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Simulating the yields of bioenergy and food crops with the crop modeling software BioSTAR: the carbon-based growth engine and the BioSTAR ET₀ method

Roland Bauböck

Abstract

Background: With a growing production and use of agricultural substrates in biogas facilities, the competition between food and energy production, environmental issues, and sustainability goals has seen an increase in the last decade and poses a challenge to policy makers. Statistical yield data has a low spatial resolution and only covers standard crops and makes no statement in regard to yields under climate change. To support policy makers and regional planners in an improved allocation of agricultural land use, a new crop model (BioSTAR) has been developed.

Results: Simulations with weather and yield data from 7 years and four regions in Lower Saxony have rendered overall good modeling results with prediction errors (RMSE and percentage) ranging from 1.6 t and 9.8% for winter wheat to 2.1 t and 11.9% for maize. The model-generated ET₀ and ET_a values (mean of four locations) are lower than ET₀/ET_a values calculated with the Penman-Monteith method but appear more realistic when compared to field trial data from northern and eastern Germany.

Conclusions: The model has proven to be a functioning tool for modeling site-specific biomass potentials at the farm level, and because of its Access® database interface, the model can also be used for calculating biomass yields of larger areas, like administration districts or states. Out of the seven crops modeled in this study, only limited yield and test site data was available for winter barley, winter rye, sorghum, and sunflower. For further improvement of model performance and model calibration, more trial data and data testing are required for these crops.

Keywords: Crop modeling; Energy crops; BioSTAR; Biomass potentials; Evapotranspiration modeling

Background

The demand for biomass from agricultural resources as an energy source is currently seeing a strong increase. This is particularly true for Germany, as the country is trying to double the share of bioenergy (agricultural, forest, and waste biomass combined) to the country's energy total by the year 2020 [1].

In 2011, 2.2 million ha of the total agricultural area (17 million ha) was already in use for either energy crop production or renewable primary products. Of this area, 800,000 ha was in use for biogas crops, mainly maize,

900,000 ha for oilseed rape (mainly for biodiesel production) and, the smallest share, 250,000 ha for starch and bioethanol production. By 2020, the agricultural area in use for renewable resource production in Germany is projected to be further expanded and will then have a share of around 20% of the country's total agricultural area. Even though Germany's food production is close to self-sufficient today, a growing competition between food production, environmental issues, sustainability goals, and the production of energy and renewable primary products is moving into the focus of policy makers and researchers. At present, the production of biogas from energy crops and agricultural wastes (manure and other residual materials) appears to be the most (land

Correspondence: rbauboe1@gwdg.de
Department of Cartography, GIS and Remote Sensing, Research Project 'BIS',
University of Göttingen, Goldschmidtstraße 5, Göttingen 37077, Germany

resource) efficient way to use agricultural areas for energy production. This is due to the relatively high energy yield of biogas per hectare [2]. This advantage of biogas is even higher when power-heat cogeneration technology is applied.

In an intensively used agricultural landscape, as it is the case in Germany, good management and farming practices and diverse crop rotation cycles are of importance, and the introduction of new energy crops into the existing crop rotation cycles can be beneficial for ecological reasons [3,4]. One research project working on this interdisciplinary topic is the currently running bioenergy project of the University of Göttingen [5].

On the contrary, using mainly maize as a substrate in biogas facilities can lead to monocultures, soil erosion, and nitrate problems in the drinking water. This is even exacerbated in areas where a lot of maize is already grown for animal feed as is the case in the western part of Lower Saxony.

Using a crop modeling tool, yield differences of different crop rotations and crops can be approximated and optimized solutions, with economical as well as ecological perspectives in view, can be found out.

Crop models have been in existence for about four decades now [6]. Resource capture of an agricultural crop can be implemented in a model in different ways. Commonly used approaches are either carbon-based [7], radiation use efficiency (RUE)-based [8], water productivity-based (WP) [9], or transpiration-based (BTR) [10].

BioSTAR's primary growth engine is carbon-based, and it uses an asymptotic exponential light response curve [11]. Among the well-known crop models, the RUE approach is probably the one which is most often used. Examples for crop models with this type of growth engine are CropSyst [12], APSIM [13], CERES (DSSAT) [14], and LINTUL. Carbon-based growth engines are used in all of the older models from Wageningen such as WOFOST and in the model CROPGRO (DSSAT).

The water productivity approach is relatively new [15], and it has been implemented in the model AquaCrop [16]. The transpiration-based growth engine (BTR) is used as a second growth engine in the model CropSyst. Because the Tanner-Sinclair relationship becomes unstable at low VPD, the RUE method is used as a main growth engine in the model CropSyst.

Even though there are numerous crop models in existence today, no single model can claim to adequately cover all possible demands a user might put to such a model. One big advantage of developing a new model is the ability to structure and build the model according to user specifications and to be able to modify it and add on to it to suit future demands.

The crop model Biomass Simulation Tool for Agricultural Resources (BioSTAR) [17,18] has been developed

to simulate climate and soil-dependent biomass yields for bioenergy crops, but obviously it can also be used to predict yields for food crops like wheat or rye. The model's software is built in such a way that, depending on the resolution of the input data, large-scale (single plots or farms) or small-scale (larger areas with many input datasets) yield predictions can be generated very easily. Novelties in the BioSTAR crop modeling software are a MS Access® database connection for fast data editing and organization and the possibility to choose between four different growth engines and four ET₀ methods. Validation runs for several agricultural crops grown in Lower Saxony have proven the models' capability to serve as a user-friendly biomass simulation tool for small- and large-scale agricultural planning.

Results and discussion

Biomass yields

To validate the model BioSTAR, yield, soil, and climate data from five different locations in Lower Saxony, Germany have been used. The first two locations are farm plots in Hedeper and in Troegen. The other two are field trial sites of the Chamber of Agriculture of Lower Saxony (LWK), situated in Poppenburg and in Werlte. Winter wheat and maize were grown at all four localities, sunflower, sorghum, winter rye, and winter barley only in Poppenburg and Werlte, and sugar beet only in Hedeper.

The overall simulation results (all have been performed with the carbon-based growth engine and the BioSTAR ET₀ method) have shown that the model predicts biomass yields at a good level of accuracy, though differences between cultures exist (Table 1). For the culture sugar beet (in the following referred to as beet), the analysis has been divided up into three parts: (1) all soil types, (2) clay soil types, and (3) no clay soils. This has been done to distinguish the unique reaction (overestimation) of beet to soils with high clay contents. The model produced the lowest error values (root-mean-square error (RMSE) and percentage error) for winter wheat (RMSE = 1.6 t and 10.1%), sorghum (RMSE = 1.0 t and 5.9%), winter barley (RMSE = 1.8 t and 11.0%), winter rye (RMSE = 1.9 t and 10.4%). Beet (clay), beet (no clay), and beet (all) simulation results show up with errors of 10.7%, 10.8%, and 11.4%, respectively, and an RMSE of 1.7 t on clay and 2.4 t for the other two. Sunflower and maize results show errors of 12.0% and 11.9% and RMSE values of 1.6 and 2.1 t, respectively. All crops combined in one analysis show up with mid-range error values (RMSE 2.1 t and 12.2%). The percentage error values have been calculated by dividing the RMSE by the mean observed yield (both are in tons per hectare).

Looking at the other statistical measure for model prediction accuracy, the Willmott index of agreement, the

Table 1 Mean for observed and simulated yields, RMSE, percentage error, and WIA for tested crops

	Mean observed	Mean simulated	RMSE	Number	Percentage error	WIA
Maize	17.7	18.2	2.1	31	11.9	0.94
Winter wheat	15.8	16.1	1.6	102	10.1	0.86
Beet (all)	21.0	21.8	2.4	40	11.4	0.77
Beet (clay)	15.9	21.1	1.7	8	10.7	0.94
Beet (no clay)	22.3	21.9	2.4	32	10.8	0.85
Winter barley	16.3	16.1	1.8	6	11.0	0.64
Winter rye	18.3	18.7	1.9	6	10.4	0.73
Sunflower	13.3	13.4	1.6	9	12.0	0.56
Sorghum	17.0	17.3	1.0	5	5.9	0.78
All crops	17.2	17.7	2.1	198	12.2	0.92

WIA, Willmott index of agreement (1 = perfect agreement, 0 = no agreement). Mean observed, mean simulated, and RMSE (root-mean-square error) given in tones dry mass per hectare.

resulting order of the crops is a different one. Now maize and beet (clay) are ranked first, both with a WIA of 0.94 followed by winter wheat (0.86), beet (no clay) (0.85), and sorghum (0.78). The lower ranks are now occupied by beet (all) (0.77), winter rye (0.73), winter barley (0.64), and sunflower (0.56). All crops combined in one analysis have achieved a high WIA of 0.92.

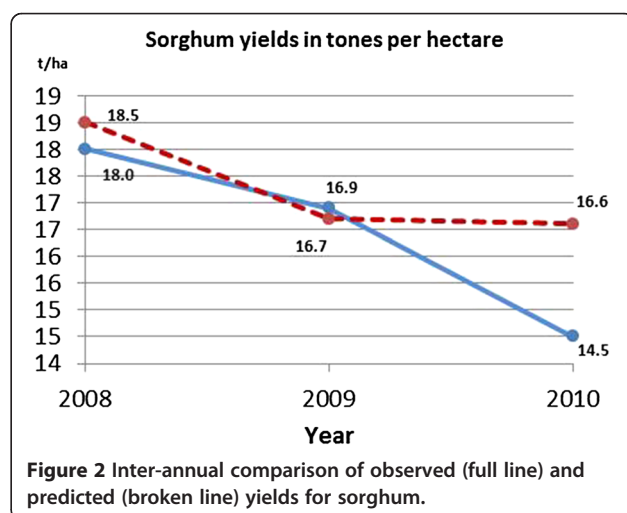
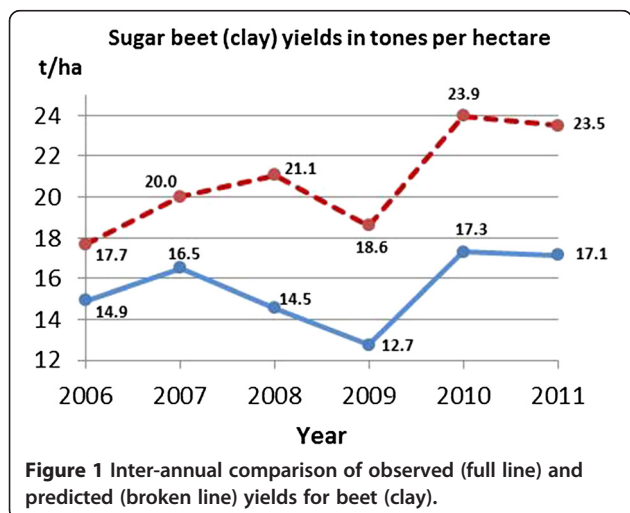
The low WIA values for the winter grains (other than winter wheat) can be explained by an approximately equal over- and underestimation of the observed results (and possibly a low number of samples), whereas the predicted biomass for beet on clay type soils is exclusively overestimated at a similar level (Figure 1). Sorghum yields have been calculated well for the years 2008/2009 but were then overestimated at a high level in 2010 (Figure 2). Sunflower's biomass yield is predicted well in 4 years and then overestimated highly in 2007 (Figure 3). To some extent, this could be the result of a fungus infection (*Sclerotinia sclerotiorum*) which has reportedly [19] damaged the sunflower crops in the extremely rainy summer of 2007.

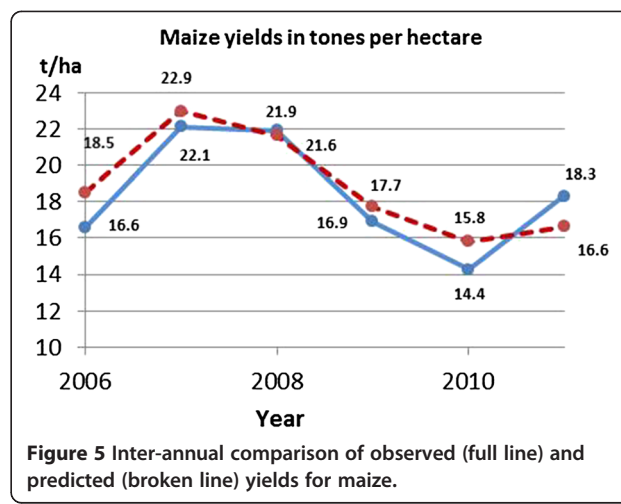
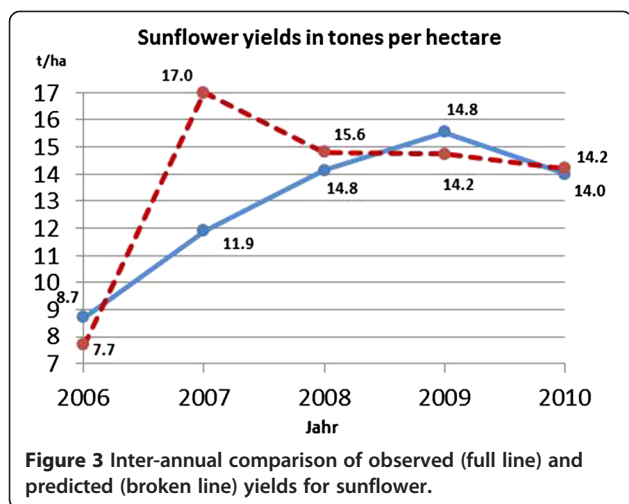
The overall reaction of the model in response to inter-annual climatic variations is at a good level of accuracy with the curves of the predicted vs. the observed biomass yields following the same pattern (Figure 4). This is particularly true for maize (Figure 5), winter barley and winter rye (Figure 6), winter wheat (Figure 7), and sugar beet (no clay) (Figure 8). The corresponding curves of beet (clay), beet (all) (Figures 1 and 9), sorghum (Figure 2), and sunflower (Figure 3) display some deviations from the inter-annual trend.

For all crops combined in one analysis, a linear regression analysis has been performed. The R^2 value (0.71) for the whole dataset (observed vs. predicted yields) is at a satisfactory level (Figure 10) and has a high correlation (Pearson correlation coefficient of 0.845 at a highly significant level of $\alpha \leq 0.01$).

Evapotranspiration levels

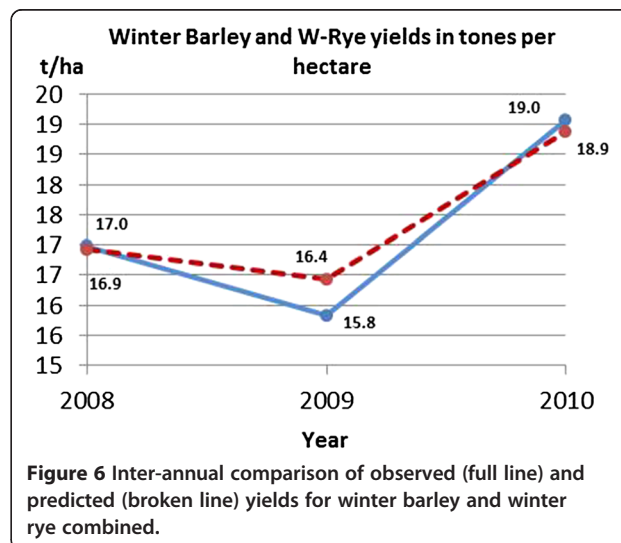
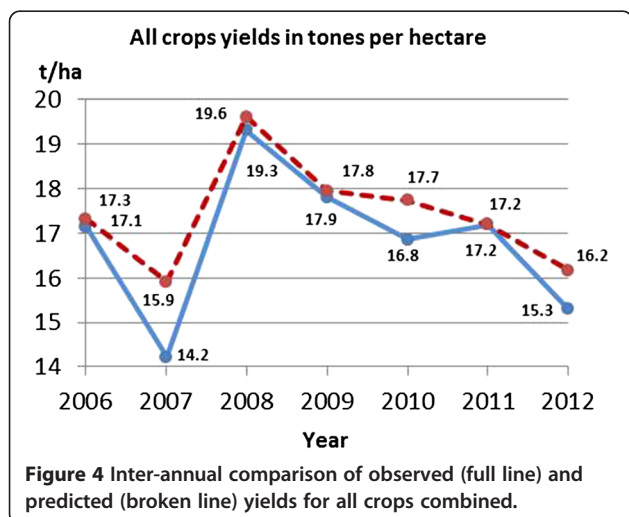
Unlike other crop models, BioSTAR can generate its own crop and phenology-dependent potential transpiration

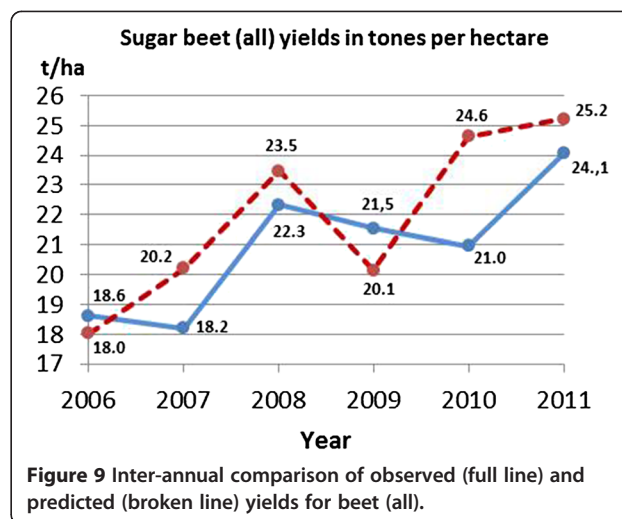
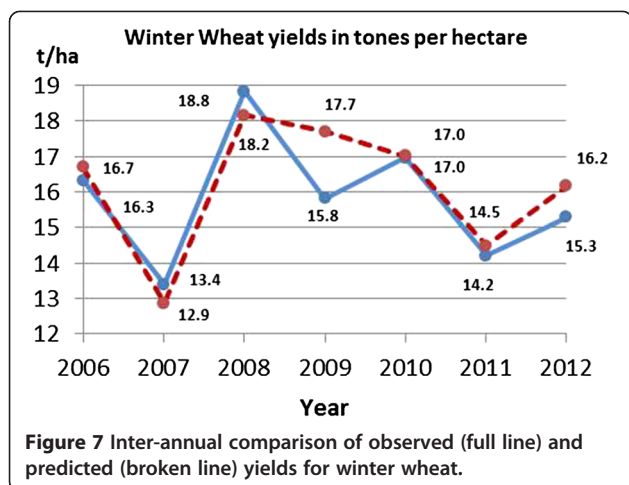




rates (see ‘Main model processes’) to which a leaf area-dependent soil evaporation value is added. In Figure 11, the mean values of all four locations of the simulation and all 7 years of the BioSTAR ET_0 (potential evapotranspiration) and ET_a (actual evapotranspiration) method are displayed along with the corresponding Food and Agriculture Organization (FAO) (Penman-Monteith) values calculated for these years. For both calculations a maize crop with a cropping period from the end of April until the beginning of September was chosen. ET_0 values calculated with the BioSTAR method are considerably lower than their FAO method equivalents. To a lesser extent, this is also true, when the ET_a values of the two methods are compared. The BioSTAR ET_0 and ET_a values range from 543 mm (2008) to 430 mm (2007) and from 423 mm (2007) to 349 mm (2012), respectively. The FAO curves for ET_0 and ET_a follow a similar inter-annual trend but at levels which are approximately 200 mm (ET_0) and 50 mm (ET_a) above the BioSTAR values. The high ET_0 values of

the FAO calculation can be explained by the fact that no crop or phenology parameters have been considered here (grass reference evapotranspiration). Looking at the literature data for ET_a values for northern and eastern Germany, the FAO values appear to be overestimated. Haferkorn [20] and Zenker [21] give ET_a values for various crops measured by lysimeters in eastern Germany, ranging from 280 to 530 mm (April until September), with average values around 350 mm. The DVWK [22] estimates the share of the evapotranspiration from May until September to be about 70% of the year’s total precipitation. Since Germany’s climate is of a humid character and average annual precipitation values range between 600 and 800 mm, annual evapotranspiration for this climate is not likely to be higher than 600 mm. In fact the DVWK gives an average annual evapotranspiration value (ET_a) of 433 mm for northern Germany. Eulenstein et al. [23] give annual ET_0 values for eastern Germany for the years 1971 to 1998 ranging from 420 to 680 mm (the approximate mean is





around 570 mm). Additionally it needs to be mentioned that eastern Germany has a more arid and continental climate than Lower Saxony.

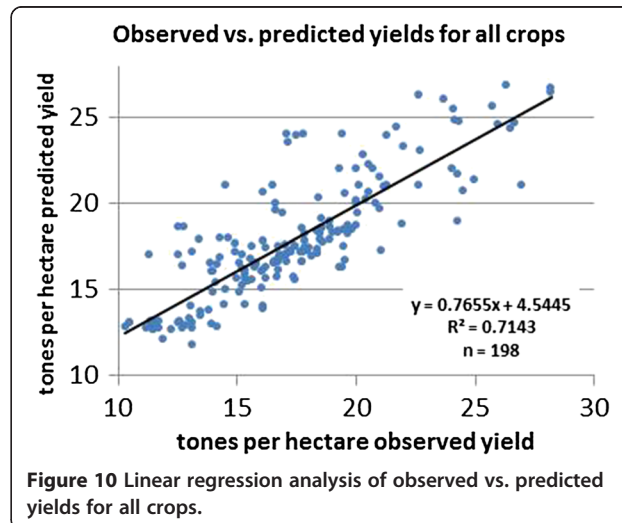
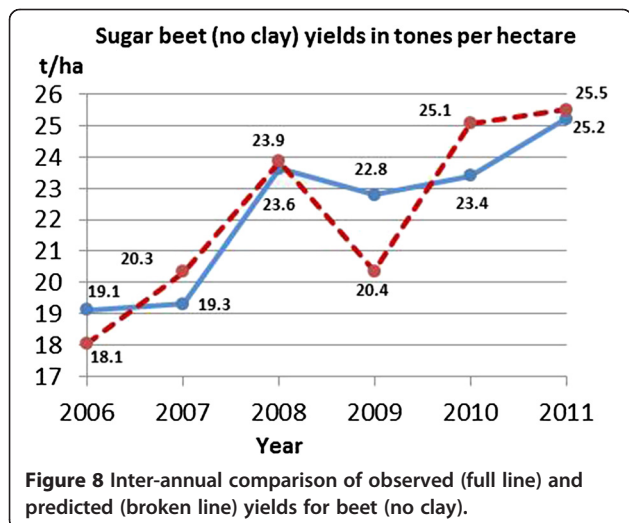
In comparison with this data, the BioSTAR ET_0 and ET_a values seem to be more realistic than the FAO values and underline the relevance of this ET method for the computation of crop biomass potentials.

Conclusions

The performance of the crop model BioSTAR has been tested with datasets from four locations in Lower Saxony, Germany for seven agricultural crops. The model predicts biomass yields for all crops combined at a satisfactory level (mean error of 12.1%). The yields of all crops have been predicted by the model with errors ranging from 8.4% (winter wheat) to 12.1% (maize). The model has proven to be a functioning tool for modeling site-specific biomass potentials at the farm level. Because of its Access® database interface, the model can also

easily be used for the prediction of potential biomass yields of larger areas, like administration districts or states and can therefore serve as a decision support tool when questions of regional and trans-regional crop planning are concerned. Because the model reacts adequately to inter-annual climatic differences, transferability to different climates is probably possible but still needs to be validated. BioSTAR offers its own method for calculating evapotranspiration during the course of crop growth. The model-generated evapotranspiration levels are lower than the ones calculated using the Penman-Monteith approach but seem to be closer to actually measured ET values in northern and eastern Germany.

Out of the seven crops modeled in this study, only limited yield and test site data was available for winter barley, winter rye, sorghum, and sunflower. For further improvement of model performance and model calibration, more trial data and data testing are required here.



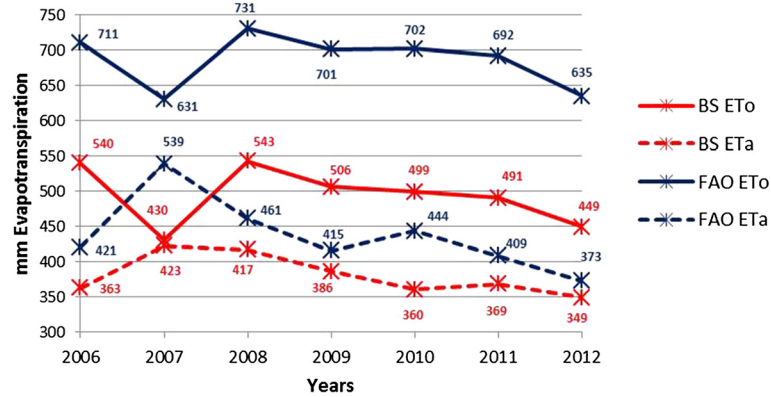


Figure 11 Inter-annual comparison of ET₀ and ET_a values calculated with the BioSTAR and FAO (Penman-Monteith) methods.

The reaction of the sugar beet yield development on clay-type soils still needs to be investigated further and improved in the model. Up to date (September 2013), the model is capable of simulating the general reaction of crops to water and nitrogen stress. To further expand the models' range of application, soil salinity content and related salinity stress reaction of plants should be implemented in the model.

Grasses and perennial cultures like the cup plant (*Silphium perfoliatum*) or short rotation coppices like poplar or willow are potential cultures for bioenergy production in the German agricultural sector. Up to date (September 2013), the model BioSTAR is capable of modeling these cultures, but calibration and validation still have to be performed before the model can be used for yield prediction of these cultures.

Methods

Main model processes

BioSTAR's primary growth engine is carbon-based (see above) and calculates a radiation and temperature-dependent gross CO₂ exchange rate in mmol CO₂ m⁻² s⁻¹ (Equation 1).

Photorespiration (maintenance and growth) and nitrogen-induced photosynthesis inhibition are accounted for in a second step. The remaining fraction of CO₂ (net photosynthesis) is then used to calculate a net photosynthesis-dependent transpiration rate. This is done using the gradients of the water vapor pressure and of the CO₂ concentration inside the leaves to the corresponding pressures of the atmosphere (Equations 2 to 5). Due to this calculation procedure, BioSTAR does not need a separate ET₀ calculation (e.g., Penman, FAO, Turc, or other) to compute crop transpiration (Figure 12):

$$P_G = P_{\max} \times 1 - \exp^{(-Q_e \times \text{PPFDI} / P_{\max})}, \quad (1)$$

where P_G is the gross photosynthesis rate (mmol CO₂ m⁻² s⁻¹), Q_e is the initial light use efficiency (mmol CO₂ mol⁻¹ light quantum), PPFDI is the intercepted photosynthetic active radiation (mmol m⁻² s⁻¹), and P_{\max} is the maximum photosynthesis rate (mmol CO₂ m⁻² s⁻¹).

$$H_2O_{\text{grad}}: ((VP_{\text{def}} \times Vol_{\text{mol}}) / 18) \times 1,000 \quad (2)$$

$$CO_{2\text{grad}}: (CO_{2\text{con}} - (CO_{2\text{con}} \times C_i / C_a)) / 1,000 \quad (3)$$

$$Wat_{\text{use}}: (H_2O_{\text{grad}} / CO_{2\text{grad}}) \times 1.56 \quad (4)$$

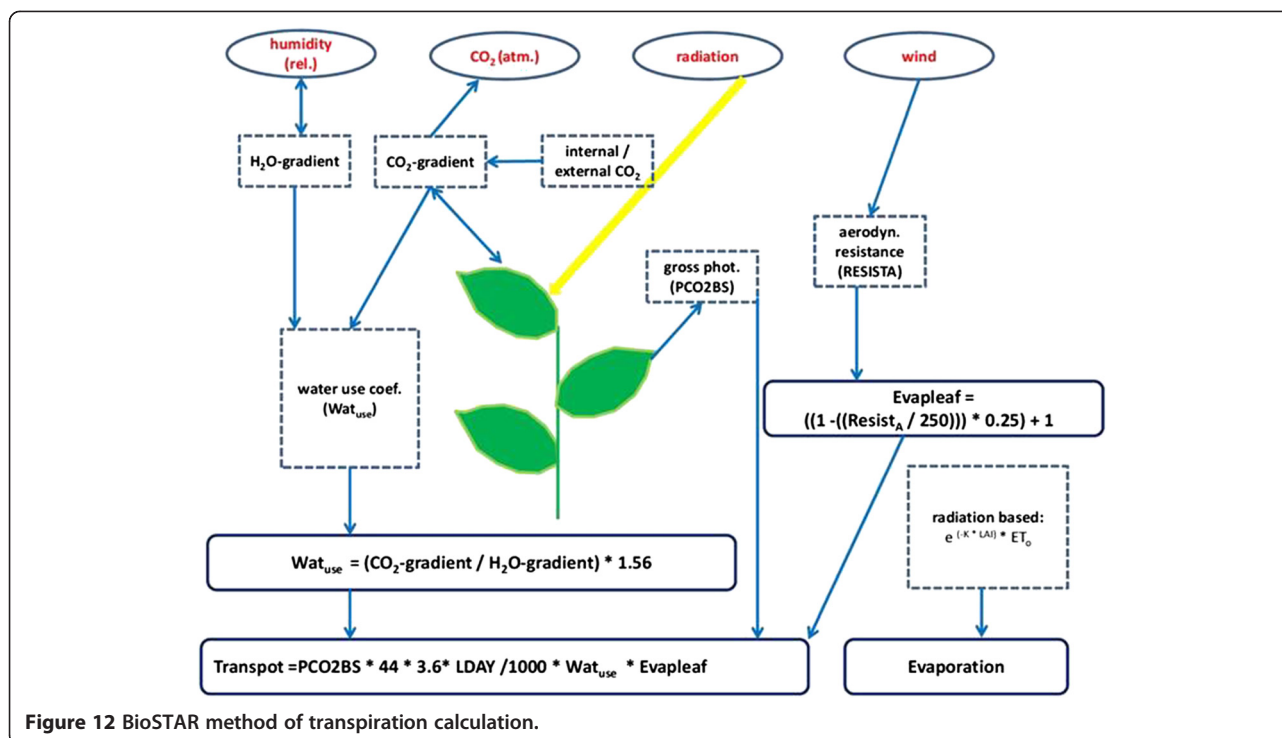
$$\text{Transpot}: (P_{\text{rate}} \times 3.6 \times L_{\text{day}} \times 44 \times 1,000) \times Wat_{\text{use}} \quad (5)$$

$$\text{Evapleaf}: \{(1 - (\text{Resist}_A / 250)) \times 0.25\} + 1 \quad (6)$$

$$P_{\text{reduct}}: P_{\text{net}} \times (ET_a / ET_0) \times S_{\text{reduct}}, \quad (7)$$

where H_2O_{grad} is the H₂O gradient from leaf to atmosphere (mmol mol⁻¹), VP_{def} is the vapor pressure deficit of the air (g m⁻³), Vol_{mol} is the volume of 1 mol dry air, $CO_{2\text{grad}}$ is the CO₂ gradient from leaf to atmosphere (mmol mol⁻¹), $CO_{2\text{con}}$ is the CO₂ concentration of the atmosphere (ppm), C_i / C_a is the internal-external CO₂ ratio dimensionless, range approximately 0.1 to 1.0, Wat_{use} is the H₂O-CO₂ evolution ratio dimensionless, Transpot is the CO₂ assimilation-dependent potential transpiration rate (L day⁻¹), P_{rate} is the CO₂ assimilation rate (mmol CO₂ m⁻² s⁻¹), L_{day} is the daylight hours, Evapleaf is the aerodynamic resistance-dependent multiplier for leaf evaporation, Resist_A is the aerodynamic resistance (s m⁻¹), P_{reduct} is the stomata conductance-induced photosynthesis reduction (g day⁻¹), P_{net} net photosynthesis (after respiration and nitrogen-induced reduction) (g day⁻¹), and S_{reduct} is the function for water stress-induced photosynthesis reduction.

The transpiration rate calculated by Equation 5 is multiplied by a dimensionless factor (Evapleaf) to account for aerodynamic resistance and leaf evaporation



(Equation 6) and then added to a leaf area-dependent soil evaporation value. The resulting evapotranspiration value (ET_0) is then used in the soil sub-model to check if enough water for evapotranspiration is available in the rooted layers of the soil profile. Soil water availability is defined by each layer's individual soil water retention curve. If the available soil water, available for evapotranspiration (ET_a), is smaller than the calculated ET_0 , biomass accumulation is lowered correspondingly (Equation 7).

Crop development and leaf area index (LAI) development are temperature driven and divided into two main stages: emergence until anthesis (development stages 0 to 1) and anthesis until ripeness (development stages 1 to 2). Maximum LAI is reached at development stage 1, and the curve of LAI development is modeled as a Gaussian integral (normal distribution).

Software architecture and model features

The BioSTAR software is written in Java and uses a connection to Microsoft Access® database tables to read input data and write output data (Figure 13 and Table 2).

Data can easily be imported into these tables from spreadsheets like Excel®, and output data can be exported to a GIS for spatial visualization via the dbf format. One advantage of this software architecture is that all relevant data for running simulations is stored in one Access® database which contains different tables storing location, weather, crop, and soil texture variables. For each simulation run (combination of location and weather data), a new result table is generated in the

database. Because all parameters (for crops and soil) are stored in the same database file, editing and comparison of the contents is easily done. Running the model on a PC or laptop requires an installed version of Microsoft Access® (versions 2007 or later) and the installation of Java runtime environment (freeware). The model software itself is contained in an executable JAR file and does not need to be installed on the computer.

Model calibration and input data

The model has been calibrated and tested for different sites and years in Lower Saxony for the winter cereals wheat, rye, triticale, and barley, for maize, sorghum, and sugar beet, and for sunflower. Further cultures which have been implemented in the model are canola (oilseed rape), cup plant (*S. perfoliatum*), and the short rotation coppices poplar and willow, although no validation for these cultures has been performed so far.

For model calibration, harvest and weather data (5 years) and soil data from two locations (Poppenburg and Werlte) in Lower Saxony has been used (Table 1). At these two locations, regular field trials are carried out by the LWK (Chamber of Agriculture Lower Saxony). For further testing of the model, additional harvest and weather data (7 years) from two farms in Lower Saxony (Hedeper and Trögen) were used. Soil qualities at these four locations cover a wide range from deep silt and silt loams to more shallow sands and sand loams and clays. Model testing has been performed for maize, winter wheat, winter barley, winter rye, sugar beet sunflower,

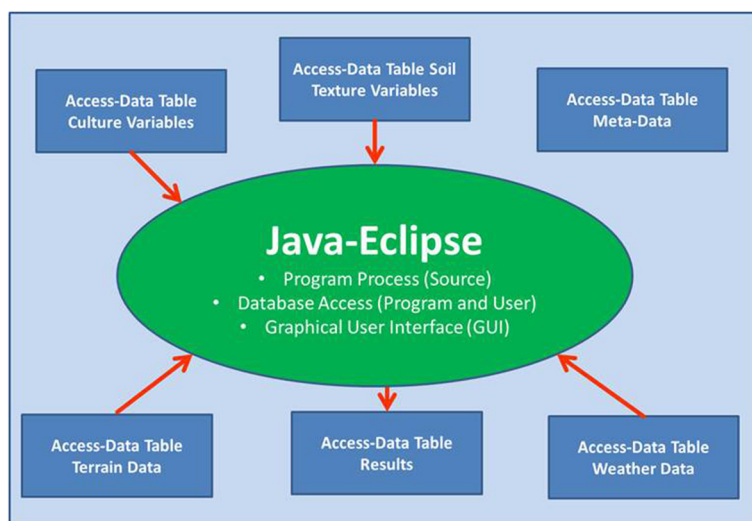


Figure 13 Software architecture of the BioSTAR model.

and sorghum. The growth engine and ET_0 method settings used for these tests are CO_2 and BioSTAR (see above).

Statistical methods used for data analysis

For the interpretation of the model output data (model performance), the *Willmott index of agreement* [24] (Equation 8) and the RMSE (root-mean-square error) (Equation 9) values have been calculated for all tested crops individually as well as all crops combined in one analysis (Table 1). For all crops combined, a linear regression and the corresponding R^2 value have been calculated (Figure 10). To see how the model reacts to inter-annual variations in climate, an inter-annual comparison of the observed and simulated yields has additionally

been done for all crops combined and individually (Figures 1, 2, 3, 4, 5, 6, 7, 8, 9).

$$d = 1 - \frac{\sum_{i=1}^n [(P_i - \bar{O}) - (O_i - \bar{O})]^2}{\sum_{i=1}^n [(|P_i - \bar{O}|) + (|O_i - \bar{O}|)]^2} \quad (8)$$

$$RMSE = \left[n^{-1} \sum_{i=1}^n (P_i - O_i)^2 \right]^{-0.5}, \quad (9)$$

where P_i is the instance of predicted value, O_i is the instance of observed value, \bar{O} is the mean of observed values, RMSE is the root-mean-square error, and d is the Willmott index of agreement (0 = no agreement, 1 = perfect agreement).

Table 2 Summary of model features

	Features
Software	
Data storage	Fast data reading, writing, and editing due to MS Access® data table interface
Multiple sites	Capability to process either individual sites or large datasets
Program type	Program runs from an executable Java file
Data organization	Soil, weather, crop, and result data are all kept in one database
Crop model	
Growth engines	User can choose between four growth engines and four ET_0 methods
Time step	Daily or monthly climate data can be processed
Minimum data	If data availability is limited, the model can be run with only daily mean temperature
Perennial crops	Modeling of perennial crops like short rotation coppices or cup plant is possible
Soil model	Computation of soil water budget in a one-dimensional 2-m soil profile with decimeter layer increments using van Genuchten soil texture parameters
Crop water stress	Crop water stress simulation enhancement with crop-specific stress phase modeling
Crop development	Crop development tracking with BBCH (EC) stages

Abbreviations

APSIM: agricultural production simulator; AquaCrop: FAO crop model; BBCH/EC scale: growth scale of monocot and dicot plants; BioSTAR: Biomass Simulation Tool for Agricultural Resources; CERES: crop model in the DSSAT family; CROPGRO: crop model in the DSSAT family; CropSyst: cropping systems model; DSSAT: decision support system for agronomy transfer; ET_a : actual evapotranspiration rate; ET_0 : potential (reference) evapotranspiration rate; FAO: Food and Agriculture Organization; LINTUL: crop model in the Wageningen family; LWK: Landwirtschaftskammer (Niedersachsen); RMSE: root-mean-square error; RUE: radiation use efficiency; VPD: vapor pressure deficit of the air; WIA: Willmott index of agreement; WOFOST: crop model in the Wageningen family.

Competing interests

The author declares that he has no competing interests.

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