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Estimating the water use efficiency of spring barley using crop models

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Abstract

In the current study, simulations by five crop models (WOFOST, CERES-Barley, HERMES, DAISY and AQUACROP) were compared for 7–12 growing seasons of spring barley (*Hordeum vulgare*) at three sites in the Czech Republic. The aims were to compare how various process-based crop models with different calculation approaches simulate different values of transpiration (Ta) and evapotranspiration (ET) based on the same input data and compare the outputs of these simulations with reference data. From the outputs of each model, the water use efficiency (WUE) from Ta (WUE_{Ta}) and from actual ET (WUE_{ETa}) was calculated for grain yields and above-ground biomass yield. The results of the first part of the study show that the model with the Penman approach for calculating ET simulates lower actual ET (ET_a) sums, at an average of 250 mm during the growing season, than other models, which use the Penman–Monteith approach and simulate 330 mm on average during the growing season. In the second part of the current study, WUE reference values in the range 1.9–2.4 kg/m^3 were calculated for spring barley and grain yield. Values of WUE_{Ta}/WUE_{ETa} calculated from the outputs of individual models for grain yields and above-ground biomass yields ranged from 2.0/1.0 to 5.9/3.8 kg/m^3 with an average value of 3.2/2.0 kg/m^3 and from 3.9/2.1 to 10.5/6.8 kg/m^3 with an average value of 6.5/4.0 kg/m^3, respectively. The results confirm that the average values of all models are nearest to actual values.

Introduction

Climate change impacts on agriculture and their implications for crop production are increasingly becoming the main themes of many case studies. These studies often emphasize that water may become one of the principal limiting factors for crop production in many areas (Blum 2005; Trnka *et al.* 2007, 2014; Hlavinka *et al.* 2009; Kang *et al.* 2009; Asseng *et al.* 2013; Ashofteh *et al.* 2014; Iglesias & Garrote 2015; Cammarano *et al.* 2016; Carlton *et al.* 2016; Gohar & Cashman 2016; Mall *et al.* 2016; Gosain 2017). Crop productivity is commonly determined by the availability of water (Hsiao & Acevedo 1974; Steduto 1996; Cossani *et al.* 2012). Water availability is limited and cannot be indefinitely supplied by irrigation in all locations (Hartmann 1981; Steduto *et al.* 1986; Howell 2001; Nawarathna *et al.* 2001). Therefore, it is crucial to focus on the consumption of water by plants for areas with insufficient reserves. Water use efficiency (WUE) may be one of the key issues for agriculture: it is the ability of a crop to produce biomass per unit of water transpired and is often considered an important determinant of yield. In a purely hydrological context, WUE has been defined as the ratio of the volume of water used productively (Stanhill 1986; Siddique *et al.* 1990; Stewart & Steiner 1990). Water use efficiency can be calculated as the ratio of biomass or grain yield to water supply, evapotranspiration (ET) or transpiration (Ta) on a daily or seasonal basis (Sinclair *et al.* 1984). Actual crop yield and actual ET (ET_a) depend on physiological processes (e.g. the stomata need to open for carbon inhalation and vapour exhalation). For an individual crop and climate, there is a well-established linear relationship between plant biomass produced and Ta (Steduto *et al.* 2007; Drechsel *et al.* 2015). Different types of crops are more water-efficient in terms of the ratio between biomass and Ta: C3 crops, such as wheat and barley, are less water-efficient than C4 crops, such as maize and sorghum. These differences are explained by the relationship between photosynthesis and stomatal conductance realized on the leaf level, which is specific for each species (Huang *et al.* 2006; Katerji *et al.* 2008; Drechsel *et al.* 2015). Wheat and barley usually have an average WUE value of approximately 1.5 kg/m^3, while maize and sorghum have an average WUE value of approximately 2.0 kg/m^3 (Katerji *et al.* 2008; Cossani *et al.* 2012; Drechsel *et al.* 2015; Fritsch & Wylie 2015; Greaves & Wang 2016). A knowledge of WUE is also necessary for evaluating individual crops and their demands for water. The WUE values of species whose market values are related to fresh weight (tomatoes, potatoes) are higher than those observed for species with a dry yield weight such as grain crops (Katerji *et al.* 2008).

Experimentally determined water consumption is difficult to obtain for a large number of locations, therefore, crop models have been used for this purpose. Among the outputs of crop models are data regarding Ta, ET and grain yield or above-ground biomass (Palosuo *et al.* 2011; Rötter *et al.* 2012), all of which are used to calculate WUE. The current study compares five crop models: WOFOST, CERES-Barley, HERMES, DAISY and AQUACROP. The selected crop models differ from each other in complexity, algorithms and approaches regarding the major processes determining crop growth and development (Eitzinger *et al.* 2002; Palosuo *et al.* 2011; Rötter *et al.* 2012). The differences between the parameterizations and configurations of each model lead to different results.

The primary aim was to compare the WUE values calculated using different process-based crop models. Another purpose was to examine the consistency of estimates based on individual models, with the hypothesis that the ensemble arithmetic mean (EAM) or the total ensemble (TE, range of all model values) is superior to individual models. Another aim was to quantify ranges in WUE values calculated using actual Ta/ET and grain and biomass yields.

Material and methods

Study locations and input data for crop models

The selected crop models were applied to three different soil-climate locations in the Czech Republic: Lednice (48°48′51″N, 16°48′46″E, altitude 171 m a.s.l.), Věrovany (49°27′39″N, 17°17′42″E, altitude 210 m a.s.l.) and Domanínek (49°31′42″N, 16°14′13″E, altitude 560 m a.s.l.) (Fig. 1). The simulated crop was spring barley, as it is widely grown in the Czech Republic.

The Czech Republic comprises various soil types and climatic conditions. The selected locations represent three basic regimes. Lednice is a warm and relatively dry spring barley growing region. Věrovany is located in the most fertile area of the country, with warm temperatures and generally sufficient rainfall conditions, and Domanínek represents the coolest and wettest of all three sites. The main characteristics of each location are summarized in Table 1.

The first step included the calibration and subsequent validation of a crop model ensemble. Within the calibration, parameters for length of the vegetative and reproductive development stages were modified manually using sensitivity analysis. Calibration and validation were performed using experimental data from the Central Institute for Supervising and Testing in Agriculture (SIAST) multi-year field experiments in the selected locations. These data were combined with data from a 4-year field experiment for the spring barley variety ‘*Tolar*’ in 2011 and 2012 and a variety with the same properties, ‘*Bojos*’, in 2013 and 2014 in Domanínek (Table 2). The lengths of the growing season and the flowering stage (growth stage [GS] 61, Zadoks *et al.* 1974), time to maturity (GS 90) and grain yields were recorded for all years and all study locations. Above-ground biomass yields were not available (Fig. 2).

Measurements

In the second step, the ET (Figs 3 and 4), Ta (Figs 3 and 4) and soil water balance (SWB) (Figs 5 and 6) were compared based on model outputs. Simulated values of ET_a, reference ET (ET_o) and SWB were compared with measured values (ET_a, ET_o, SWB) for Domanínek from 2011 to 2014 (Figs 4 and 5). The data, which were used as reference data for ET (ET_a, ET_o), were measured from data by two meteorological stations permanently located on turfgrass at Domanínek (49°31′28″N, 16°14′30″E and 540 m asl; 49°31′18″N, 16°14′10″E and 575 m asl). The actual evapotranspiration of the turfgrass was measured using the Bowen ratio energy balance method. Measurements and data processing have been extensively described in a previous study by Fischer *et al.* (2013). Temperature and humidity gradients were measured by combined EMS 33 instruments placed in AL 070/1 radiation shields (EMS

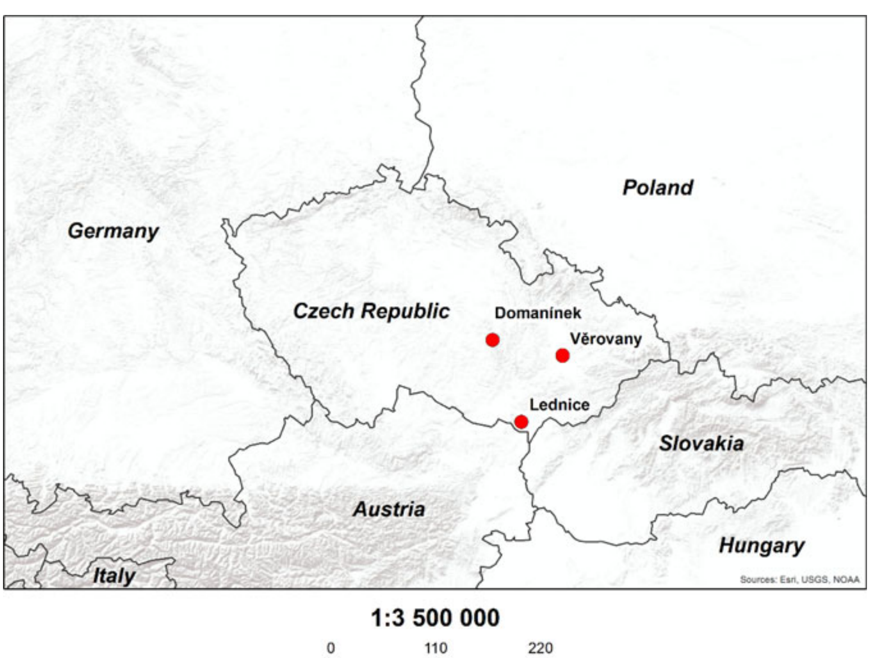

Fig. 1. Map of the Czech Republic indicating the study locations.

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Table 1. Basic characteristics of the study locations. The climate data are derived from the years 1971–2000 (Tomiška *et al.* 2003; Tolasz 2007; Hájková & Dahl 2012)

Location	Lednice		Věrovany		Domanínek	
Latitude (N)	48°48′		49°27′		49°31′	
Longitude (E)	16°47′		17°17′		16°14′	
Production area	Maize		Sugarbeet		Potato	
Altitude (m a.s.l.)	171		210		560	
Ø annual temperature (°C)	9.6		8.7		6.8	
Ø date of emergence of spring barley	18 April		18 April		28 April	
Ø date of full ripeness of spring barley	28 June		28 June		13 August	
Ø duration of Ø daily air temperature of 10 °C and more (number of days)	180		170		140	
Ø annual temperature during the growing season (°C)	16.4		16.0		14.5	
Ø annual precipitation (mm)	461		502		575	
Ø annual precipitation during the growing season (mm)	291		316		309	
Soil type	Chernozem		Chernozem		Cambisol	
Textural type	Loamy clay		Loamy		Loamy	
Soil depth (m)	1.50		1.50		1.50	
Ø maximum capillary capacity (%)	38.6		37		36.9	
Ø wilting point (m^3/m^3)	14		14.6		13.5	
Ø bulk density (g/m^3)	1.54		1.53		1.62	
	m	%	m	%	m	%
Clay	0–0.30	0.223	0–0.28	0.169	0–0.24	0.158
	0.30–0.82	0.251	0.28–0.64	0.219	0.24–0.66	0.263
	0.82–1.02	0.198	0.64–0.94	0.247	0.66–0.94	0.186
	1.02–1.50	0.151	0.94–1.22	0.184	0.94–1.30	0.133
			1.22–1.50	0.180	1.30–1.50	0.129
Silt	0–0.30	0.606	0–0.28	0.664	0–0.24	0.500
	0.30–0.82	0.575	0.28–0.64	0.637	0.24–0.66	0.461
	0.82–1.02	0.628	0.64–0.94	0.617	0.66–0.94	0.387
	1.02–1.50	0.645	0.94–1.22	0.658	0.94–1.30	0.196
			1.22–1.50	0.632	1.30–1.50	0.262
Sand	0–0.30	0.171	0–0.28	0.167	0–0.24	0.342
	0.30–0.82	0.174	0.28–0.64	0.144	0.24–0.66	0.276
	0.82–1.02	0.174	0.64–0.94	0.136	0.66–0.94	0.493
	1.02–1.50	0.204	0.94–1.22	0.158	0.94–1.30	0.382
			1.22–1.50	0.187	1.30–1.50	0.452

Brno, Czech Republic). The net radiation was measured by an NR 8110 net radiometer (Philipp Schenk GmbH Wien, Austria), and the soil heat flux was monitored by an HFP01 sensor (Hukseflux Thermal Sensors, Netherlands). Measurements were taken every minute and logged as half-hour averages. Raw data of latent heat flux were subjected to quality control filtering according to Guo *et al.* (2007). Gaps in the flux data were filled using the algorithm of Reichstein *et al.* (2005), as implemented in the R package REddyProc (http://r-forge.r-project.org/projects/reddyproc/). The soil water balance was measured using the time domain reflectometry (TDR) method, (CS 616, Campbell Scientific Inc., Shepshed, UK): TDR sensors were placed vertically to monitor the SWB from the surface to a depth of 0.3 m in field experiments with spring barley in Domanínek at the central time during the growing seasons from 2011 to 2014 (Fig. 5).

Crop models and methods for calculating evapotranspiration and soil water balance

The current paper describes various results from the selected models. The models and approaches for the calculations used in the current study are described as follows (Table 3).

Table 2. Overview of years and study locations from which simulation outputs of crop models were used

Year / Locality	1998	1999	2000	2001	2002	2003	2004	2005	2006	2007	2008	2009	2010	2011	2012	2013	2014
Lednice																	
Věrovany																	
Domanínek																	

Approaches for calculating evapotranspiration

Approaches to ET calculations (Table 3) vary from quite simple (empirical or semi-empirical) requiring only information on monthly average temperatures, to complex (more physical), requiring daily data on maximum and minimum temperature, solar radiation, humidity and wind speed, as well as characteristics of the vegetation (Eitzinger *et al.* 2002; Fischer 2012). The model computes daily net solar radiation. Evapotranspiration (combination of soil evaporation and plant Ta) can be limited by low solar radiation and cool temperatures (low leaf area index, low soil water content, low root length density and their distributions relative to each other) (detailed in Ritchie 1972).

WOFOST (WOrld FOod STudies), as one of the selected models, uses the Penman (P) approach (Penman 1956), adapted according to Frère & Popov (1979), to calculate ET. In WOFOST, the actual crop Ta is determined by the potential ET time correction factors for the degree of light interception, the degree of water stress and the crop in general (Wolf & De Wit 2003). Weather data must include wind and humidity data (Doorenbos & Pruitt 1977). The P approach is elucidated by the following equation:

$$ET = \frac{\Delta R_{n,a} + \gamma E_a}{\Delta + \gamma}$$

where ET is the evapotranspiration rate, $R_{(n,a)}$ is the net absorbed radiation (expressed in equivalent evaporation), Ea is the evaporative demand, Δ is the slope of the saturation vapour pressure curve and γ is a psychometric constant (Supit *et al.* 1994).

CERES-Barley calculates ET based on the Priestley–Taylor (PT) approach in the current study. The PT equation is useful for the calculation of daily ET in case when weather inputs for the aerodynamic term (relative humidity, wind speed) are unavailable. This radiation-based method approach requires only daily solar radiation and temperature (Ritchie 1972). The equation is given as:

$$\lambda ET = \alpha \frac{S}{S + \gamma} (R_n - G)$$

where ET is evapotranspiration, λ is the latent heat of vaporization, α is a model coefficient (which Priestley and Taylor allowed to vary for drying conditions), S is the slope of the saturation vapour density curve, γ is a psychrometric constant, R_n is the net radiation, and G is the soil heat flux (Priestly & Taylor 1972; Flint & Childs 1991; Ngongondo *et al.* 2013).

The approach of Penman–Monteith (PM) is used to calculate ET for the remainder of the selected models: HERMES, DAISY and AQUACROP. Unlike the original P model, in the PM model, the mass-transfer evaporation rate is calculated based on physical principles (Ponce 1989). The 'full-form' PM equation can be expressed as follows:

$$ET = \frac{\Delta (R_n - G) + \rho_a c_p \ (e_s - e_a)/r_a}{(\Delta + y\ (1 + (r_s/r_a)))\rho_w \lambda}$$

where ET is the evapotranspirative flux expressed as depth per unit time, Δ is the slope of the saturation vapour pressure *v.* temperature curve, R_n is the net radiation flux density at the surface, G is the sensible heat flux density from the surface to the soil (positive if the soil is warming), ρ_a is the air density, c_p is the specific heat of moist air at a constant pressure, e_s is the saturation vapour pressure at air temperature, e_a is the actual vapour pressure of the air, r_a is the

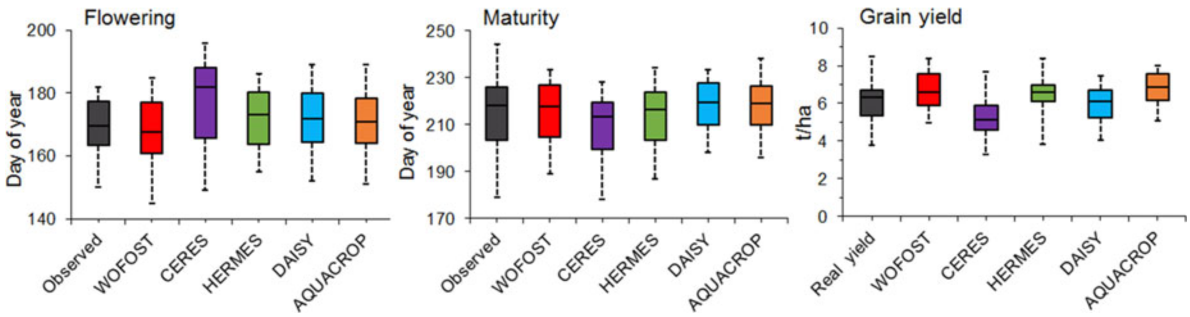

Fig. 2. A comparison of the observed and simulated onset of phenological phases and grain yields for the study locations and the years referenced in Table 1. Boxplots delimit the inter-quartile range (25–75 percentiles) and show the minimum value, maximum value and median.

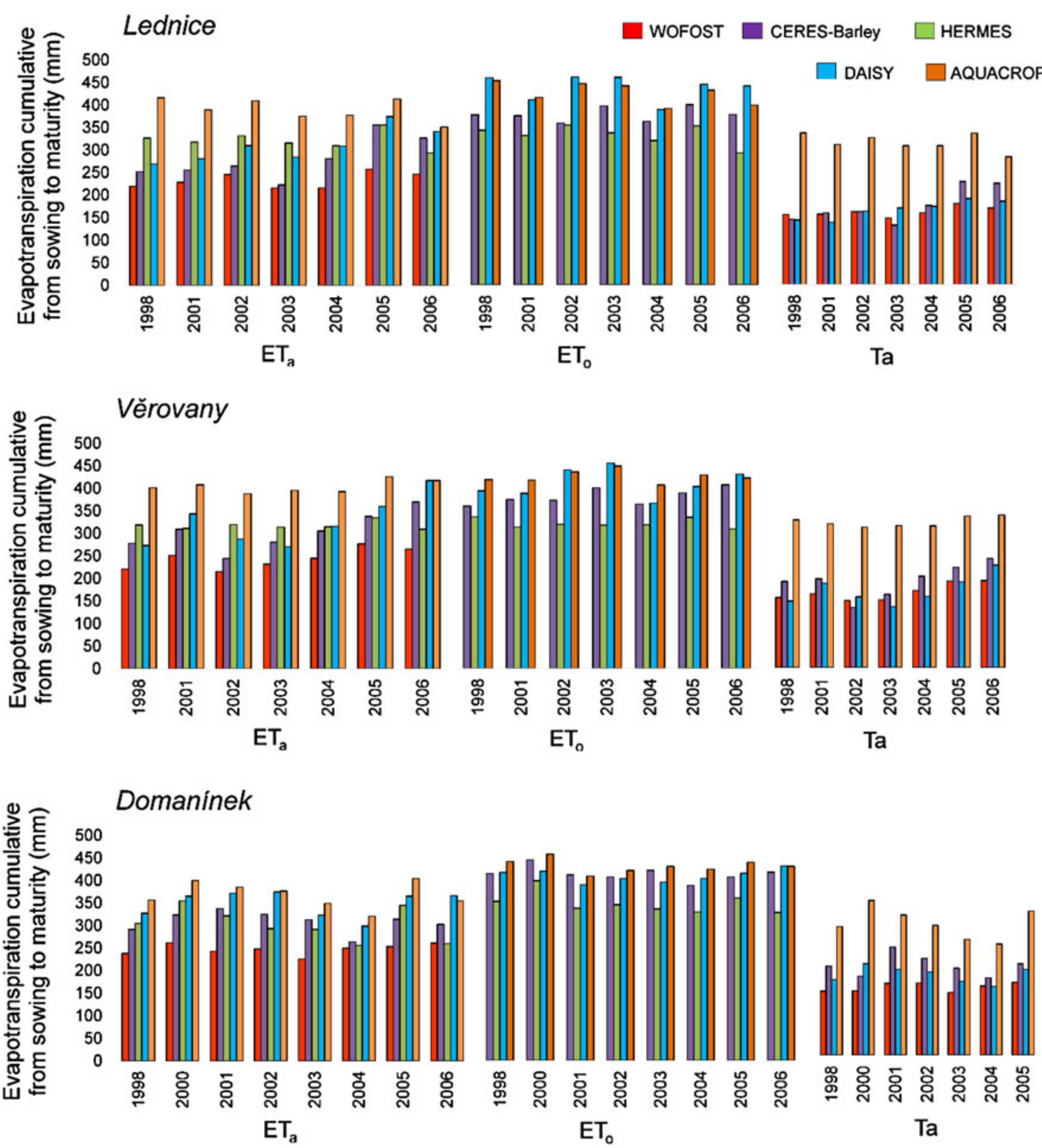

Fig. 3. Simulated components of evapotranspiration (ET_a = actual evapotranspiration, ET_o = reference evapotranspiration, Ta = actual transpiration) by five crop models, accumulated from sowing to maturity, at three locations during the years given in *X*-axis.

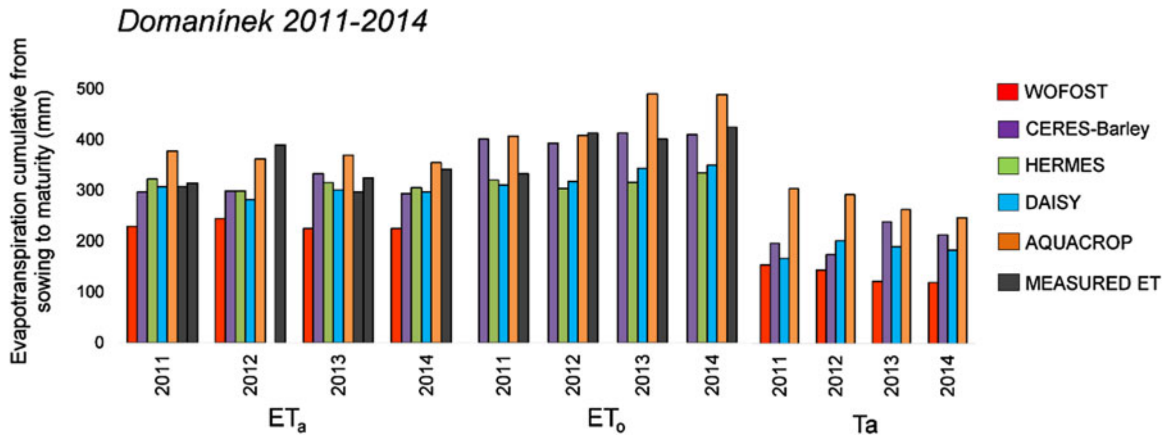

Fig. 4. Simulated and measured components of evapotranspiration (ET_a = actual evapotranspiration, ET_o = reference evapotranspiration, Ta = actual transpiration) for the study location Domanínek from 2011 to 2014. Measured ET_o was obtained from data of one meteorological station and measured ET_a from data of both stations. For 2012 and 2014, relevant seasonal data for both meteorological stations are not available. Therefore, measurement were performed for only one of the stations. The measured ET_a and ET_o values for the turfgrass were used as reference data.

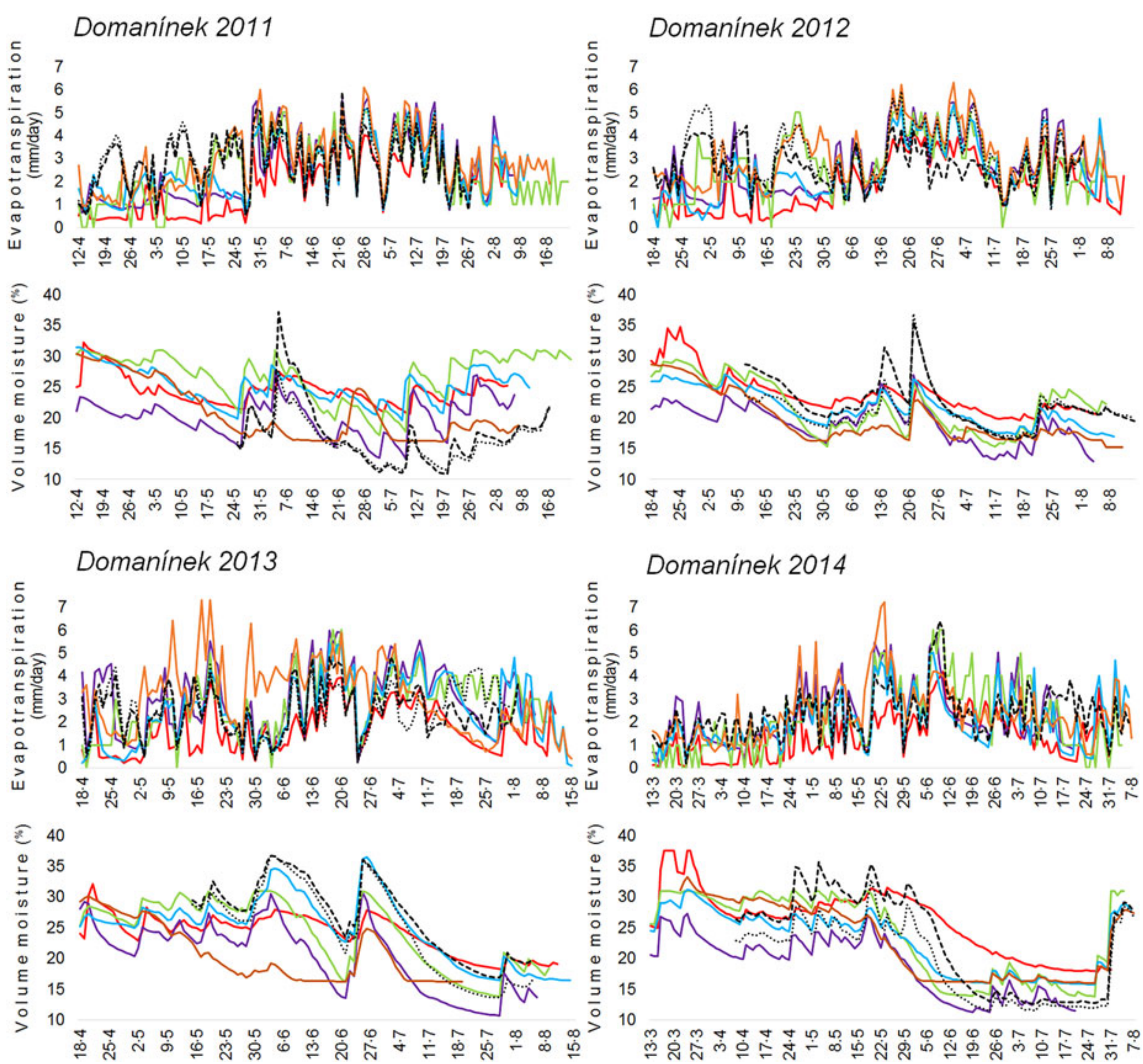

Fig. 5. Comparison between the simulated and measured actual evapotranspiration (ET_a) and soil water balance (SWB) for spring barley from soil layer 0–0.3 m between sowing and maturity at the study location Domanínek from 2011–2014. Values measured ET_a were obtained from data of two meteorological stations. For 2012 and 2014, relevant seasonal data for both meteorological stations are not available. Therefore, measurements were performed for only one of the stations.

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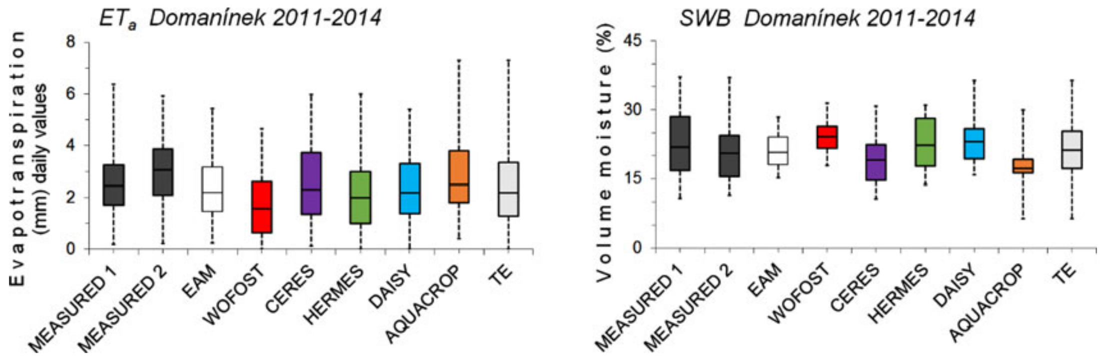

Fig. 6. Comparison between the simulated and measured actual evapotranspiration (ET$_a$) and soil water balance (SWB) for spring barley for the study location Domanínek from 2011 to 2014. Boxplots delimit the inter-quartile range (25–75 percentiles) and show the minimum value, maximum value and median. EAM is ensemble arithmetic mean, TE is total ensemble.

Table 3. Modelling approaches regarding the main processes determining crop growth and development

Model	Version	(a)	(b)	(c)	(d)	(e)	(f)
WOFOST	7.1.3	T, DL	PRT, B	P	C	D	P-R
CERES-Barley	4.6	T, DL	HI(Gn), B	PT	C	S	RUE
HERMES	2.01.1	T, DL	PRT	PM	C	D	P-R
DAISY	4.01	T, DL	PRT	PM	R	D	P-R
AQUACROP	4.0	T	HI	PM	C	S	TE

(a) Crop phenology as a function of: T = temperature, DL = photoperiod (daylength), (b) Yield formation depending on: B = above-ground biomass, Gn = number of grains, HI = harvest index, PRT = partitioning during reproductive stages, (c) Approaches for calculating evapotranspiration: P = Penman approach, PM = Penman–Monteith approach, PT = Priestley–Taylor approach, (d) Water dynamics approach: C = capacity approach, R = Richards approach, (e) Leaf area development and light interception: D = detailed approach (e.g. layers of canopy), S = simple approach (e.g. LAI), (f) Light utilization: RUE = radiation use efficiency approach, P-R = gross photosynthesis–respiration), TE = transpiration efficiency biomass growth.

aerodynamic resistance to turbulent heat or vapour transfer from the surface to some height z above the surface, y is a pyschrometric constant, r_s is the bulk surface resistance describing the resistance to flow of water vapour from inside the leaf, vegetation canopy or soil to outside the surface, ρ_w is the density of water, and λ is the latent heat of vaporization (Allen *et al.* 2006).

Depending on approaches for calculating ET, crop models require different meteorological data (Palosuo *et al.* 2011).

Approaches for calculating soil water balance

Soil water balance is one of the most important parts of the models. According to the models, the soil profile is divided into root zone layers with different water supplies. Each layer has an associated horizon, defining the unique physical properties of that layer (Abrahamsen & Hansen 2000). Accordingly, the incoming and outgoing water flows are simulated. WOFOST, CERES-Barley, HERMES and AQUACROP calculate the water balance using the capacity approach (Table 3). This works on the basis of estimated water consumption by ET$_a$, which depends on the course of the meteorological elements, soil moisture availability and characteristics of the vegetation cover or surface (Boogaard *et al.* 1998).

WOFOST has the simplest approach for calculating soil water balance among the selected models. The model considers three soil layers: the rooted zone between the soil surface and the actual rooting depth, the lower zone between the actual rooting depth and the maximum rooting depth, and the sub-soil below the maximum rooting depth. The available soil water contained in the rooted zone, which is directly at the disposal of the crop, is defined as the product of the rooting depth and the current available soil water content (van Diepen *et al.* 1988; Eitzinger *et al.* 2004). WOFOST does not consider the possible influence of groundwater or its potential capillary rise and treats the soil as a homogeneous layer (Supit *et al.* 1994; Eitzinger *et al.* 2004).

The most comprehensive approach among the selected models is that of DAISY, which calculates the water balance between the surface and the soil. DAISY determines the movement of water in soil using a numerical solution of Richards' equation (Abrahamsen & Hansen 2000; van Dam & Feddes 2000), which can simulate the water balance at the desired depth (Richards 1931). DAISY simulates the movement of water in the soil based on potential theory. The ability of a soil to supply water is determined by the simulated potential infiltration rate, which is based on conditions in the soil. Transpiration is determined by the water intake of roots, depending on the depth of rooting and root density.

More details about model construction and functioning can be found in the literature, e.g. Jones & Kiniry (1986); van Diepen *et al.* (1988); Kersebaum (1995); Ritchie *et al.* (1998); Tsuji *et al.* (1998) or Hsiao *et al.* (2009).

A comparative analysis was used to compare the simulations ET$_a$ and SWB for Domanínek 2011–2014. Simulation results of crop models were subjected to statistical analysis by means of descriptive statistical indices and statistical parameters such as maximum, minimum and mean value; standard deviation; coefficient of variation and variance; root mean square error (RMSE), which describes the average absolute deviation between the observed and modelled values; the mean bias error (MBE) as an indicator of the average systematic error (Davies & McKay

1989) and index of agreement (IA), developed by Willmott (1981), was used as a more general indicator of modelling efficiency (Table 4). MBE, RMSE and IA can be calculated as follows:

$$\mathrm{MBE} = \frac{\sum_{i=1}^{n}(S_i - O_i)}{n} \quad \mathrm{RMSE} = \sqrt{\frac{\sum_{i=1}^{n}(O_i - S_i)^2}{n}}$$

$$\mathrm{IA} = 1 - \frac{\sum_{i=1}^{n}(S_i - O_i)^2}{\sum_{i=1}^{n}(|\dot{S}| + |\dot{O}|)^2}$$

where S_i is the simulated value of the variable, O_i is the measured value of the variable, n is the number of pairs of observed and estimated values, $\bar{S}$ is the average simulated value of the variable, $\bar{O}$ is the average measured value of the variable and $\dot{S} = |S_i - (S_i - \bar{S})|$ and $\dot{O} = |O_i - (O_i - \overline{O})|$.

Calculation of water use efficiency

Water use efficiency can be defined and calculated in a variety of different ways (Blum 2009; Medrano *et al.* 2015; Cammarano *et al.* 2016). In the current work, calculation and comparison of WUE used simulated outputs of Ta, ET_a, dry matter of above-ground biomass and grain yield of spring barley. An equation for calculating WUE was determined as follows:

$$WUE\ (\mathrm{kgDM/m^3H_2O}) = \frac{Dry\ weight\ of\ yield\ (\mathrm{kg/ha})}{Crop\ water\ supply\ (\mathrm{m^3\ H_2O/ha}) = ETa\ or\ Ta}$$

Water use efficiency is represented in units of kg/m^3, where crop production is measured in kg/ha and water use is estimated as mm of water applied or received as rainfall, converted to m^3/ha (1 mm = 10 m^3/ha) (Drechsel *et al.* 2015).

The combination of two separate processes whereby water is lost from the soil surface by evaporation and from the crop by Ta is referred to as ET (Allen *et al.* 1998). In a purely hydrological context, WUE has been defined as the ratio of the volume of water used productively (Stanhill 1986). Above-ground biomass accumulation, and consequently grain yield, has been shown to be inextricably linked to Ta (Sinclair *et al.* 1984). Water use efficiency should therefore be calculated from Ta. However, evaporation is the main factor affecting the total amount of water consumed during the growing season. In the current study, WUE has been calculated using both Ta (WUE_{Ta}, Fig. 7) and ET_a (WUE_{ETa}, Fig. 8).

The percent deviation (D_i) between measured and simulated ET_a and calculated WUE_{ETa} was determined as follows (Table 5)

Table 4. Descriptive statistics calculated for the ET_a and SWB and results of models comparison with the measured values for Domanínek 2011–2014

	MEASUREMENT	WOFOST	CERES-Barley	HERMES	DAISY	AQUACROP	EAM
ET_a (mm)							
Min	0.18	0.00	0.13	0.00	0.00	0.70	0.32
Max	6.38	4.65	5.97	6.00	5.41	7.30	5.42
Av	2.74	1.66	2.60	2.55	2.38	2.94	2.42
Median	2.68	1.53	2.27	2.50	2.18	2.70	2.23
SD	1.18	1.25	1.46	1.43	1.28	1.38	1.16
Var.	1.39	1.26	2.14	2.04	1.63	1.90	1.34
CV	0.43	0.75	0.56	0.56	0.53	0.47	0.48
MBE		−1.11	−0.16	−0.26	−0.37	0.21	−0.33
RMSE		1.69	1.26	1.00	1.16	1.33	1.04
IA		0.62	0.78	0.84	0.78	0.71	0.81
SWB (%)							
Min	11.19	17.90	10.68	13.76	15.86	5.08	14.77
Max	36.71	31.50	30.77	31.00	36.44	30.01	31.08
Av	21.64	24.04	18.77	22.71	22.85	16.08	21.38
Median	21.30	24.20	19.00	22.23	23.04	17.20	21.19
SD	6.56	1.68	4.56	5.55	4.46	7.89	4.10
Var.	42.95	10.24	20.71	30.66	19.85	26.79	13.99
CV	0.30	0.07	0.24	0.24	0.20	0.49	0.19
MBE		2.39	−2.86	1.07	1.21	−5.56	−0.75
RMSE		5.34	5.54	5.49	4.69	8.28	5.18
IA		0.72	0.75	0.78	0.81	0.76	0.73

EAM, ensemble arithmetic mean; Min, minimum; Max, maximum; Av, mean value; SD, standard deviation; Var, variance; CV, coefficient of variation.

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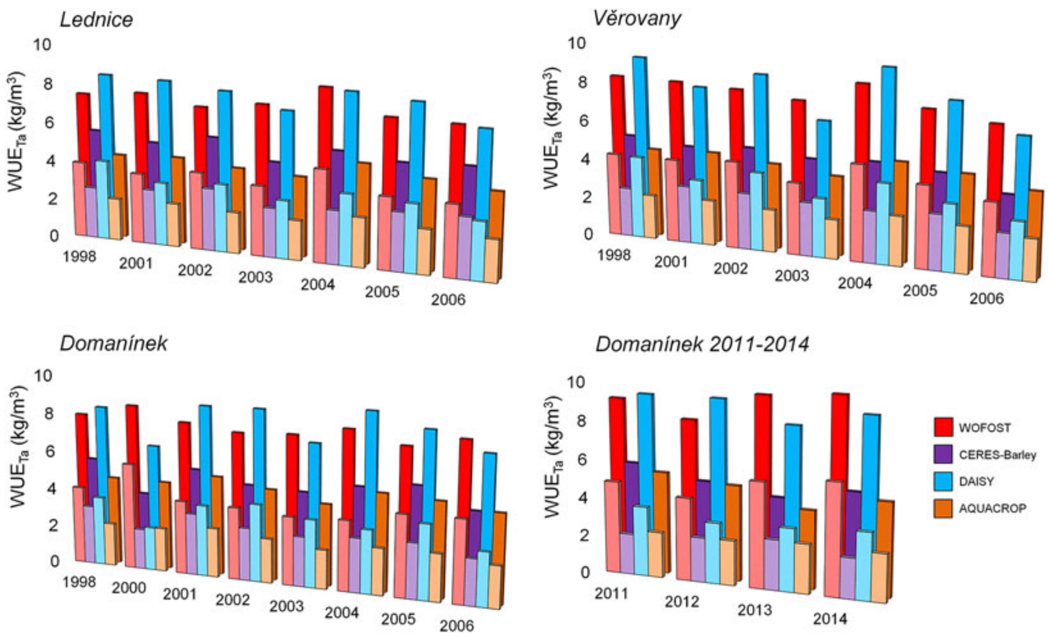

Fig. 7. Comparison of water use efficiency (WUE) values calculated from simulated transpiration (Ta) and grain yield (lower column) and above-ground biomass (higher column) with colours as given in list of models, by four crop models at three study locations for 1998 and 2001–2006 at Lednice and Věrovany and for 1998 and 2000–2006 at Domanínek, and additional at Domanínek during 2011–2014.

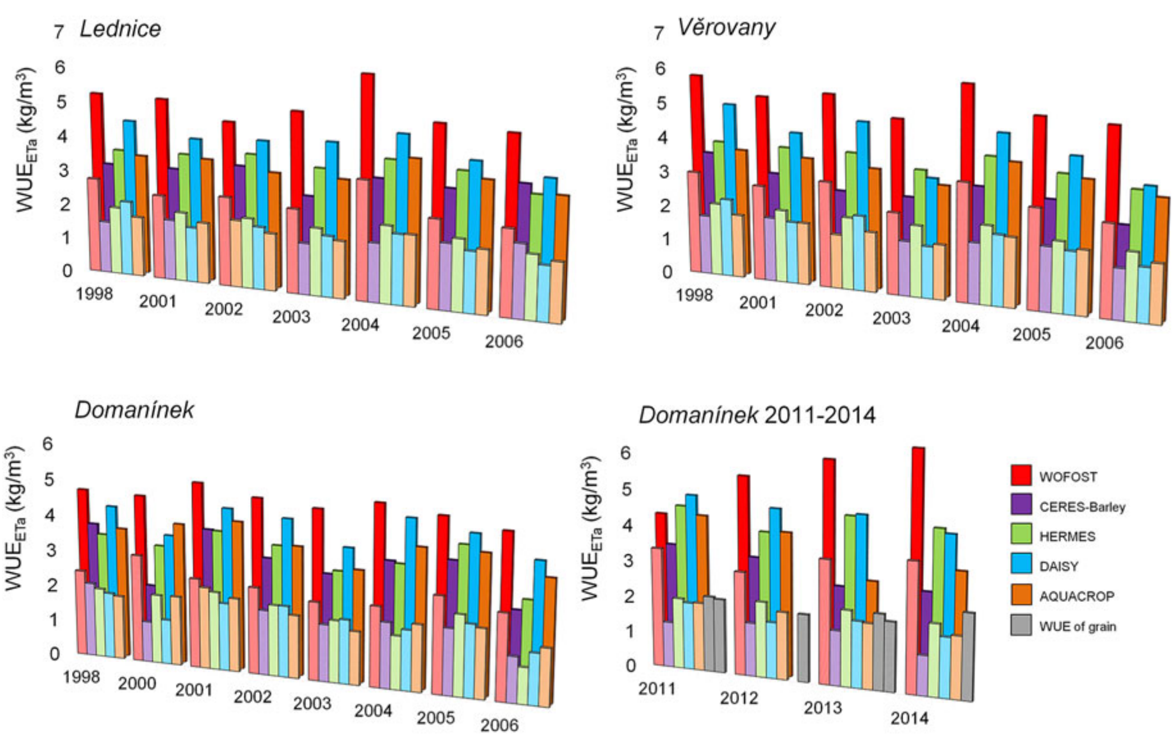

Fig. 8. Comparison of water use efficiency (WUE) values calculated from simulated and measured actual evapotranspiration (ET_a) and grain yield (lower column) and above-ground biomass yield (higher column) with colours as given in list of models, by five crop models at three study locations for 1998 and 2001–2006 at Lednice and Věrovany and for 1998 and 2000–2006 at Domanínek, and additional at Domanínek during 2011–2014. WUE of grain was calculated from the measured values. Graph 'Domanínek 2011–2014' show calculated results WUE_{Eta} from measured ET_a. Values measured ET_a were obtained from data of two meteorological stations. For 2012 and 2014, relevant seasonal data for both meteorological stations are not available. Therefore, measurements were performed for only one of the stations.

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(Bitri & Grazhdani 2015):

$$D_i = (simulated\ value - measured\ value) \times \frac{100}{measured\ value}$$

The arithmetic mean of the crop models simulations as EAM and the total range of crop models simulations as TE was shown by the use of boxplots (Figs 6, 9 and 10).

Results

Flowering, maturity and grain yield

The crop models were calibrated and validated based on approximations of the observed phenological phases (flowering and maturity) and grain yields, to produce simulated phenological phases and grain yields (Fig. 2).

The simulation results for spring barley with respect to the phenological phase of flowering (GS 61) in the Czech Republic showed a slight deviation from the observations, from −1 to +9 days. CERES-Barley simulated later flowering dates than the other models. Phenological phase maturity (GS 90) was less variable among the models, with differences of −7 to +5.5 days as compared with the observations. These results indicate that the simulated length of the growing season is different for each individual model. The simulation results for grain yield showed deviations from the real grain yield ranging from −1 to +1.28 t/ha. Detailed calibration and validation results can be found in the Supplementary Material.

Evapotranspiration and soil water balance

Evapotranspiration was calculated for all study years and study locations (Tables 1 and 2) by the different approaches incorporated within the selected crop models (Table 3). The obtained values of cumulative ET can be found in Figs 3 and 4.

In the current study, the sum of ET_a during the growing seasons ranged from 201.5 to 426.2 mm among the applied approaches, while ET_o ranged from 226.9 to 490 mm. The deviation of ET_a from ET_o is evident. The crop matures and the canopy cover declines during the growing season, therefore, the ET_a is lower. Crop models using the PM approach to calculate the sum of ET often produced higher values than models with a different approach. With the exception of AQUACROP (PM approach), which simulated the highest values, and WOFOST (P approach), which simulated the lowest values, the results are within a relatively small range. Transpiration, part of ET_a, is an important factor for water balance. Different approaches can cause deviations in the results, which are clearly shown in Figs 3 and 4, particularly for AQUACROP.

The success of individual models can be compared on the basis of ET_a and SWB reference data from Domanínek 2011–2014 (Figs 4–6, Tables 4 and 5). The results of statistical parameters showed that crop models HERMES ($IA_{ETa/SWB}$ 0.84/0.78), DAISY ($IA_{ETa/SWB}$ 0.78/0.81) and CERES-Barley ($IA_{ETa/SWB}$ 0.78/0.75) showed the closest conformity. The crop model WOFOST ($IA_{ETa/SWB}$ 0.62/0.72) showed the poorest conformity. The values of $IA_{ETa/SWB}$ for EAM were 0.81/0.73. When compared $RMSE_{ETa/SWB}$ and $IA_{ETa/SWB}$ as indicators, it was found that several models, such as HERMES, DAISY and CERES-Barley, do almost as well as the EAM (Tables 5 and 6, Figs 6 and 9).

The largest D_{iETa} between measured and simulated values was in 2012. The maximum D_i with value −45% was reached by WOFOST (Table 5). The zero D_i was achieved in one case in 2011 by DAISY and EAM.

Water use efficiency

The differences in the simulations of seasonal Ta, ET_a, length of growing season and yield of individual models resulted in different WUE values for spring barley. The outputs of the HERMES model did not include Ta.

The values of WUE_{Ta} ranged from 3.9 to 10.5 kg/m^3 for above-ground biomass yield and from 2.0 to 5.9 kg/m^3 for grain yield (Fig. 7). The values of WUE_{ETa} were lower, ranging from 2.1 to 6.8 kg/m^3 for above-ground biomass yield and from 1.0 to 3.8 kg/m^3 for grain yield (Fig. 8).

Figure 8 also shows the WUE_{ETa} values calculated from measurements for use as reference data. These values ranged from 1.9 to 2.4 kg/m^3 for grain yield.

The highest WUE values were calculated from outputs of the crop model WOFOST, which simulated the lowest Ta/ET among all selected models. The lowest WUE values were calculated from outputs of the models CERES-Barley and AQUACROP.

For the WUE_{ETa} values calculated from simulations and measurements, the best agreements were shown by the HERMES model, with an average D_i −0.83%, and AQUACROP, with an average D_i 10.50%. The values of WUE_{ETa} calculated from simulations of the WOFOST and CERES-Barley models showed the poorest agreement (average D_i of 67.33 and −33.16%, respectively; Fig. 9 and Table 5).

Finally, Fig. 10 shows a comparison of the WUE values calculated from simulations of the crop models. The results confirm that the WUE calculated from the outputs of the WOFOST model is overestimated compared with that of other models, often with the largest variation. The values of WUE_{Ta} calculated from the outputs of CERES-Barley and AQUACROP are nearly the same. The values of WUE_{ETa} for CERES-Barley, HERMES, DAISY and AQUACROP also show strong agreement with each other.

Discussion

The results of the first part of the study show that the WOFOST model, using the P approach, simulates low ET_a sums compared with the other models, which use the PM approach. Sums of ET_a values during the vegetative season were 240 mm, on average, for WOFOST. For models using the PM approach, the sum values of ET_a were 340 mm on average. This finding is similar to those reported by Eitzinger *et al.* (2002), where sums of ET_a simulated with WOFOST were low, at 205 mm on average, and the highest sums of ET_a, 330 mm on average, were simulated with models using the PM approach, as in the current study. WOFOST was also shown to underestimate ET_a compared with other models in a study by Rötter *et al.* (2012), where DAISY, HERMES and CERES-Barley simulated the highest ET_a values, with high similarity among the values, as in the current study. AQUACROP simulated the highest Ta of the models. The value of Ta was calculated as 78% of ET_a on average. A similar result was reported by Zeleke *et al.* (2011), in which AQUACROP produced a Ta value of 75% of ET_a. The largest D_{iETa} is from 2012 may be due to the fact that the ET_a reference value was measured at only one

Table 5. Comparison between measured and simulated seasonal sums of actual evapotranspiration (ET_a) and water use efficiency (WUE_{ETa}) for the study location Domanínek from 2011 to 2014. Measured ET_a was obtained from data of two meteorological stations. For 2012 and 2014, relevant seasonal data for both meteorological stations are not available. Therefore, comparison was performed for only one of the stations in these years

MEASURED		WOFOST		CERES-Barley		HERMES		DAISY		AQUACROP		EAM	
Year	ET_a	ET_a	D_i (%)	ET_a	D_i (%)	ET_a	D_i (%)	ET_a	D_i (%)	ET_a	D_i (%)	ET_a	D_i (%)
2011	307	235	−23	296	−4	322	5	307	0	378	22	308	0
2011	314	235	−25	296	−6	322	3	307	−2	378	20	308	−2
2012	389	213	−45	298	−23	299	−23	282	−27	362	−7	291	−25
2013	296	212	−28	333	12	315	6	301	2	369	24	306	3
2013	324	212	−34	333	3	315	−3	301	−7	369	13	306	−5
2014	341	216	−36	294	−14	305	−11	297	−13	354	4	293	−14
MEASURED		WOFOST		CERES-Barley		HERMES		DAISY		AQUACROP		EAM	
Year	WUE_{ETa}	WUE_{ETa}	D_i (%)	WUE_{ETa}	D_i (%)	WUE_{Eta}	D_i (%)	WUE_{ETa}	D_i (%)	WUE_{ETa}	D_i (%)	WUE_{ETa}	D_i (%)
2011	2.11	3.25	53	1.27	−40	1.98	−6	1.88	−11	1.90	−10	2.06	−2
2011	2.07	3.25	57	1.27	−38	1.98	−5	1.88	−9	1.90	−8	2.06	−1
2012	1.89	3.33	75	1.50	−21	2.12	12	1.58	−16	1.89	0	2.08	10
2013	2.13	3.68	72	1.54	−27	2.14	0	1.87	−12	1.84	−13	2.21	3
2013	1.95	3.68	89	1.54	−20	2.14	9	1.87	−4	1.84	−5	2.21	13
2014	2.41	3.80	58	1.12	−53	2.02	−15	1.69	−29	1.75	−27	2.08	−13

EAM, ensemble arithmetic mean; D_i, deviation, sums of ET_a (mm), WUE_{ETa} (kg/m^3).

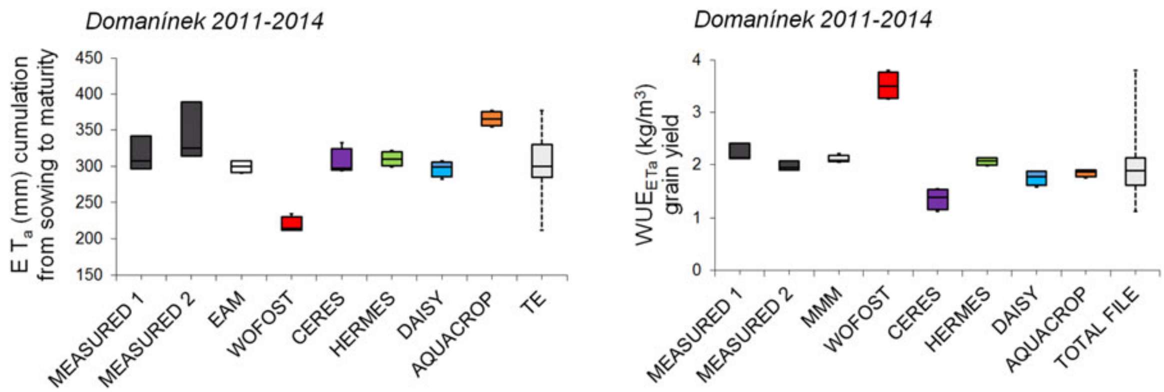

Fig. 9. Comparison of the seasonal sums of ET_a and water use efficiency (WUE_{ETa}) for grain yield of spring barley, calculated from simulated and measured ET_a values for selected crop models at the study location Domanínek from 2011 to 2014. Boxplots delimit the inter-quartile range (25–75 percentiles) and show the minimum value, maximum value and median. EAM is ensemble arithmetic mean, TE is total ensemble.

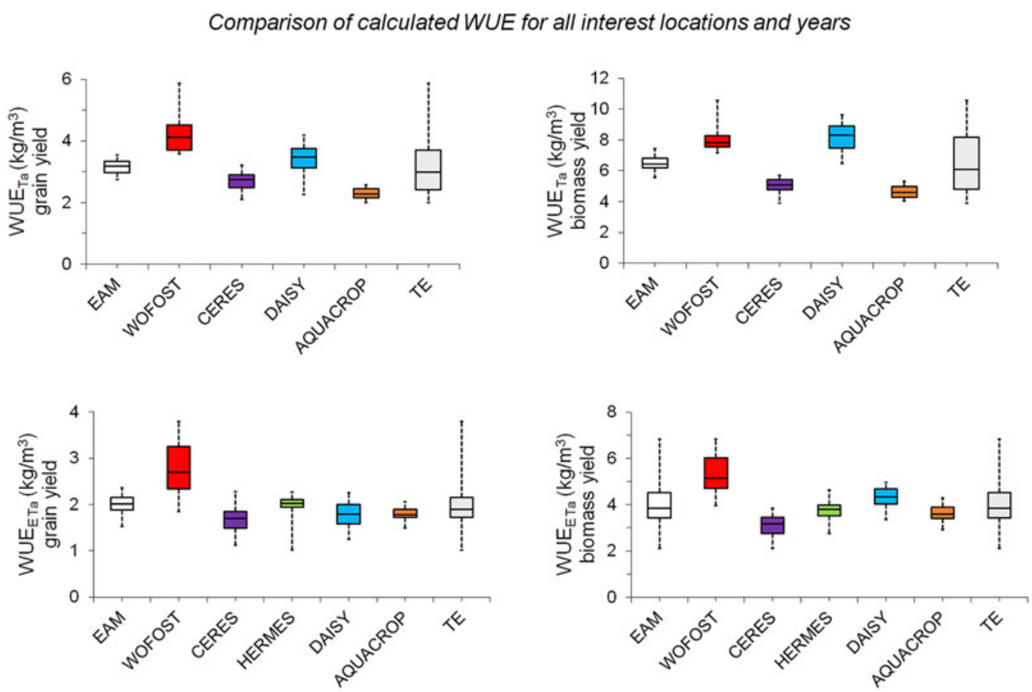

Fig. 10. Comprehensive comparison of calculated WUE_{Ta} values and WUE_{ETa} values for the study locations: Lednice for 1998 and 2001–2006, Věrovany for 1998 and 2001–2006, Domanínek for 1998, 2000–2006 and 2011–2014. Boxplots delimit the inter-quartile range (25–75 percentiles) and show the minimum value, maximum value and median. EAM is ensemble arithmetic mean, TE is total ensemble.

Table 6. An overview of the range of water use efficiency (WUE) values calculated from the outputs of individual models (WUE_{Ta}/WUE_{Eta})

	Grain yield			Biomass yield		
$WUE_{Ta/ETa}$ (m^3/ha)	Min	Max	Mean	Min	Max	Mean
Reference	1.9	2.4	2.1			
EAM	2.0/1.0	5.9/3.8	3.2/2.0	3.9/2.1	10.5/6.8	6.5/4.0
WOFOST	3.6/1.9	5.9/3.8	4.2/2.8	7.1/3.9	10.5/6.8	8.1/5.3
CERES	2.1/1.1	3.2/2.3	2.7/1.7	3.9/2.1	5.7/3.8	5.0/3.1
HERMES	1.0	2.3	2.0	4.6	2.7	3.7
DAISY	2.3/1.3	4.2/2.3	3.4/1.8	6.5/3.4	9.6/4.9	8.2/4.3
AQUACROP	2.0/1.5	2.6/2.1	2.3/1.8	4.0/2.9	5.3/4.3	4.6/3.6

EAM, ensemble arithmetic mean.

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Table 7. Overview of the range of water use efficiency (WUE) values for other important crops

WUE (kg/m^3)	Min	Max	Mean	Location	Reference
Barley	0.7	2.3	1.5	Catalonia	Cossani *et al.* (2012)
	1.5	2.8	1.7	Mediterranean	Katerji *et al.* (2008)
	3.0[a]	4.7[a]	3.4[a]	Australia	Kemanian *et al.* (2005)
	1.0	2.3	1.7	Mediterranean	Cantero-Martinez *et al.* (2003)
	1.6	1.6	1.6	Merredin	Siddique *et al.* (1990)
Mean	**1.2**	**2.3**	**1.6**		
Cotton	0.8	1.3	1.1	Lebanon	Karam *et al.* (2006)
	0.5	0.7	0.6	Turkey	Yazar *et al.* (1999)
Mean	**0.7**	**1.0**	**0.9**		
Chickpea	0.5	1.1	0.8	Australia	Fritsch & Wylie (2015)
Maize	1.8	2.8	2.3	Taiwan	Greaves & Wang (2016)
	1.6	3.9	2.7	lowland areas	Drechsel *et al.* (2015)
	1.7	2.2	1.9	Turkey	Dağdelen *et al.* (2006)
	1.4	2.0	1.7	North China	Zhang *et al.* (2004)
	1.4	1.9	1.7	Lebanon	Karam *et al.* (2003)
	1.4	1.8	1.6	Italy	Nouna *et al.* (2000)
Mean	**1.6**	**2.3**	**1.9**		
Oat	0.1	0.5	0.3	North China	Zhang *et al.* (2015)
Potato	0.3	1.5	0.9	North China	Zhang *et al.* (2015)
	1.6	1.9	1.8	Italy	Katerji *et al.* (2003)
Mean	**1.0**	**1.7**	**1.4**		
Rape	0.5	0.9	0.7	Australia	Sadras & McDonald (2012)
Rice	0.2	1.2	0.7	lowland areas	Drechsel *et al.* (2015)
Sorghum	1.0	1.8	1.4	Australia	Fritsch & Wylie (2015)
	0.7	1.6	1.2	Italy	Mastrorilli *et al.* (1995)
Mean	**0.9**	**1.7**	**1.3**		
Soybean	0.5	0.7	0.6	Mediterranean	Jaoudé *et al.* (2008)
	0.4	0.5	0.5	Lebanon	Karam *et al.* (2005)
	0.5	0.8	0.7	Italy	Katerji *et al.* (2003)
Mean	**0.5**	**0.7**	**0.6**		
Sugar beet	6.6	7.0	6.8	Italy	Katerji *et al.* (2003)
Wheat	0.9	1.5	1.2	Australia	Fritsch & Wylie (2015)
	0.8	1.6	1.2	lowland areas	Drechsel *et al.* (2015)
	1.0	2.3	1.6	Catalonia	Cossani *et al.* (2012)
	2.0	2.2	2.1	Mediterranean	Sadras & Angus (2006)
	1.1	1.6	1.4	Italy	Katerji *et al.* (2005)
	1.0	1.5	1.3	North China	Zhang *et al.* (2004)
	1.3	1.5	1.4	Turkey	Sezen & Yazar (1996)
Mean	**1.1**	**1.8**	**1.5**		

[a]WUE values were calculated from Ta.

meteorological station. There is no other reference value that would allow for verification of measurement accuracy.

As in the studies of Federer *et al.* (1996), Eitzinger *et al.* (2002) and Rácz *et al.* (2013), the differences between ET calculation approaches (P, PT, PM) in the current study amounted to hundreds of millimetres per growing season. The PM approach had on average the highest match from measured ET. The PT approach performed slightly poorer while the P approach had

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the highest discrepancy with the reference data, as was also the case in the studies of Xu & Singh (2002) and Xing *et al.* (2008). Weaknesses can be found in P, PT and PM approaches. The P approach was mainly developed for a short crop, such as grass. In semi-arid areas, simulated Ta may also be too low. Further, wind velocity was solved empirically (Penman 1948; Wolf & De Witt 2003; Subedi & Chávez 2015); therefore, the P approach may not work properly under all climatic conditions. The PT approach does not take account of saturation vapour pressure, therefore is useful for mild and humid tropical climates but not very suitable for arid and windy areas (Novák 1995; Schneider *et al.* 2007; Fischer 2012; Rácz *et al.* 2013). The PM approach is considered as one of the best methods for ET calculation. It contains all the parameters included in the energy exchange process that can be used globally without the need for special modifications. However, the PM approach has the greatest data demands (Allen *et al.* 1998; Ngongondo *et al.* 2013; Remesan & Holman 2015).

The accuracy of a given approach depends on the climatic and soil conditions (SWB) of the study location (Nash 1989; Rácz *et al.* 2013) and model parameterization. The variability among simulations of crop models in ET and SWB indicates that there are differences in the way the processes that affect water use are modelled. Crop models use either a simpler capacity approach or a more detailed Richards approach. Simulated SWB is not dependent only on model approaches for calculating water balance. For example, individual crop models, which have different approaches to simulating soil water extraction by roots (e.g. the maximum rooting depth is important) deal also with the soil profile at different degrees of resolution (De Wit & Van Keulen 1987; Wu & Kersebaum 2008; Palosuo *et al.* 2011; Cammarano *et al.* 2016). The same methods of calculation can produce different results, caused by different parameterizations in the various models (Eitzinger *et al.* 2002). The total range of crop model simulations shows the range and variability of simulations.

Similar results are described with other studies such as Eitzinger *et al.* (2004); Hlavinka *et al.* (2010); Andarzian *et al.* (2011); Palosuo *et al.* (2011); Abrha *et al.* (2012); Rötter *et al.* (2012) or Wang *et al.* (2013). The aforementioned studies dealt with crop models and SWB modelling: values for the statistical parameter IA_{SWB} were in the range 0.59 (WOFOST) to 0.93 (CERES-Barley) and for $RMSE_{SWB}$ (%) were in the range 0.70 (CERES-Barley) to 13.05 (AQUACROP). In the current study, the statistical parameter IA_{SWB} was in the range 0.72 (WOFOST) to 0.81 (DAISY) and $RMSE_{SWB}$ (%) was in the range 4.69 (DAISY) to 8.28 (AQUACROP), corresponding with the range of the results for the aforementioned studies.

WOFOST was most distant to SWB measurements and closest to the measured values were DAISY and HERMES, as well as in the study by Rötter *et al.* (2012). Otherwise, it was in the study of Palosuo *et al.* (2011) where measured values were the closest to the WOFOST and HERMES simulations, while CERES and DAISY simulated SWB overstated.

Some of the deviation within the SWB measurements could be connected with the TDR sensors, which have shortcomings (e.g. lower measured soil volume, limited use in soil with a high salinity content and in soils with high electrical conductivity, sensitivity to soil cracks or air pockets) (Hlavinka *et al.* 2010; Litschmann 2010).

The last part of the study concerns WUE. The values of WUE have ranged from 0.7 to 2.8 kg/m^3 in studies on spring barley: for example, Katerji *et al.* (2008) reported variability in WUE, with values for barley ranging from 1.5 to 2.8 kg/m^3. Cossani *et al.* (2012) reported lower WUE values for grain and biomass, ranging from 0.7 to 2.3 kg/m^3. Cantero-Martinez *et al.* (2003) found average WUE values for grain and biomass of 2.3 kg/m^3 and 1.0 to 1.5 kg/m^3, respectively, and Siddique *et al.* (1990) measured WUE at a value of 1.6 kg/m^3. In the current study, WUE reference values in the range 1.9–2.4 kg/m^3 were calculated for spring barley and grain yield. These values correspond to a narrower range of results than the aforementioned studies.

The values of WUE for spring barley, as calculated from simulations, ranged from 2.1 to 10.5 kg/m^3 for above-ground biomass yield and 1.0–5.9 kg/m^3 for grain yield.

The values of WUE were calculated in two ways, therefore, the resulting values show greater deviation. The values of WUE based on ET_a were more accurate. The reference values were closest to the WUE values obtained from the simulation models HERMES, AQUACROP and DAISY, followed by and CERES-Barley, with the poorest agreement for WOFOST. Average WUE_{ETa} values of EAM would be with D_i 1.6% included after HERMES.

Table 7 shows WUE values from world studies with an average WUE value of 1.6 kg/m^3 for spring barley. This value is slightly lower than the reference WUE value calculated for the study location Domanínek, with an average of 2.1 kg/m^3. This discrepancy can be explained by the fact that the other studies on WUE were often performed in semi-arid areas.

Conclusion

The aims of the current study were to compare values calculated from simulations of selected process-based crop models with observational results. Differences were observed between individual models. Some models predicted values that were closer to recordings than others. No model was clearly superior or more robust in terms of WUE accuracy. If average values are taken into account, EAM proved to be the best predictor. However, EAM reduces variability and the result is simplified. In the predictions of the different scenarios, it is important to know the extreme values and the range of uncertainty between different approaches. The degree of variability of the simulated values increases by incorporating the 'less successful' models into an ensemble simulation. Simulations are not constant, due to the variety of environmental conditions. For this purpose, it is good to choose a TE approach, which provides a better estimation of the uncertainty of simulation outputs. To lower the level of the degree of uncertainty further research is needed, especially for model inter-comparisons and site-specific model evaluation.

Supplementary material. The supplementary material for this article can be found at https://doi.org/10.1017/S0021859618000060.

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