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Designing cropping systems that are well-adapted to water-limited conditions is one challenge of adapting agriculture to climate change. It requires estimating impacts of current and future cropping practices on crop water use and water resource availability in agricultural areas. Crop models such as AqYield are useful tools for evaluating effects of climate, soil and crop practices on evapotranspiration (ET) and drainage that directly impact soil available water (AW). AqYield is a simple model with few input data that has already been satisfactory evaluated for spring crops in southwestern France. Our main objective was to evaluate the ability of AqYield to predict components of soil water balance at the field level for crop rotations. First, we calibrated and evaluated AqYield predictions for winter wheat in France under a wide range of contrasting climatic and soil conditions. Fifty experimental situations (site × year × management) were chosen for calibration. AqYield was evaluated (i) for winter wheat in nine experimental situations, using daily drainage and ET data, and (ii) for two crop rotations on two fields with 7-years of continuous measurements of daily ET flux. During calibration, AqYield predicted soil AW in the contrasting situations with a model efficiency of 0.83, in the same range of accuracy as those of other widely published models. AqYield also predicted ET accurately from calibration and validation datasets, with a model efficiency of 0.84 and 0.69, respectively, for monthly ET. AqYield predicted daily and monthly drainage less accurately, although the range of drainage during the cropping period was predicted well. At the crop-rotation scale, AqYield yielded acceptable predictions of ET for contrasting climate conditions and crops. Whereas AqYield is simple and requires only a few input data, it accurately predicted ET of cropping systems. It therefore could be useful as a module in more complex modeling approaches.

1. Introduction

Southern Europe is subject to global changes that will affect the future of available water resources for agriculture. Climate change is expected to decrease annual precipitation and increase its inter-annual as well as its inter-seasonal variability. This will increase water stress caused by a combination of decreased water resource availability (lower precipitation and increased evapotranspiration (ET)) and increased water use pressure resulting from economic growth and urban expansion (García-Ruiz et al., 2011). Baseline evapotranspiration is expected to increase, especially in winter and spring, which may have higher temperatures (Moratiel et al., 2011; Saadi et al., 2015). This will result in increased water demand and consumption, soil evaporation and crop transpiration, which will affect surface water balance and the partitioning of rainfall between ET, runoff, and groundwater fluxes (García-Ruiz et al., 2011). The latter is a particularly concerning issue since drought is already relatively severe in several areas, inducing limited irrigation (Mishra and Singh, 2010). The response of agricultural systems to water scarcity depends on the management practices adopted, such as crop rotations, which directly impact the amount and availability of soil water (Tubiello et al., 2000). The ability to estimate the influence of current and future cropping practices on crop water use and, in turn, on water resource availability, is a great challenge in agricultural areas (Mazzega et al., 2014; Murgue et al., 2015). Quantifying the ET and drainage of irrigated and rainfed crops is crucial for water resource management in areas where water is predicted to be

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Abbreviations, definitions and units of variables in water balance equations. Units are mm unless otherwise specified

Irr	Daily irrigation
PET	Daily potential evapotranspiration
R	Daily rainfall
Drain	Daily amount of water loss by drainage
EVA	Daily amount of evaporation from the soil
Kc	Crop coefficient, index of foliar expansion (unitless)
RootAWC	Available Water Content in the layer explored by roots on a given day
$RootAWC_{max}$	Maximum Available Water Content in the layer explored by roots on a given day
SurfAWC	Available Water Content in the shallow layer on a given day
$SurfAWC_{max}$	Maximum Available Water Content in the shallow layer
TotAWC	Available Water Content in the soil on a given day
TR	Daily actual crop transpiration
TR_{max}	Daily maximum crop transpiration

or is already scarce. These predictions can be used to design cropping systems better adapted to water-limited conditions.

In this context, crop models are valuable tools to predict effects of climate, soil characteristics and crop management on the water balance in actual and future cropping systems. Evapotranspiration, soil available water (AW), and drainage are crucial water balance components that have a direct impact on water availability in cropping systems; therefore, it is essential to predict them with crop models (Eitzinger et al., 2004). Several models of crop functioning have been developed for a variety of climatic and soil conditions with multiple levels of complexity (Kollas et al., 2015; Palosuo et al., 2011; Rötter et al., 2012). Most were developed and/or evaluated to predict yields. Only a few focus on simulating water flux components or run at the fine time resolution of one day (needed to optimize irrigation) or at the crop-rotation scale (needed for a more integrative approach to field functioning).

Crop models, like AqYield, that simulate dynamic water balance components (ET, AW) can be coupled with hydrological models to study interactions between agricultural practices and physical characteristics of watersheds (Ferrant et al., 2011; Martin et al., 2016). Predictions at the watershed level help in monitoring aquifer depletion and understanding changes in water use induced by land use. They also help to optimize irrigation and, specifically, to predict impacts of water regulation strategies. This could enable stakeholders to allocate AW better among agricultural, urban and environmental uses (Anderson et al., 2012; Martin et al., 2016; Mazzega et al., 2014). The MAELIA platform, on which the AqYield soil-crop model was implemented (Gaudou et al., 2014; Martin et al., 2016; Mazzega et al., 2014; Therond et al., 2014), was developed to accurately spatialize and simulate water flux components at the watershed level to assess water and land use management strategies. It is useful for analyzing scenarios of water and land use management strategies at the watershed level in combination with global changes. In this platform, the AqYield crop model predicts water fluxes in fields at the watershed level. AqYield was chosen because it is a simple model (simple equations and empirical processes), requiring few input data. It only requires four soil properties, three daily climate features and dates for crop managements (Constantin et al., 2015). Consequently, it has shorter calibration and calculation times and requires only basic input data, which are more easily collected than detailed data at a watershed level. Moreover, simple models, like AqYield, have the advantage to avoid “black box” effect (transparency of internal structure and behavior of the model) and to ease communication with various stakeholders (Voinov and Bousquet, 2010). AqYield was recently found to predict AW (Constantin et al., 2015) of spring crops as accurately as a more complex crop model such as STICS (Brisson et al., 2003). In this recent study, AqYield predictions were evaluated for three rainfed and irrigated spring crops (sunflower, maize, and sorghum) at four sites in a region with dry summers in southwestern France. An evaluation of AqYield's performance for new crop species and at the crop-rotation scale is thus required. Extending evaluation of model performance to the rotation scale is a priority since crop rotation is the minimum temporal scale that makes sense for environmental assessment of cropping systems (Beaudoin et al., 2008; Yin et al., 2017).

The objective of our study was to evaluate the ability of AqYield to predict water balance components for crop rotations. We first calibrated and validated the model for winter wheat under a range of contrasting climatic and soil conditions in France. We then evaluated its ability to reproduce the daily ET flux measured for seven contrasting climate years for two typical crop rotations in southwestern France.

2. Materials and methods

2.1. AqYield overview

AqYield is a simple dynamic soil-crop model based on pattern modeling (Grimm and Railsback, 2012) of field-level water fluxes and crop yield. The model simulates water balance components (AW, evaporation, transpiration and drainage) at a daily time step, phenological stages and yield. The main inputs are i) soil properties (clay content, soil water holding capacity and soil depth), ii) climate data (daily mean temperature, rainfall and reference ET (ET_0) calculated by Penman-Monteith formula) and iii) crop management data such as irrigation practices (dates and amounts), sowing and harvest dates, and tillage date and depth. The influence of crop development on water fluxes is considered using only a crop coefficient (Kc); no biomass is simulated. The Kc is function of degree-days, crop phenology and water stress; it thus varies according to crop and situation. The Kc influences evaporation, maximum transpiration and root growth, which determine the soil water available for the crop. Soil is represented using a classic tipping-bucket approach and the concept of AW capacity. The equations used to predict water balance components are given in the Appendix A complete description of AqYield is provided in the Appendix of Constantin et al (2015).

2.2. Compilation of databases for wheat calibration and validation

We calibrated and validated the model for winter wheat (durum wheat and soft wheat). We selected AW, ET and/or drainage data from 14 experimental sites monitored in France to consider a wide range of contrasting soil, climate and crop management (mainly irrigation) situations which correspond to various European climates. Situations were distributed between calibration and validation databases to have contrasting situations (years) in both databases. We chose sites not limited by N (at least 110 kg N ha^{-1} added from fertilizers or manure), since AqYield does not represent N stress. For calibration, a total of 50 situations (site × year × management) were simulated; these situations had contrasting soil features, ranging from 10 to 50% clay content, 0.8–2.0 m soil depth and 81–313 mm of AW capacity (Table 1). Mean monthly temperature during the wheat cropping period (November to June) ranged from 6.7 to 11.9 °C. For each situation, water deficit (WD) was calculated from wheat sowing to harvest dates as cumulative daily rainfall (R) minus ET_0, excluding irrigation. Mean WD during the cropping period ranged from −187 to 132 mm among sites. WD varied among years for a given site; for example, at Fagnières it ranged from −110 to 81 mm (in 2011 and 1998, respectively). Wheat was not

Table 1
Descriptions of the sites in the wheat calibration and validation databases (dataset A).

Database	Site	Latitude/ Longitude	Clay content (%)	AW capacity (mm)	Mean temperature Nov-Jun (°C)	Range of WD during cropping period (mm)	Range of irrigation (mm)	Range of sowing dates	Range of harvest dates	No. of situations[a] (No. of daily observations)	Observed data[b]	Harvest years
Calibration	Auradé	43.6/ 1.1	32	128	9.8	[-87; -31]	0	[27 Oct; 19 Nov]	[29 Jun; 13 Jul]	2 (482)	ET	2006; 2010
	Lamasquère	43.5/ 1.2	50	130	10.3	[-208; -11]	0	[18 Oct; 3 Nov]	[2 Jul; 15 Jul]	2 (513)	ET	2007; 2011
	Fagnières	49.0/ 4.3	10	281	7.8	[-110; 81]	0	[14 Oct; 31 Oct]	[12 Jul; 5 Aug]	6 (1627)	drainage	1985; 1989;1998; 2005; 2006; 2011
	Bois-Joly	46.2/ -0.46	33	81	11.5	[-16; 153]	[0; 118]	[26 Oct; 28 Oct]	[26 Jun; 8 Jul]	5 (36)	AW	2002-2004
	Pouilly	49.7/ 3.6	20	142	6.7	132	53	24 Oct	30 Jul	1 (5)	AW	1991
	Magneraud	46.2/ -0.46	33	156	10.5	[-16; 153]	[0; 90]	[26 Oct; 28 Oct]	[26 Jun; 8 Jul]	5 (36)	AW	2002-2004
	Auzeville	43.5/ 1.5	25	180	11.0	[-266; 41]	0	[3 Nov; 24 Nov]	[30 Jun; 12 Jul]	9 (19)	AW	2004; 2006; 2007; 2010; 2012; 2015
	StGilles	43.7/ 4.4	20	200	11.9	[-304;- 146]	[0; 105]	30 Oct	4 Jul	4 (12)	AW	2006-2008
	Villamblain	48.0/ 1.8	27	205	8.5	[-230;- 64]	[0; 286]	[22 Oct; 7 Nov]	[18 Jul; 24 Jul]	7 (20)	AW	1996-1997
	Aulnois	49.6/ 3.6	13	218	8.2	113	0	24 Oct	27 Jun	1 (18)	AW	1989
	Estrées-Mons	49.9/ 3.0	17	238	8.3	[108; 144]	0	[5 Oct; 7 Oct]	[25 Jul; 28 Jul]	2 (17)	AW	1994-1995
	Grignon	48.8/ 1.9	23	267	9.1	51	109	23 Oct	17 Jul	1 (5)	AW	1995
	Bruyères	49.5/ 3.7	20	269	7.4	[-170; 31]	0	[5 Oct; 15 Oct]	[30 Jul; 15 Aug]	5 (16)	AW	1996-1998
	Minière	48.8/ 2.1	14	313	8.9	−72	0	26 Oct	29 Jul	1 (3)	AW	2002
Validation	Auradé	43.6/ 1.1	32	128	10.5	[-147; 49]	0	[26 Oct; 27 Oct]	[10 Jul; 14 Jul]	2 (519)	ET	2008;2012
	Lamasquère	43.5/ 1.2	50	130	10.6	−23	0	19 Nov	13 Jul	1 (236)	ET	2009
	Fagnières	49.0/ 4.3	10	281	8.5	[-197; 81]	0	[8 Oct; 12 Nov]	[20 Jul; 13 Aug]	6 (1693)	drainage	1987; 1998; 2004; 2009; 2010; 2012

[a] One situation represents a combination of site × year × management. WD is water deficit, ET is evapotranspiration (in mm), AW is soil available water for plant in the soil (in mm).
[b] Only one kind of data was available on each site (ET, drainage or AW).

usually irrigated, but some irrigation occurred in certain experiments, with a maximum of 286 mm during wheat development at Villamblain. The runoff was not simulated but all fields were flat, except at Auradé (2–3% slope).

Soil available water data were available for 41 situations, for a total of 187 observations (daily measurements of AW, ET or drainage) during crop development. Three experimental sites provided daily drainage and ET data. Daily drainage was measured with a lysimeter for 12 situations during the crop development period (Constantin et al., 2016), for a total of 3320 observations (1627 for calibration and 1693 for validation). Daily ET was measured by eddy covariance (e.g. Béziat (2009) and Béziat et al. (2010) at Lamasquère and Auradé) for 7 situations (site × year), for a total of 1750 observations (995 for calibration and 755 for validation). In total, the calibration database included 2809 observations, and the validation database included 2448 observations.

The validation database for wheat consisted of 9 situations (site × year) from the same three experimental sites with ET and drainage measurements as those in the calibration database, but corresponded to different years in order to express various climatic conditions.

2.3. Model calibration and optimization

Each simulation was initialized a few days or weeks before sowing (1 September to 30 October, depending on the site) with the AW estimated from soil water content (%) measured with soil moisture sensors (CS615 or CS 616, Campbell Scientific Inc, Logan, UT, USA) at each site on this date. To estimate the observed AW, we subtracted the water content at wilting point from the soil water content measurements. According to the site, the water content at wilting point was estimated by i) measuring the water content with an application of a −1.5 MPa potential (especially for the main three sites Auradé, Lamasquère and Fagnières) or ii) implementing pedotransfer functions. We converted soil water content into an amount of water based on soil depth and bulk density. No AW data were available at the Fagnières site to initialize the model; consequently, we used AW predicted by STICS in several years of continuous simulations from a previous study (Constantin et al., 2016).

Only two crop parameters were optimized (specifically for wheat) and only one global parameter of evaporation (one generic value for all crops). The first step in calibrating the model for wheat was to optimize the prediction of phenological stages by improving representation of the interacting effects of photoperiod and cumulative temperature. In AqYield, plant development is driven by cumulative temperature. Specific sums of effective temperature are needed to reach phenological stages, depending on species and cultivar. Development of winter crops slows during winter due to decreasing day length, which AqYield represents by using a photoperiod coefficient to calculate a vegetation scale (*Vscale*):

$$Vscale_{(d)} = (Vscale_{(d-1)} + \frac{(Tm-T0)}{SumTflo})^{*} K_{phot}$$

where Tm is daily mean temperature, T0 is the base temperature of the crop (0 °C for winter wheat), SumTflo is the cumulative effective temperature needed to reach flowering (Constantin et al., 2015), and K_{phot} is the photoperiod coefficient (active for crops growing during winter), which is applied only during a given period (generally from sowing to February, depending on the latitude). The end date of K_{phot} application (End_{Kphot}) is estimated as follows:

$$End_{K_{phot}} = 45 \times (\frac{DLindex}{0.28})^{1.5}$$

where DL_{index} is the day length index, calculated as:

$$DL_{index} = (\frac{latitude}{80})^{3} + 0.12$$

By trial and error, we optimized K_{phot} for winter wheat to predict the flowering dates observed in the calibration database more accurately. The K_{phot} was optimized for all simulations in order to have a generic value (K_{phot} of winter wheat = 0.43).

In a second step, we optimized the coefficient α, which influences soil evaporation (see Appendix for details). By trial-and-error, we optimized α based on measured AW, daily ET and drainage in the calibration database. This coefficient is generic for all crops; we thus took care to check that predictions for previously evaluated spring crops (Constantin et al., 2015) were not negatively impacted by this calibration.

Finally, by trial-and-error, we optimized the root-growth coefficient (RootG, in °C mm^{-1}), which influences root exploration in the soil, to 8.0 for durum wheat and 9.0 for soft wheat, based on measured AW, daily ET and drainage in the calibration database.

2.4. Crop rotations and site descriptions used to evaluate ET

We evaluated predicted daily and cumulative ET at the crop-rotation scale by comparing them to observed data from two of the experimental sites: Auradé and Lamasquère. These sites are part of the Integrated Carbon Observation System (ICOS) network (Paris et al., 2012) as FR-Aur and FR-Lam, respectively. For the evaluation, we ran AqYield continuously from sowing of the first crop to harvest of the last crop in each rotation. Since data from these two sites had been used to calibrate the model from wheat sowing to harvest (dataset A, Table 1), we excluded these calibration data when calculating statistical criteria used to evaluate predictions of the crop rotation (dataset B, Table 2).

Auradé followed mainly a winter wheat/rapeseed rotation, sown in September or October and harvested in June or July, with mineral fertilization (annual average of 140 kg N ha^{-1}), straw incorporated into the soil and no irrigation. Sunflower was grown at this site in 2007. Lamasquère followed a winter wheat/maize rotation, with mineral and organic (manure or slurry) fertilizer (annual average of 277 kg N ha^{-1}). Irrigation was applied to maize (50–148 mm $year^{-1}$). The required meteorological data at a daily time-step (temperature, ET_0, rainfall) were obtained from data initially recorded at a 30-minute time step at each experimental site. Daily ET was calculated from 30-minute ET fluxes recorded from 2006 to 2012, corresponding to seven cropping years (Table 2). Eddy covariance was used to continuously monitor ET, and included a system with a fast (20 Hz) infra-red gas analyzer (Li7500, Licor) and a 3D sonic anemometer (CSAT, Campbell Scientific Ltd). Filtering, quality controls and gap filling were performed following CarboEurope-IP recommendations (Aubinet et al., 2012). Ultimately, the dataset contained 4498 observations (2455 for Auradé and 2043 for Lamasquère). No data were recorded at Lamasquère from 1 January to 15 March 2011 due to instrument failure. We also calculated cumulative ET from sowing of a given crop until the sowing of the subsequent crop (including the fallow period between them). WD showed contrasting years of AW at both sites, since 2011 and 2012 were extremely dry and 2008 was wet (Table 2).

2.5. Statistical criteria used for model calibration and evaluation

Three statistical criteria — mean deviation (MD), relative root mean square error (rRMSE) and model efficiency (Ef) — were calculated to assess the quality of model calibration and evaluation:

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

$$rRMSE = \frac{\sqrt{\frac{1}{n}\sum_{i=1}^{n}(P_i - O_i)^2}}{\bar{o}} \tag{2}$$

Table 2
Management dates and climate features of the two crop rotations for the Auradé and Lamasquère sites. Total N applied is the total amount of N provided by fertilizers (and manure for the Lamasquère site) during the year. Water deficit (WD) equals the annual sum of daily rainfall minus reference evapotranspiration.

Site	Year	Crop	Sowing date	Harvest date	Total N applied (kg N ha^{-1})	Total irrigation (mm)	Annual WD (mm)	Data used to model wheat (dataset A)	Dataset for crop rotations evaluation (dataset B)
Auradé	2006	Wheat	27 Oct 2005	29 Jun 2006	124	0	−247	calibration	excluded
	2007	Sunflower	10 Apr 2007	15 Sep 2007	100	0	−137	/	used
	2008	Wheat	26 Oct 2007	10 Jul 2008	110	0	−45	validation	used
	2009	Rapeseed	04 Sep 2008	30 Jun 2009	167	0	−172	/	used
	2010	Wheat	19 Nov 2009	13 Jul 2010	195	0	−213	calibration	excluded
	2011	Rapeseed	29 Sep 2010	30 Jun 2011	150	0	−434	/	used
	2012	Wheat	27 Oct 2011	14 Jul 2012	147	0	−379	validation	used
Lamasquère	2006	Maize	01 May 2006	31 Aug 2006	395	148	−268	/	used
	2007	Wheat	18 Oct 2006	15 Jul 2007	352	0	−209	calibration	excluded
	2008	Maize	20 May 2008	10 Nov 2008	224	50	−1	/	used
	2009	Wheat	19 Nov 2008	13 Jul 2009	234	0	−249	validation	used
	2010	Maize	21 Apr 2010	17 Oct 2010	246	130	−320	/	used
	2011	Wheat	03 Nov 2010	02 Jul 2011	260	0	−375	calibration	excluded
		Wheat volunteers	01 Sep 2011	06 Dec 2011	0	0	/	/	used
	2012	Maize	27 Apr 2012	23 Aug 2012	230	115	−383	/	used

$$Ef = 1 - \frac{\sum_{i=1}^{n} (P_i - O_i)^2}{\sum_{i=1}^{n} (O_i - \bar{o})^2} \quad (3)$$

where n is the number of observations, O_i and P_i are observed and predicted values, respectively, and $\bar{o}$ is the mean of observed values. MD provides model deviation from the line $x = y$. rRMSE provides the relative absolute error and ranges from 0 to infinity, with 0 corresponding to the ideal. Ef represents model accuracy relative to the mean of observed data (ranges = -∞ to 1). As it approaches 1, the match between observed and predicted values increases; it becomes negative when the mean of observed values lies closer to observed values than predicted values do. We also calculated the R^2 for the linear regressions between observed and predicted data. We also calculated the median difference between observed and predicted values in absolute value and relative to the mean of observed values. Except for daily drainage (which had many observed values of zero), daily, monthly (cumulative) and cropping-period (cumulative) predictions of ET and drainage were evaluated using the same steps.

3. Results

3.1. Water balance component predictions for wheat

3.1.1. Soil available water for wheat

During calibration (dataset A), AqYield predicted AW during the wheat cropping period well, with Ef = 0.83, rRMSE = 0.23 (corresponding to 31 mm) and MD = 13 mm (Fig. 1). Model predictions of AW ranged from 9 to 311 mm, while observations ranged from 0 to 314 mm. The model predicted most situations well (median difference of 16 mm in absolute value; 13% in relative value), although it tended to overpredict the low and medium observed AW slightly.

3.1.2. Daily, monthly and cumulative evapotranspiration for wheat

During calibration (dataset A), AqYield predicted daily ET for wheat relatively well overall, with Ef = 0.54, rRMSE = 0.55 (corresponding to 0.7 mm) and MD = −0.1 mm for the four situations combined. The median difference between daily predicted and observed values was 0.34 mm in absolute value (25% in relative value). Prediction quality varied according to the situation, however, with Ef from 0.23–0.73, rRMSE from 0.45-0.65 and MD from −0.3 to 0.3 (Fig. 2).

Generally, daily ET was predicted well at the beginning of wheat

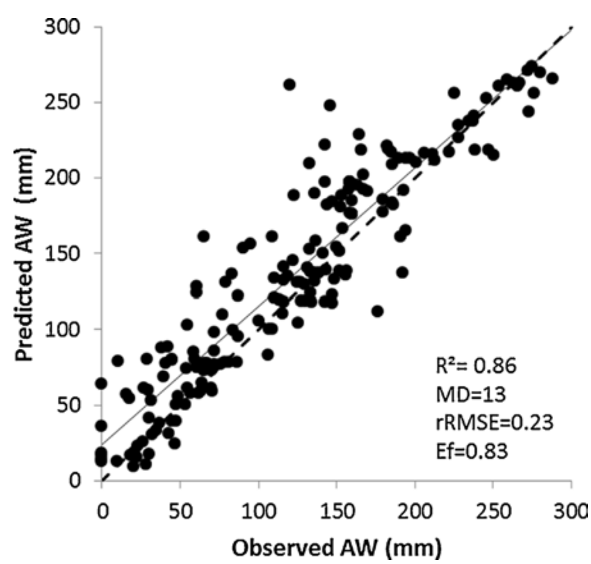

Fig. 1. Observed vs. predicted available water (AW) in the soil under wheat after model calibration. The data came from 14 sites in dataset A (Table 1). "MD" is the mean deviation, "rRMSE" is the relative root mean square error and "Ef" is the model efficiency.

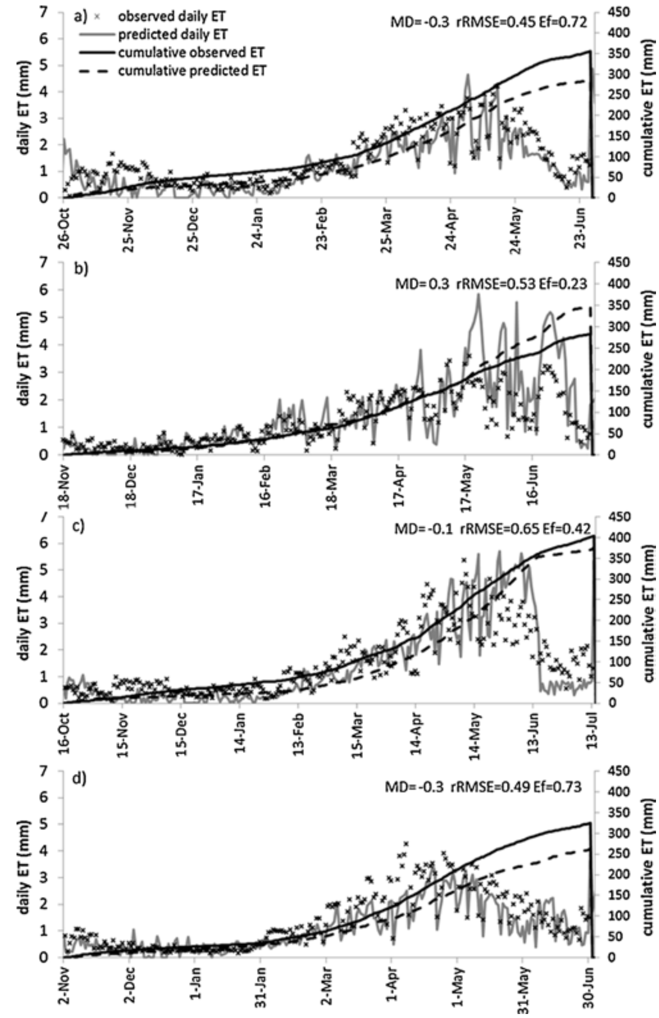

Fig. 2. Observed and predicted daily and cumulative evapotranspiration (ET) during the cropping period of wheat after model calibration for four site × year situations: a) Auradé in 2006, b) Auradé in 2010, c) Lamasquère in 2007 and d) Lamasquère in 2011. The statistical criteria shown were calculated for daily predictions. The data came from dataset A (Table 1). “MD” is the mean deviation, “rRMSE” is the relative root mean square error and “Ef” is the model efficiency.

growth, when ET is low in winter. Accuracy of predicted daily ET tended to decrease in spring and summer, when daily ET was higher and varied greatly. Consequently, for Auraudé in 2010, predicted cumulative ET followed the observed value until mid-May, when it became overpredicted (Fig. 2b). Conversely, AqYield tended to underpredict cumulative ET for the other three situations. Overall, cumulative ET during the cropping period ranged from 264 to 376 mm for predictions and 282–403 mm for observations. The median difference between observed and predicted cumulative ET was 62 mm in absolute value (18% in relative value). The differences ranged from − 67 mm to + 63 mm among the four situations.

During calibration, AqYield predicted monthly ET well, with Ef = 0.84, rRMSE = 0.31 (corresponding to 12 mm) and MD = − 2.9 mm (Fig. 3). Predicted monthly ET ranged from 3 to 115 mm, while observed monthly ET ranged from 4 to 119 mm. The model predicted most situations well (median difference of 7.7 mm in absolute value, 20% in relative value).

During validation, AqYield predicted daily ET sufficiently well, with Ef = 0.49, rRMSE = 0.57 (corresponding to 0.7 mm) and MD = 0.0 mm (data not shown). Cumulative ET during the cropping period ranged from 290 to 356 mm for predictions and 336–470 mm for observations (data not shown). The median difference between observed and predicted cumulative ET during the cropping period was 64 mm in absolute value (16% in relative value). During validation, the model predicted monthly ET nearly as well as it had during calibration, with Ef = 0.69, rRMSE = 0.41 (corresponding to 16 mm) and MD = − 0.6 mm (Fig. 3). The median difference between observed and predicted monthly ET was 6.6 mm in absolute value (19% in relative value).

3.1.3. Drainage for wheat

Observed cumulative drainage at Fagnières during the cropping period ranged from 0 to 287 mm, depending on the situation. During calibration, AqYield predicted cumulative drainage well, since it predicted no drainage for the two situations (out of six in dataset A) in which no drainage occurred during the cropping period (data not shown). For the four situations in which drainage occurred, the model accurately predicted the range of cumulative drainage, despite an overprediction in 1998 (Fig. 4).

The median difference between observed and predicted cumulative drainage during the cropping period was 6 mm in absolute value (8% in relative value) for all situations and 18 mm in absolute value (16% in relative value) for the four situations in which drainage occurred. The differences ranged from − 11 mm to 61 mm. The dynamics of predicted and observed drainage differed greatly: predicted drainage occurred in one event, while observed drainage was more spread out over several days (Fig. 4).

During calibration, AqYield predicted monthly drainage relatively well, with a good Ef (0.63) and a small bias (MD = 1.0 mm), but the model accuracy was poor (rRMSE = 1.4; corresponding to 10 mm) (Fig. 5). Of the 60 months of data, only 28 recorded monthly drainage > 1 mm, indicating that the other 32 had no drainage. Monthly drainage ranged from 0 to 86 mm for predictions and 0–85 mm for observations. When situations with no observed drainage were excluded, the median difference between observed and predicted monthly drainage was 2.4 mm in absolute value (15% in relative value). For all situations, including those with no drainage, the difference was 0.8 mm in absolute value (9% in relative value).

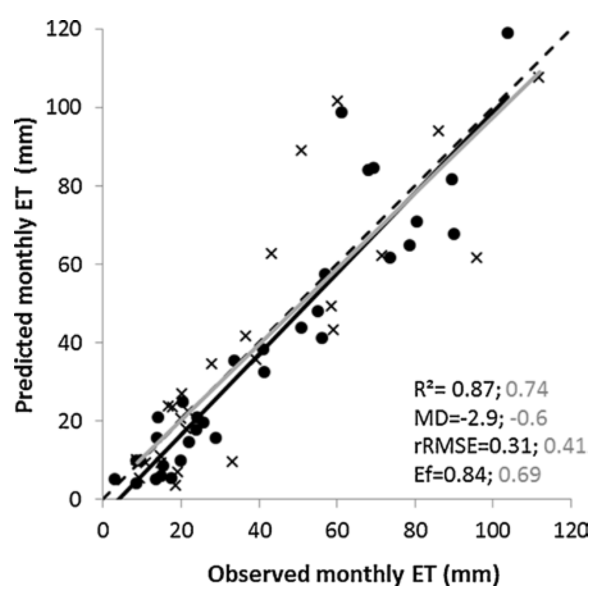

Fig. 3. Observed vs. predicted monthly evapotranspiration (ET) for wheat at Lamasquère and Auradé for model calibration and validation. For calibration, the data are black points, the regression line is the black solid line and statistical criteria are in black. For validation, the data are crosses, the adjustment line is gray and statistical criteria are gray. The 1:1 line is black and dashed. The data came from dataset A (Table 1). “MD” is the mean deviation, “rRMSE” is the relative root mean square error and “Ef” is the model efficiency.

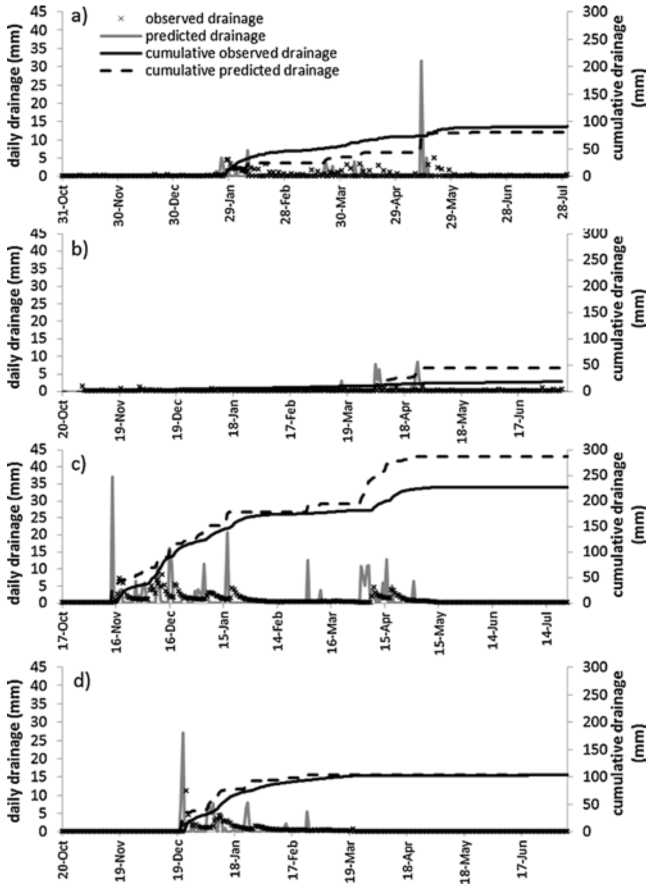

Fig. 4. Observed and predicted daily drainage and cumulative drainage during the cropping period of wheat after model calibration for four situations at the Fagnières site: a) 1985, b) 1989, c) 1998 and d) 2011. The data came from dataset A (Table 1).

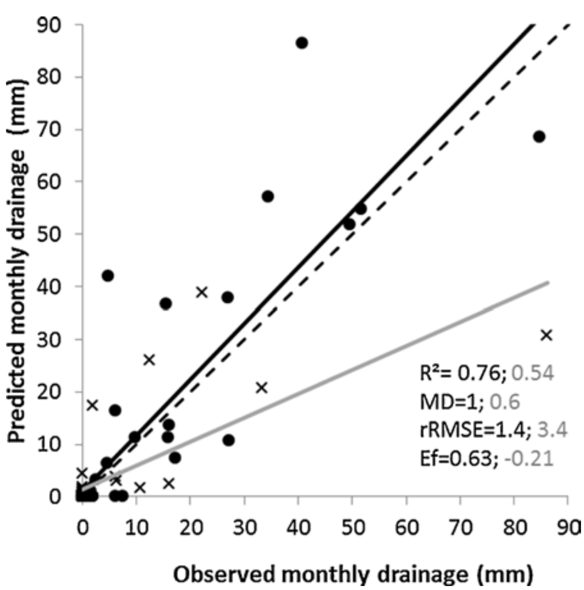

Fig. 5. Observed vs. predicted monthly drainage for wheat for model calibration and validation. For calibration, the data are black points, the adjustment line is the black solid line and statistical criteria are in black. For validation, the data are crosses, the adjustment line is gray and statistical criteria are gray. The 1:1 line is black and dashed. "MD" is the mean deviation, "rRMSE" is the relative root mean square error and "Ef" is the model efficiency.

In the validation dataset for Fagnières, cumulative drainage during the cropping period ranged from 0 to 121 mm for predictions and 0–88 mm for observations. Among the six situations at Fagnières, only two cropping periods with drainage were recorded, which had a median difference between observations and predictions of 20.5 mm in absolute value (26% in relative value) and differences ranging from −13 to 54 mm (data not shown). During validation, AqYield did not predict monthly drainage at Fagnières as well, with Ef = −0.21, rRMSE = 3.4 (corresponding to 9 mm) and MD = 0.6 (Fig. 5). The median difference between observed and predicted monthly drainage was 0.1 mm in absolute value (4% in relative value) for all six situations, increasing to 14.6 mm (62% in relative value) when excluding situations with no observed drainage.

3.2. Predicted evapotranspiration for two crop rotations

Overall, AqYield predicted daily ET during crop rotations relatively well for fallow and cropping periods at the two sites (Lamasquère and Auradé) (Fig. 6). However the model predictions were less accurate in the end of cropping period when ET was high. At Auradé, ET was overpredicted for wheat in 2010 and underpredicted for wheat in 2008 and for rapeseed in 2009. At Lamasquère, ET was underpredicted for maize in 2010 and slightly in 2012. Nevertheless, ET was predicted well for most other crops, such as rapeseed in 2011, sunflower in 2007 and wheat in 2006, 2012 at Auradé (Fig. 6a) and maize in 2006 and 2008 at Lasmaquère (Fig. 6c). Over the 7-year crop rotation at Auradé, AqYield predicted daily ET relatively well, with Ef = 0.63, rRMSE = 0.51 (corresponding to 0.7 mm) and MD = −0.2 mm. For Lamasquère, it predicted daily ET less well, with Ef = 0.48, rRMSE = 0.68 (corresponding to 0.9 mm) and MD = −0.2 mm.

For cumulative ET (from sowing of a given crop until sowing of the subsequent crop), predictions and observations ranged from 293 to 652 mm and 333–700 mm at Lamasquère, respectively, and from 351 to 602 mm and 348–652 mm at Auradé, respectively. AqYield underpredicted cumulative ET for all crops at Lamasquère by 44 mm (median difference), ranging from −125 to −20 mm, depending on the crop (Fig. 6d). It also tended to underpredict cumulative ET at Auradé, except for wheat in 2010, for which it was overpredicted (Fig. 6b). The median difference between observed and predicted cumulative ET at Auradé was 70 mm in absolute value (14% in relative value), ranging from -164 to + 70 mm, depending on the crop and fallow period.

At the crop-rotation scale, AqYield predicted monthly ET well over seven years (excluding wheat calibration periods) for both sites together (Ef = 0.72, rRMSE = 0.36 (corresponding to 16 mm) and MD = −7.0 mm) (Fig. 7) and separately (Ef = 0.76 and 0.69, rRMSE = 0.38 and 0.40, and MD = −7.0 and −7.0 mm for Auradé and Lamasquère, respectively). The model predicted the ranges of monthly ET (9–133 mm for Auradé and 10–132 mm for Lamasquère) well, with a median difference between observed and predicted values of 8.8 mm in absolute value (19% in relative value). Generally, the model tended to underpredict monthly ET slightly, especially low values.

4. Discussion

4.1. AqYield's ability to predict dynamics of winter wheat water flux components

With only few input data and simple equations, AqYield accurately predicted the amount of AW in the soil during wheat cropping periods in a variety of contrasting situations (soil, climate and management practices). It slightly overpredicted AW in certain situations, especially those with low AW, which might have been due in part to uncertainty in observed AW. Observed AW was calculated as the amount of water available for the crop, subtracting water content at wilting point from soil water content measurements. Determining the wilting point and its uncertainty for each experimental field can thus influence the observed

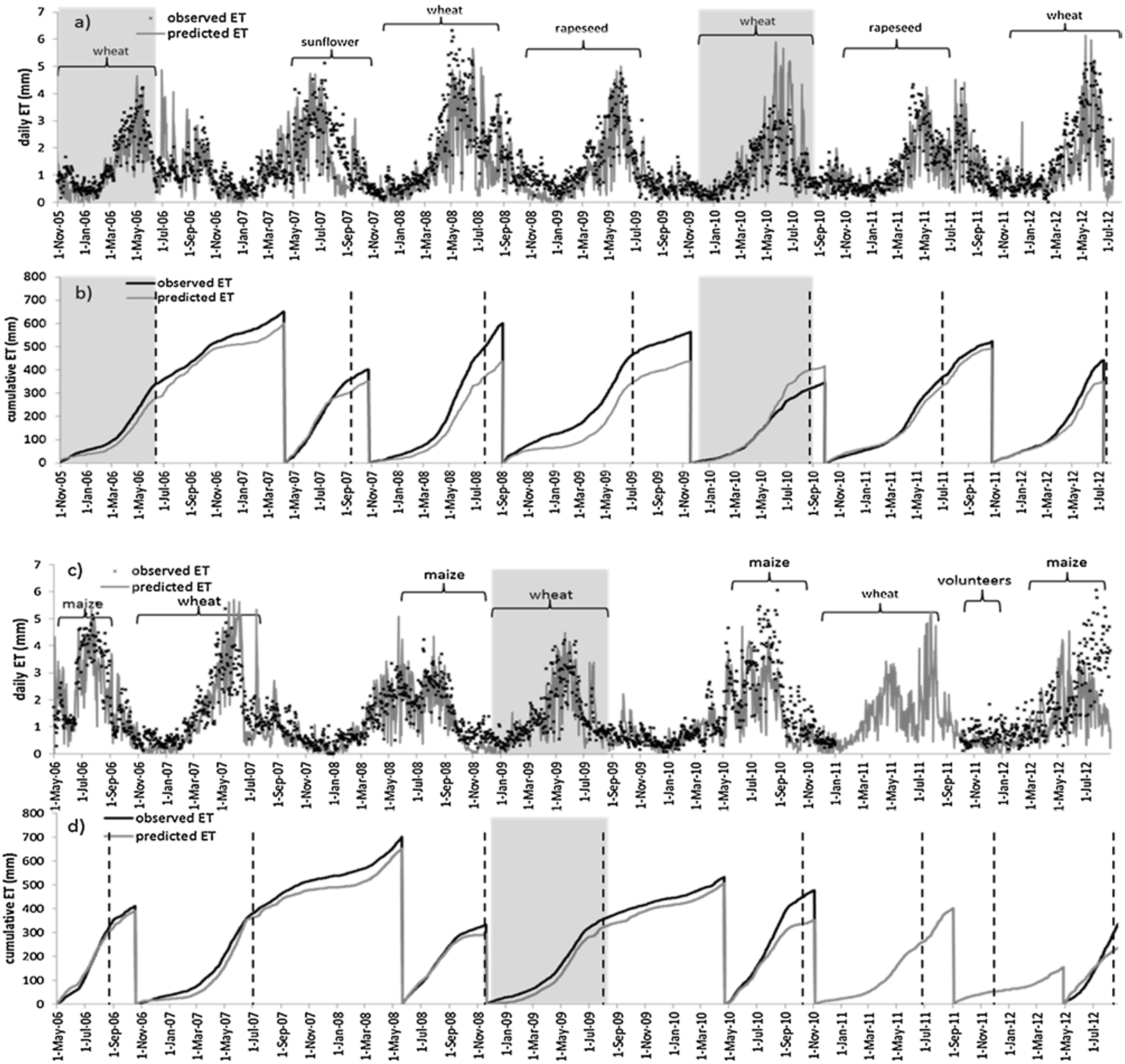

Fig. 6. (a, c) Daily and (b,d) cumulative observed and predicted evapotranspiration (ET) during fallow and cropping periods for two crop rotations at the (a, b) Auradé and (c, d) Lamasquère sites from 2006-2012. Vertical dashed lines represent harvest dates. Input data used for this analysis came from dataset B (Table 2). Gray areas represent wheat crops used for model calibration (dataset A).

AW used in the model. The accuracy of AqYield's soil water predictions was similar to those of other widely published crop models, despite the little information required for inputs and the simple equations used. The STICS model, which is frequently used in agronomic research (e.g. Beaudoin et al., 2008; Justes et al., 2009; Jégo et al., 2010; Tribouillois et al., 2016; Yin et al., 2017), predicted soil water variables (soil water humidity in % and amount in mm) for wheat with the same range of model efficiency: 0.70–0.90 for STICS vs. 0.83 for AqYield (Coucheney et al., 2015). This comparison is also consistent with results of Constantin et al. (2015), who compared STICS and AqYield predictions for spring crops (sunflower, maize and sorghum) and found similar model efficiencies in predicting soil AW content (0.53 for STICS vs. 0.57 for AqYield). Moreover, AqYield seemed to predict AW slightly better for winter crops than for spring crops. Another example is the widely used FAO AquaCrop model, which predicted soil water content for wheat with a MD similar to that of AqYield, albeit slightly overpredicting low water contents (Mkhabela and Bullock, 2012). AqYield predicted soil water content with the same range of variability as FAO AquaCrop (RMSE = 31 and 49 mm, respectively; mean difference between observations and predictions = 16 and 10 mm, respectively).

We focused model evaluation on water fluxes (ET and drainage) because they are processes that directly impact soil water content. For wheat, AqYield predicted ET accurately from the calibration and validation datasets. However, the difference between observations and predictions increased when observed ET increased, which usually corresponded to the end of a cropping period. This could be due to AqYield's difficulty in representing processes that occur during plant senescence and their influence on soil evaporation (Dunin et al., 1989). AqYield predicted daily drainage less accurately, overpredicting it immediately after rainfall events, because the model drains all excess water within one day, while observed rainfall events drained over several days. Notably, AqYield does not consider the saturated hydraulic conductivity of soil, a property that can decreases the rate of vertical water flux. For cumulative drainage during the cropping period, however, AqYield accurately distinguished situations with and without drainage during wheat development. It accurately predicted

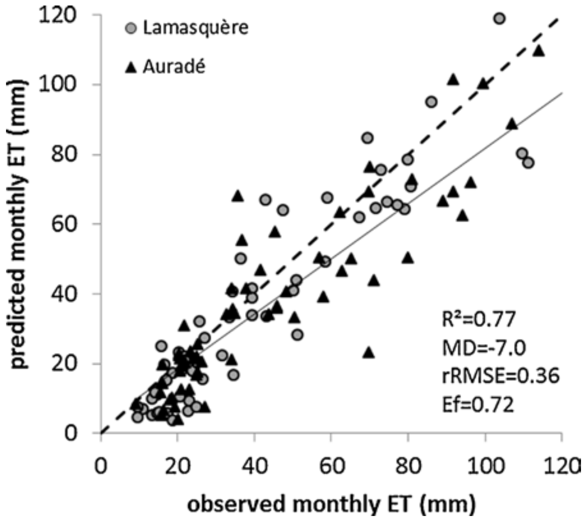

Fig. 7. Observations vs. predictions of monthly evapotranspiration (ET) for two crop rotations at Auradé and Lamasquère for model validation. Input data came from dataset B (Table 2). "MD" is the mean deviation, "rRMSE" is the relative root mean square error and "Ef" is the model efficiency.

the total amount of drainage during the cropping period, which is a concern for water management and cropping system issues at this temporal scale. When simulating at the annual or cropping period scale, accurate AW is required to initialize the simulation in order to predict drainage accurately, especially the beginning of the drainage period. Initial AW thus requires careful measurement or estimation from multi-year simulations, even though AqYield can predict other variables accurately without knowing the initial AW, as shown by Constantin et al. (2015). However, at the crop-rotation scale, when several years are simulated (without initialization each year), knowing the observed AW is less necessary because AqYield predicts it accurately.

4.2. Model efficiency in predicting evapotranspiration at the crop-rotation scale

Model evaluations of ET at the crop-rotation scale are rare and are generally excluded in model comparison studies, especially due to insufficient data (Bassu et al., 2014; Kollas et al., 2015; Rötter et al., 2012; Salo et al., 2016; Yin et al., 2017). In our study, AqYield simulated a 7-year crop rotation at two sites, predicting daily, monthly and cropping-period ET well. It adequately reproduced intra- and inter-annual variability in ET, and accurately predicted low and high ET for a variety of crops and contrasting climatic years. Despite its simple equations and empirical processes, AqYield accurately predicted water fluxes such as ET at a fine time scale. Contrasting ET values in winter or fallow periods (low ET) and in summer or at the end of cropping periods (high ET) were always predicted well. Howevern ET at the end of cropping periods was slightly underpredicted.

AqYield did not accurately simulate dynamics of the "barrier effect" after flowering, due to soil covering or mulching, which can impact soil evaporation (Ding et al., 2013; Dunin et al., 1989). In AqYield, soil evaporation after flowering is reduced according to the same coefficient as that at flowering (maximum barrier effect due to maximum soil cover), thus assuming that the maximum barrier effect is maintained. In reality, we assume that this effect may decrease (higher soil evaporation) for some species. Senescence can decrease soil cover (if leaves do not fall to the ground) by shrinking vegetation and decreasing the amount of radiation it intercepts, thus increasing soil evaporation. Including this process in AqYield could substantially improve its predictions, even though they are currently satisfactory.

Daily ET predictions at Auradé were as accurate or more accurate for certain years than those of the spatially distributed TNT2 model, which was evaluated using the same dataset from 2006 to 2010 (Ferrant et al., 2014). For example, AqYield overpredicted ET within the same range as TNT2 for the wheat in 2010 and both models underpredicted daily ET in the late sunflower cropping period in July 2007. The agreement between the two models indicates that a limiting factor exists that was not represented by either model. Another source of discrepancy between observations and predictions is the measurement of ET itself. Béziat (2009) showed that the uncertainty in ET measurements increases with ET intensity when using eddy covariance. It is difficult to obtain accurate daily ET, due to the use of heavy instruments that are subject to failure or calibration drift, the complexity of calculating flux from data measured in the field that rely on turbulence assumptions, and data filtering and processing, including filling data gaps using statistical models that are also subject to uncertainties. AqYield also does not consider water transfer within soil macropores, which can influence AW and thus ET. At Lamasquère, soil anoxia was sometimes observed due to an increase in groundwater level induced by heavy rainfall; AqYield does not consider groundwater rise, which may explain some differences between predictions and observations of daily ET.

AqYield predicts the two fluxes that constitute ET: soil evaporation and crop transpiration. We did not know, however, their relative contributions to observed ET, which restricted analysis and accurate calibration of ET predictions; in addition, runoff was not simulated. Despite these limitations, AqYield predictions were sufficiently accurate to predict ET during crop rotations.

4.3. Validity range of AqYield

Model calibration of wheat predictions was based on datasets from several experimental sites across France. For most of these sites, several years were used, which represent contrasting soil and climate conditions. The validity range for wheat predictions is thus temperate climates with a large gradient of dryness, especially in summer, and without strong nutrient limitations or pest impacts. Predictions of daily ET in cropping systems were validated only for southwestern France, which has a temperate climate with dry summers. Global radiation, which varies by location, is not included in AqYield because the model does not represent biomass. Low global radiation decreases crop growth, which consequently influences water balance and fluxes. Adding global radiation as input data for AqYield, however, would increase the complexity of this simple model. AqYield was developed to predict only at the species level and not at the cultivar level. It was calibrated using several cultivars as a "mean species" to increase its genericity. More generally, the fact that water stress is the only limiting factor in AqYield could limit its utility for studying agroecological practices such as low-input cropping systems. Despite its limitations and simple and empirical equations, AqYield remains reliable for predicting water fluxes and balances in a variety of situations.

4.4. Applications for cropping system evaluation

Our results indicate that AqYield adequately predicts water balance during crop rotations with the same accuracy as other published crop models that are more complex and require larger amounts of input data. A simple and accurate crop model such as AqYield, which requires only a few input data, seems useful as a module in more complex modeling approaches at the watershed level. For example, it can be implemented in the modeling platform MAELIA (Gaudou et al., 2014; Martin and Isaac, 2015; Mazzega et al., 2014; Therond et al., 2014). AqYield has been calibrated and evaluated as sufficiently accurate for wheat (main winter crop) and spring crops (Constantin et al., 2015). Its ability to predict ET in crop rotations including rapeseed was also satisfactory, although it requires more complete evaluation for this crop. Thus, AqYield is useful for simulating several agroecological practices in a variety of cropping system scenarios and their impacts on water balance, as well as management practices under actual and future climates at the watershed level.

5. Conclusion

In the present study, the AqYield crop model was calibrated for winter wheat, and its predictions of ET were evaluated by comparing them to ET measured during 7-year crop rotations at each of two sites. Although the model is simple and requires only a few input data, it was as accurate as other more complicated crop models widely used and evaluated in the agronomic literature, such as STICS or AquaCrop. AqYield, whether alone or in more complex modeling approaches such as an agro-hydrological modeling platform, could be used to predict water fluxes during crop rotations at field and watershed levels to support innovative cropping systems or to design water management strategies.

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Appendix A. Equations for water balance components

Soil evaporation

Evaporation is calculated using an empirical equation based on potential evapotranspiration (PET), a crop coefficient (K_c) and Available Water Content of the shallow soil compartment (SurfAWC). With a minimum value of 0, it is calculated as follows:

$$EVA_{(d)} = PET_{(d)} \times \left(1 - \frac{Kc_{(d-1)}}{Kcoff}\right) \times \left(\frac{SurfAWC_{(d-1)}}{SurfAWC_{max_{(d-1)}}} \times CoefCC + 1 - CoefCC\right)^{\alpha}$$

where *Kcoff* is the value of Kc at which evaporation stops (default value = 1.2), and *CoefCC* is an empirical coefficient that represents evaporation capacity of the soil (default value = 0.6). Initially a value of 3.0, the coefficient α was optimized to 2.0. This coefficient was optimized for all simulations of wheat but also of spring crops (database coming from Constantin et al., 2015) in order to be generic. It is not site- or species-dependent. After flowering, $Kc_{(d-1)}$ remains at the maximum value (that of Kc at flowering) until harvest.

Crop transpiration

Daily maximum transpiration (TR_{max}) is calculated as:

$$TR_{max_{(d)}} = (PET_{(d)} - EVA_{(d)}) \times Kc_{(d)}$$

Actual transpiration is an empirical function of TR_{max}, available water for roots, soil clay content (%) and vegetation scale (Vscale, calculation presented in Material and Method section):

$$TR_{(d)} = TR_{max_{(d)}} \times \left(1 - \left(1 - \frac{RootAWC_{(d)} - SurfAWC_{(d)}}{RootAWC_{max_{(d)}} - SurfAWC_{max\,(d)}}\right)\right)^{\left(\frac{120}{[Clay]+15}\right)^{\wedge Vscale}}$$

Drainage

Drainage is calculated as the excess amount of water above the maximum available water content ($TotAWC_{max}$) after considering all other water flows.

$$If\ TotAWC_{(d)} + R_{(d)} + Irr_{(d)} - Eva_{(d)} - TR_{(d)} - TotAWC_{max_{(d)}} > 0,\ Drain_{(d)} = TotAWC_{(d)} + R_{(d)} + Irr_{(d)} - Eva_{(d)} - TR_{(d)} - TotAWC_{max}$$

Irr	Daily irrigation
PET	Daily potential evapotranspiration
R	Daily rainfall
Drain	Daily amount of water loss by drainage
EVA	Daily amount of evaporation from the soil
Kc	Crop coefficient, index of foliar expansion (unitless)
RootAWC	Available Water Content in the layer explored by roots on a given day
$RootAWC_{max}$	Maximum Available Water Content in the layer explored by roots on a given day
SurfAWC	Available Water Content in the shallow layer on a given day
$SurfAWC_{max}$	Maximum Available Water Content in the shallow layer

TotAWC	Available Water Content in the soil on a given day
TR	Daily actual crop transpiration
TR_{max}	Daily maximum crop transpiration

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