–2019 cropping seasons; they included early and medium-maturity cultivars (Table 1). Experiments were designed in a randomized block with four replicates, with one replicate plot size = $8.0 \text{ m} \times 1.5 \text{ m}$. Sowing and harvest methods, as well as crop practices, were typical of wheat and barley production in the GDL. Winter barley and wheat are generally sown between the end of September and the end of October. Plant densities ranged from 200 to 250 plants m^{-2} and 170 to 200 plants m⁻² for winter wheat and winter barley, respectively, with sowing depths varying between 1 and 2 cm for both crops. Nitrogen fertilizers were applied three times: the first applications were generally made between the end of February and early March; the second nitrogen fertilizer was applied during the first fortnight of April (which corresponds to the first node stage); and the third and last application of nitrogen fertilizer was made during the second half of May (which corresponds to the period when the flag leaf emerges). Growth regulators are often applied from the end of April to early May, in conjunction with herbicides or fungicides. Herbicides were typically applied from the end of March to early April. The application and frequency of fungicide application depend on the prevalence and severity of foliar disease at earlier growth stages, and the prevailing weather conditions.

2.2. Data

Daily weather data (mean air temperature, relative humidity, and precipitation) were recorded at an automatic weather station located within 1 to 2 km of each experimental field. Mean air temperature and relative humidity were measured at 2 m above the soil surface. Total precipitation was measured at 1 m above the soil surface. The raw weather variables, recorded at 10 min intervals, were automatically retrieved from the web-based database system (www.agrimeteo.lu) and processed using an automatic data processing chain within which data were quality checked [33]. The mean daily weather variables by month during the 2014–2019 period for each of the study sites are presented in Figure 1.

Site	Year		Wheat						Barley				
		Cultivar	CC ^a	Sowing Date	Previous Crop	Tillage	N Rate (N kg/ha) ^b	Cultivar	CC ^a	Sowing Date	Previous Crop	Tillage	N Rate (N kg/ha)
Bettendorf	2014	Kerubino	4	9 October 2013	Oilseed rape	No	150	Leibniz	6	24 September 2013	Wheat	Yes	220
	2015	Kerubino	4	15 October 2014	Oilseed rape	No	170	California	6	28 September 2014	Oilseed rape	Yes	220
	2016	Kerubino	4	09 October 2015	Oilseed rape	No	160	California	6	28 September 2015	Maize	Yes	220
	2017	Kerubino	4	12 October 2016	Oilseed rape	No	160	California	6	30 September 2016	Winter wheat	Yes	220
		Achat	6	12 October 2016	Oilseed rape	No	160			-			
	2018	Kerubino	4	19 October 2017	Oilseed rape	Yes	150	California	6	30 September 2017	Winter wheat	Yes	220
		Desamo	5	19 October 2017	Oilseed rape	Yes	150						
	2019	Kerubino	4	24 October 2018	Oilseed rape	No	150	California	6	28 September 2018	Winter wheat	Yes	220
		Desamo	5	24 October 2018	Oilseed rape	No	150						
Burmerange	2014	Asano	4	3 October 2013	Oilseed rape	No	185	Sandra	5	27 September 2013	Wheat	No	140
	2015	Asano	4	4 October 2014	Maize	No	190	Leibniz	6	18 September 2014	Wheat	No	140
	2016	Kerubino	4	4 October 2015	Maize	No	200	Leibniz	6	18 September 2015	Wheat	No	140
	2017	Kerubino	4	17 October 2016	Oilseed rape	No	190	Wotan	5	15 October 2016	Wheat	Yes	140
	2018	Reform	6	12 October 2017	Oilseed rape.	Yes	140	Wotan	5	15 October 2017	Winter wheat	No	140
	2019	Kerubino	4	18 October 2018	Oilseed rape	Yes	140	California	6	27 September 2018	Spring triticale	No	140
Everlange	2014	Privilege	6	3 October 2013	Oilseed rape	No	160	Meridian	5	26 September 2013	Oilseed rape	No	150
	2015	Desamo	5	25 October 2014	Maize	No	180	Souleika	6	24 September 2014	Triticale	Yes	170
	2016	Desamo	5	25 October 2015	Maize	No	170	Tamina	6	20 September 2015.	Spring wheat	Yes	160
	2017	Manitou	6	13 October 2016	Maize	Yes	160	Tamina	6	29 September 2016	Ryegrass	Yes	160
	2018	Genius	5	14 October 2017	Peas	Yes	140	Meridian	5	25 September 2017	Oilseed rape	Yes	150
	2019	Kerubino	4	16 October 2018	Oilseed rape	Yes	140	Higgins	5	28 September 2018	Grass seed	Yes	150
Reuler	2014	Kerubino	4	20 October 2013	Maize	Yes	180	California	6	30 September 2013	Wheat	Yes	200
	2015	Kerubino	4	1 October 2014	Oilseed rape	Yes	190	California	6	30 September2014	Spelled	Yes	200
	2016	Kerubino	4	30 October 2015	Maize	Yes	200	California	6	29 September 2015	Wheat	Yes	200
	2017	Kerubino	4	3 October 2016	Maize	Yes	190	California	6	22 September 2016	Oilseed rape	Yes	200
	2018	Kerubino	4	19 October 2017	Maize	No	140	California	6	25 September 2017	Oilseed rape	Yes	200
	2019	Kerubino	4	12 October 2018	Oilseed rape	Yes	140	California	6	27 October 2018	Maize	No	150

Table 1. Agronomic information for the commercial winter wheat and winter barley fields at the study sites used for investigating the effect of phyllotherm on leaf
emergence during the 2014–2019 cropping seasons in the Grand-Duchy of Luxembourg.

^a: Cultivar classification. Early-maturity cultivar: ≤4; Medium-maturity cultivar: 5–6; Late-maturity cultivar: ≥7 [32]. ^b: Nitrogen fertilizer.



Figure 1. Distribution and variability of daily mean air temperature, relative humidity and precipitation during the 2014–2019 period at the study sites in the Grand-Duchy of Luxembourg. For a given site, the boxplot represents the distribution of daily meteorological variables for each month over the 2014–2019 period. The top and bottom of the box represent the 75th and 25th percentiles, respectively; the solid line indicates the median. The whiskers on the top and bottom represent the largest and smallest values within 1.5 times interquartile range above the third and first quantiles, respectively.

Data for leaf appearance used in the study originated from plots which received no foliar fungicide throughout the cropping seasons. Ten plants per plot (40 plants total) were randomly selected and marked when delineating the experimental plots at each site. To closely monitor the emergence of the three upper leaves, a reference marking was made on each of the 10 plants at the time of selecting the plants. The mark consisted of manually cutting a small section of the leaf at the extremity of the third leaf layer. The correct number of the leaf layers was determined upon the emergence of the flag leaf (F). The percentage of emerged leaf area for each leaf layer was estimated by comparison to the total area of the preceding fully formed leaf (assumed to be 100%), and by checking the ligule of the emerging leaf (a fully visible leaf layers was estimated relative to the preceding leaf layer for each of the 40 plants. Observations were carried out weekly between March and July each year by experienced agronomists and plant pathologists. Care was also taken to ensure the same rater assessed the same replicate during each of the monitoring weeks.

The PROCULTURE model [29,31] was used to simulate the emergence of the three upper leaves. PROCULTURE is a mechanistic model used for simulating the risk of infection and progress of STB, as well as the emergence of the five upper leaves, within the DSS for managing fungal disease risks in cereals in Luxembourg [6,30]. For each cropping season and for each of the study sites, the default phyllotherm value (130 °Cd) in PROCULTURE was used to predict the emergence of F-4, F-3 and F-2 based on the sowing dates. Given that PROCULTURE allows for correction when predicting F-2 before the prediction of subsequent leaves (F-1 and F), adjustments were applied based on the date of the first report of the emergence of F-2 on the plants in the fields, and the percentage of that leaf position that had emerged, where necessary [30].

Five phyllotherm values, 100 °Cd to 160 °Cd (in 15 °Cd steps), including the default value (130 °Cd), were used for predicting the emergence of leaves F-2 to F for both winter wheat and winter barley during the 2014–2019 cropping seasons. The range was chosen based on previously reported phyllotherm values [20,22,24]. A base temperature of 0 °C was used for both crops [26,34]. As noted, the simulation of F-2 emergence was empirically corrected based on field observations (Table 2).

Table 2. Dates of observation and percentage of emerged leaf area for the F-2 leaf (where F = flag) on plants in commercial winter wheat and winter barley fields at the four study sites in the Grand-Duchy of Luxembourg during the 2014–2019 cropping seasons.

Site	Vear	Date of Ol	oservation	Percentage of Leaf Formed (%) ^a			
one	icai	Barley	Wheat	Barley	Wheat		
	2014	31 March	14 April	85	10		
	2015	16 April	22 April	70	60		
Battandarf	2016	11 April	19 April	25	50		
Detteriuori	2017	18 April	2 May	67	95		
	2018	16 April	16 April	40	9		
	2019	8 April	15 April	90	13		
	2014	21 March	14 April	5	13		
	2015	13 April	20 April	32	32		
Burmerange	2016	8 April	18 April	14	60		
Durmerange	2017	19 April	29 April	15	90		
	2018	13 April	21 April	15	2		
	2019	3 April	20 April	12	16		
	2014	5 March	14 April	80	18		
	2015	12 April	20 April	27	43		
Everlance	2016	4 April	25 April	14	89		
Lvenange	2017	12 April	2 May	43	30		
	2018	6 April	16 April	6	7		
	2019	6 April	28 April	1	5		
	2014	10 April	22 April	90	57		
	2015	13 April	4 May	36	70		
Doulor	2016	18 April	5 May	80	5		
Keuler	2017	23 April	1 May	90	5		
	2018	9 April	30 April	13	24		
	2019	5 April	28 April	5	6		

^a: The percentage of emerged leaf area for each leaf layer was estimated by comparison to the total area of the preceding fully formed leaf (assumed as 100%), and by checking the ligule of the emerging leaf (a fully visible leaf ligule corresponds to a fully emerged leaf). Thus, the percentage of the emerged area of each of the three leaf layers was estimated relative to the preceding leaf layer for each of the 40 plants.

2.4. Statistical Analyses

The predicted percentage leaf emergence (expressed as the percentage of emerged leaf area) for each of the three upper leaves during each phyllotherm was compared to field assessments (the estimated

area emerged for that leaf layer relative to the previous, fully emerged layer). The accuracy of predictions was evaluated using the mean absolute error (MAE), the root mean square error (RMSE) and the Willmott's index of agreement (WI) [35]. The three statistics were calculated as follows:

$$MAE = \frac{1}{n} \sum_{i=1}^{n} |O_i - P_i|$$
(1)

$$RMSE = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (O_i - P_i)^2}$$
(2)

$$WI = \begin{cases} 1 - \frac{\sum_{i=1}^{N} |P_i - O_i|}{2\sum_{i=1}^{N} |O_i - \overline{O}|}, \text{ when } \sum_{i=1}^{N} |P_i - O_i| \le 2\sum_{i=1}^{N} |O_i - \overline{O}| \\ \frac{2\sum_{i=1}^{N} |O_i - \overline{O}|}{\sum_{i=1}^{N} |P_i - O_i|} - 1, \text{ when } \sum_{i=1}^{N} |P_i - O_i| > 2\sum_{i=1}^{N} |O_i - \overline{O}| \end{cases}$$
(3)

where *n* is the number of field observations; O_i is the *i*th observed value; \overline{O} is the mean observed value; and P_i is the *i*th predicted value.

The smaller the value of the MAE or RMSE, the more accurate are the predictions. Values of WI closer to 1 are indicative of good agreements between predicted and observed values, and are thereby indicative of good model performance.

Considering that data were available for two winter wheat cultivars during each of the 2017 and 2019 cropping seasons at Bettendorf (Table 1), a comparison of leaf emergence using the default phyllotherm in PROCULTURE and those obtained using the best-performing phyllotherm (found after comparisons of all five phyllotherms) was made to check whether the performance of the latter phyllotherm was cultivar-sensitive.

Additionally, the ability of the best-performing pyhllotherm -adjusted PROCULTURE model (i.e., the model using the best-performing phyllotherm) to predict the point of first emergences of each of the three upper leaves F-2 to F for both winter wheat and winter barley was also investigated. Statistical scores derived from a contingency table analysis were used to evaluate the ability of the best-performing phyllotherm to predict the point of the first observed emergence of leaves F-2 to F during the 6-year period at each of the study sites. The statistical scores used were the probability of detection (POD), the false alarm ratio (FAR), and the critical success index (CSI). They were calculated as follows: POD = a/(a + c), FAR = b/(a + b), and CSI = a/(a + b + c), where a, b, and c refer to leaf emergence either observed or predicted, leaf emergence predicted but not observed, and leaf emergence observed but not predicted, respectively.

All statistical analyses and graphical representations were performed using R (v4.0.0; [36]) and SigmaPlot (v14; Systat Software Inc., San Jose, CA, USA).

3. Results

3.1. Prediction of Emergence of Leaves F-2, F-1 and F in Winter Wheat

The performance of various models differed when simulating the emergence of F-2, F-1 and F using the five different phyllotherms. Overall, accurate predictions of leaf emergence were found when using the 100 °Cd phyllotherm in all years and at all study sites, irrespective of the leaf. For F-1 and F, the MAE and RMSE were \leq 5% (Figure 2). Exceptions included the sites at Burmerange in 2017 for F-1 (MAE = 11%; RMSE = 12%), and Everlange in 2015 for F (MAE = 12%; RMSE = 15%), which indicate only modest deviations in accuracy in these cases (Figure 2). For the F-1 and F leaves, using a phyllotherm greater than or equal to 115 °Cd yielded generally greater prediction errors when compared to those found using a phyllotherm of 100 °Cd, indicating less accuracy. For example, for phyllotherms 130 °Cd, 145 °Cd and 160 °Cd, the MAE and RMSE values were most often \geq 20% for all sites and in all years, indicating less accuracy in prediction (Figure 2). With regard to F-2, the 100 °Cd and 115 °Cd phyllotherms, and to a lesser extent the 130 °Cd phyllotherm, resulted in a similar model performance (Figure 2). However, prediction errors were more frequent (\geq 10% on

average) for phyllotherms greater than 130 °Cd, indicating less accuracy when compared to the 100 °Cd, 115 °Cd and 130 °Cd phyllotherms.



Figure 2. Mean absolute errors (MAE; left) and root mean square errors (RMSE; right) according to the phyllotherms used for predicting the emergence of leaves F, F-1 and F-2 in winter wheat in the Grand-Duchy of Luxembourg. Phyllotherms are expressed in °Cd. F is the flag leaf. In all years only values for the cultivar Kerubino were used.

Leaf emergence (% area emerged), as recorded on plants in the winter wheat fields during each of the study cropping seasons, and predicted values are provided (Figure 3, and Supplementary Materials Figures S1 and S2; results for F were presented in the text to reduce redundancy). Similarities between the curve shape based on the observed values and the curve shape based on the predicted values showed that, in most of the site–year cases, the 100 °Cd phyllotherm outperformed the other phyllotherms tested. Thus, the 100 °Cd phyllotherm appears appropriate for simulating leaf emergence in winter wheat fields under Luxembourgish conditions. The agreements between the observed and predicted leaf emergence values for F-1 and F based on the 100 °Cd phyllotherm were confirmed by the WI values; the WI values were consistently \geq 0.90, indicating close agreement (Figure 4). For phyllotherms >130 °Cd, the WIs were generally \leq 0.50 for F in all site–year cases (Figure 4). A similar pattern was observed for F-1 for phyllotherms 145 °Cd and 160 °Cd. With F-2, the WI values were all greater than 0.70 for the majority of site–year cases (Figure 4), irrespective of the phyllotherm value.



Figure 3. Observed (dashed lines) and predicted (solid lines) percentage emergence of formation of the flag leaf (F) in winter wheat during the 2014–2019 cropping seasons at the different study sites in the Grand-Duchy of Luxembourg. The percentage of emerged leaf area for each of the three leaf layers was estimated by comparison to the total area of the preceding fully emerged leaf (assumed as 100%), and by checking the ligule of the emerging leaf (a fully visible leaf ligule corresponds to a fully emerged leaf). The percentage emerged areas were estimated for each of the 40 replicate plants at each assessment. In all years only values for the cultivar Kerubino were used. Note: the curve for observed values and that for predicted values using the 100 °Cd phyllotherm appear superposed in most of the graphs.

Figure 4. Comparisons of the Willmott's index values according to the phyllotherms (100, 115, 130, 145 and 160 °Cd) used for predicting the emergence of leaves F, F-1 and F-2 in winter wheat during the 2014–2019 cropping seasons at the different study sites in the Grand-Duchy of Luxembourg. F is the flag leaf. In all years only values for the cultivar Kerubino were used.

Analyzing the simulation results for different wheat cultivars in 2017, 2018 and 2019 (Figure 5, Table S1) showed that using a phyllotherm of 100 °Cd for simulating the emergence of the upper leaves gave accurate results, regardless of the cultivar. A similar range of prediction errors were found when comparing the cultivar Kerubino to cultivars Achat (in 2017) or Desamo (in 2018 and 2019). For Kerubino, RMSE and MAE ranged from 1 to 6%, and from 1 to 3%, respectively, over the three cropping seasons (all leaves considered), indicating accurate predictions. The respective range of errors for the other cultivars was from 2 to 65%, and from 1 to 4% (Table S1). Although larger prediction errors were found with the emergence of the F-2 leaves of the cultivar Desamo in 2018 (RMSE = 11% and MAE = 10%; Table S1), the lowest prediction errors occurred when using the phyllotherm of 100 °Cd, indicating that this phyllotherm can be applied to accurately and reliably predict the emergence of the three uppermost leaves in different winter wheat cultivars in the GDL.

Figure 5. Comparisons between observed and predicted leaf emergence for the three upper leaves (F, F-1 and F-2, F being the flag leaf) for different winter wheat cultivars at Bettendorf during the 2017–2019 cropping seasons. Only results for the default phyllotherm in PROCULTURE (130 °Cd) and phyllotherm 100 °Cd are presented. Note: the curves for observed values and predicted values using the 100 °Cd phyllotherm appear superposed in some of the graphs.

3.2. Prediction of Emergence of Leaves F-2, F-1 and F in Winter Barley

The patterns of leaf emergence and prediction errors in winter barley were similar to those found for winter wheat. Good predictions were observed when using a phyllotherm of 100 °Cd for F and F-1 for the majority of the site–year cases; the MAE and RMSE were generally <5% (Figure 6). Exceptions occurred in 2014 and 2019 for F at Reuler where the MAE and RMSE were 9%. For phyllotherm \geq 115 °Cd, the prediction errors most often increased for both F and F-1 leaves, with values exceeding 20% in most cases (Figure 6). For the prediction of F-2, the errors were most often lower compared to those for F and F-1 leaves. Leaf emergence predictions using a phyllotherm of 100 °Cd outperformed those based on phyllotherms from 115 °Cd to 160 °Cd. The differences in prediction errors were generally \leq 5% for phyllotherms of 115 °Cd and 130 °Cd (Figure 6), suggesting similar accuracies.

Figure 6. Mean absolute errors (MAE; left) and root mean square errors (RMSE; right) according to the phyllotherms tested for predicting the emergence of the upper leaves F, F-1 and F-2 in winter barley at the different study sites in the Grand-Duchy of Luxembourg. Phyllotherms are expressed in °Cd. F is the flag leaf.

The analyses of the WI values corroborate these results. There was clear and strong agreement between the observed and predicted leaf emergence values for F-1 and F in all years for all the study sites (Figure 7). Similar to winter wheat, in most cases, the WI values for F-2 were greater than or equal to 0.70. Moreover, a visual inspection of the relationships between the observed or predicted emerged leaf area based on the 100 °Cd phyllotherm showed, in most cases, that the curves had very similar shapes (Figure 8, and Figures S3 and S4).

• 100 • 115 • 130 • 145 • 160

Figure 7. Comparisons of the Willmott's index values according to the phyllotherms (100, 115, 130, 145 and 160 °Cd) used for predicting the emergence of leaves F, F-1 and F-2 in winter barley at the different study sites in the Grand-Duchy of Luxembourg. F is the flag leaf.

Figure 8. Observed (dashed lines) and predicted (solid lines) percentage emergence (in this case measure as first visible appearance) of the flag leaf (F) in winter barley during the 2014–2019 cropping seasons in the Grand-Duchy of Luxembourg. The percentage of emerged leaf area for each of the three leaf layers was estimated by comparison to the total area of the preceding fully emerged leaf (assumed as 100%), and by checking the ligule of the emerging leaf (a fully visible leaf ligule corresponds to a fully emerged leaf). The percentage emerged areas were estimated for each of the 40 replicate plants at each assessment. Note: the curves for observed values and predicted values using the 100 °Cd phyllotherm are superposed in most of the graphs.

3.3. Improvement of Leaf Emergence Prediction within the DSS

We have shown that the 100 °Cd phyllotherm is an accurate and reliable basis for predicting leaf emergence for F, F-1 and F-2 in both winter wheat and winter barley. Using the 100 °Cd phyllotherm, the predicted visible emergence of the three uppermost leaves was compared to the first observed emergence. The analysis of the statistical scores indicated satisfactory levels of visible leaf emergence prediction for all the study sites during the 2014–2019 cropping seasons for both winter wheat and winter barley. POD and CSI were greater than or equal to 0.70 (a perfect score for either statistic is 1.0), with the lower values associated with the prediction of the first emergence of F (Table 3). The maximum FAR values were 0.16 for F-2 in winter wheat at Burmerange, and F-2 and F-1 in winter barley at Reuler. For the remainder of the site–crop cases, a perfect FAR score of 0.00 was obtained (Table 3).

Table 3. Probability of detecting (POD) leaf emergence, false alarm ratio (FAR), and critical success index (CSI) using a phyllotherm of 100 °Cd for winter wheat and winter barley during the 2014–2019 cropping seasons. The values of the forecasted and observed data used for the calculations of the statistical scores are provided. For 2017, 2018 and 2019, only observations for the wheat cultivar Kerubino were used. F = the flag leaf.

Crop	Site	Leaf	FE ^a	FNE ^b	NFE ^c	POD ^d	FAR ^e	CSI ^f
Winter wheat		F-2	6	0	0	1.00	0.00	1.00
	Bettendorf	F-1	6	0	0	1.00	0.00	1.00
		F	6	0	0	1.00	0.00	1.00
		F-2	6	0	0	1.00	0.00	1.00
	Burmerange	F-1	6	0	0	1.00	0.00	1.00
		F	4	0	2	0.70	0.00	0.70
		F-2	5	1	0	1.00	0.16	0.84
	Everlange	F-1	6	0	0	1.00	0.00	1.00
		F	5	0	1	0.84	0.00	0.84
		F-2	6	0	0	1.00	0.00	1.00
	Reuler	F-1	6	0	0	1.00	0.00	1.00
		F	5	0	1	0.84	0.00	0.84
Winter barley		F-2	6	0	0	1.00	0.00	1.00
	Bettendorf	F-1	6	0	0	1.00	0.00	1.00
		F	6	0	0	1.00	0.00	1.00
		F-2	6	0	0	1.00	0.00	1.00
	Burmerange	F-1	6	0	0	1.00	0.00	1.00
		F	5	0	1	0.84	0.00	0.84
		F-2	6	0	0	1.00	0.00	1.00
	Everlange	F-1	6	0	0	1.00	0.00	1.00
		F	4	0	2	0.70	0.00	0.70
		F-2	5	1	0	1.00	0.16	0.84
	Reuler	F-1	5	1	0	1.00	0.16	0.84
		F	6	0	0	1.00	0.00	1.00

^a Forecasted and emerged. ^b Forecasted but not emerged. ^c Emerged but not forecasted. ^d POD, probability of detection, it is the probability of correctly forecasting the observed event; it ranges between zero and one (perfect score = 1). ^e FAR, false alarm ratio, is the number of times an event is forecast but is not observed, divided by the total number of forecasts of that event. Perfect value = 0. ^f CSI, critical success index, considers both false alarms and missed events; it ranges between zero and one (perfect score = 1).

The performance of the prediction of first emergence based on different phyllotherms is presented in Figures 3 and 8, as well as Figures S1–S4. The predicted first emergence dates of F and F-1 based on the 100 °Cd phyllotherm generally coincided with the observed values, whereas the predicted first emergence was delayed by up to 10 days in some cases when using the default phyllotherm value (130 °Cd). This was especially so when predicting the first emergence of F in winter wheat (Figures 3 and 8). In winter barley, there was little or no delay in the prediction of the first emergence of F-1 when using either the default phyllotherm values of 130 °Cd or 100 °Cd (Figure S3).

4. Discussion

Despite its relatively small size (approximately 2586 km²), the Grand-Duchy of Luxembourg is characterized by noticeable climatic contrasts between and within its agricultural regions, which affect crop growth and the development and severity of foliar fungal diseases in winter wheat and winter barley throughout the cropping season [37,38]. The variable within- and between-season disease risks imply tailored fungicide-based crop protection to meet growers' needs to maintain yield while minimizing the cost of inputs and any adverse environmental effects of the crop protection measures. Extending the duration of the green leaf area of the upper leaves in both winter wheat and winter barley through the application of certain foliar fungicides benefits the grain filling period, that is, the fungicide effect leads to extended leaf area greenness, allowing grain filling over a longer period [7,39,40]. Such a long grain filling period could ultimately result in an increased final grain yield. In the GDL, preventive fungicide applications following a phenology-based calendar are integral to wheat and barley production [6,30]: the first treatment is applied during stem elongation to control early season fungal diseases (i.e., wheat powdery mildew and eyespot); the second treatment is typically applied at flag leaf emergence to protect against STB; and the third is occasionally applied at early flowering to protect against Fusarium head blight [6,30]. In this study, the prediction of leaf emergence of the upper leaves F-2 to F within the DSS, used for managing foliar fungal disease risks in the GDL, was assessed based on five phyllotherm values over six cropping seasons at different sites. The results indicate that the most accurate leaf emergence predictions based on the various environmental conditions and crop cultivars of winter wheat and winter barley used during the study period were based on a 100 °Cd phyllotherm for both crops, irrespective of the leaf. These findings are in agreement with previous reports (e.g., [24,41,42]), which concluded the average phyllotherms for the upper leaves were in the range 100 to 115 °Cd. The slight differences observed in the current study could be explained by environmental conditions, including variable sowing dates and varieties, variable nutrient application rates and availabilities, and differences in the effect of temperatures on leaf emergence.

Various factors, considered alone or in interaction with one another, regulate the rate of development and leaf emergence in wheat and barley, with the major variables being temperature, photoperiod and vernalization [16,26,43–48]. Nutrition (including availability of nitrogen, phosphorus and sulfur, aluminum toxicity) also affects the duration of the ontogenic phases from seedling emergence to flowering, though to a lesser extent [49–54]. Our experiments were conducted in commercial winter wheat and winter barley fields, and the responses of leaf emergence to varying sowing dates or nutrient rates in each of the cropping seasons were beyond the scope of the study's objectives, and thus were not investigated. Nevertheless, the results we present are of value and can guide future research in relation to the effects of other factors.

Although the contribution of F (the flag leaf) to grain filling and final yield in barley is almost insignificant due to its small size (hence the focus on keeping F-1 free of disease; [2]), we extended our analysis to F and F-2 because the potential severity of some diseases on F-1 might depend upon their severity in F or F-2. Thus, ensuring accurate and reliable prediction for all leaf layers (F-2 to F) could help minimize yield losses from diseases. Our analyses demonstrated that, for winter barley, as well as for winter wheat, accurate predictions of leaf emergence (i.e., the time of first appearance of the leaf) (Table 3) and subsequent leaf area development (Figures 3 and 8; Figures S1–S4), were obtained using a phyllotherm of 100 °Cd. Compared to the prediction errors when using the default phyllotherm value (130 °Cd), using a 100 °Cd phyllotherm improved the performance of PROCULTURE under the environmental conditions prevailing in Luxembourg, and thereby the overall performance of the DSS. A 100 °Cd phyllotherm allows more timely fungicide application for lasting protection [6]. Under changing climate conditions [55], and considering the continued improvements in crop breeding, it is worth re-evaluating phyllotherm variability for the uppermost leaf layers of major winter wheat and

winter barley cultivars across major cropping regions beyond Luxembourg. To this end, our findings may provide valuable insights for broader applications regarding the variability of phyllotherm within the leaf layers of these two economically important food crops.

In conclusion, our research confirms that a phyllotherm of 100 °Cd can be considered accurate and reliable for predicting the leaf emergence of the three uppermost leaf layers in winter wheat and winter barley under variable environmental and crop conditions in the GDL. The simulations of leaf emergence of F-2, F-1 and F in both crops at all the study sites were improved using the 100 °Cd phyllotherm when compared to phyllotherm values ≥ 115 °Cd, including the current phyllotherm standard of 130 °Cd used in the DSS. Moreover, based on the prediction errors when comparing the emergence of the three uppermost leaves for different winter wheat cultivars, our results indicate that the 100 °Cd phyllotherm is reliable for predicting the emergence of F-2, F-1 and F. Within the DSS, for managing disease risks based on foliar fungicide applications, leaf emergence simulations are important for efficacious crop protection. Thus, the results we present can help ensure timely fungicide applications to maximize disease control, to reduce the risk of disease and increase the likelihood of an improved yield for both winter wheat and winter barley, while minimizing the impact on the environment. Further research involving multiyear, multilocation experiments with major wheat and barley cultivars is warranted to extend the results across a broader range of conditions and cropping practices in Europe and elsewhere.

Supplementary Materials: The following are available online at http://www.mdpi.com/2073-4395/10/11/1825/s1, Table S1: Comparisons of leaf emergence predictions for different winter wheat cultivars at Bettendorf using five different phyllotherm values; Figure S1: Observed (dashed lines) and predicted (solid lines) percentage emergence of the leaf below the flag leaf (F-1) in winter wheat during the 2017–2019 growing seasons at the different study sites in Luxembourg; Figure S2: Observed (dashed lines) and predicted (solid lines) percentage emergence of the leaf below the flag leaf (F-2) in winter wheat during the 2017–2019 growing seasons at the different study sites in Luxembourg; Figure S3: Observed (dashed lines) and predicted (solid lines) percentage emergence of the leaf below the flag leaf (F-1) in winter barley during the 2017–2019 growing seasons at the different study sites in Luxembourg; Figure S4: Observed (dashed lines) and predicted (solid lines) percentage emergence of the leaf below the flag leaf (F-2) in winter barley during the 2017–2019 growing seasons at the different study sites in Luxembourg; Figure S4: Observed (dashed lines) and predicted (solid lines) percentage emergence of the leaf below the flag leaf (F-2) in winter barley during the 2017–2019 growing seasons at the different study sites in Luxembourg; Figure S4: Observed (dashed lines) and predicted (solid lines) percentage emergence of the leaf below the flag leaf (F-2) in winter barley during the 2017–2019 growing seasons at the different study sites in Luxembourg.

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