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Simulating switchgrass biomass productivity using ALMANAC. I. Calibration of soil water

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Abstract

Soil water supply plays a key role in driving switchgrass (*Panicum virgatum* L.) yield, and therefore is an important parameter for crop-model accuracy. ALMANAC (Agricultural Land Management Alternative with Numerical Assessment Criteria) model has been applied to simulating switchgrass growth with mixed results. The objective was to develop and test a calibration for ALMANAC simulating soil water dynamics in a switchgrass ('Alamo') stand under Arkansas conditions. Soil volumetric water content (SW) profiles were measured daily in switchgrass from May 2009 to February 2013. Soil, crop, and weather input data were developed based on in situ measurements. After identifying the most sensitive parameters in SW simulation, a calibration method was proposed, and the parameters initial soil water (FFC), permanent wilting point (U), field capacity (FC), sand content (SAN), silt content (SIL), pH, and maximum stomatal conductance (GSI) were modified. Daily SW simulation outputs from default and calibrated runs were compared to SW observations. Default Willmott agreement *d*-index values were lower than the calibrated *d*-index values in all years. Therefore, calibration improved simulation accuracy. Calibration accuracy was greater in 2009 and 2010 than in 2011 and 2012. Lower root mean square error of calibrated versus observed SW data confirmed the elevated *d*-index values. Lower accuracy in the latter years was related to drought periods when ALMANAC was unable to mimic switchgrass drought adaption by lowering GSI. Calibration of SW in ALMANAC was aided by using site-specific soil data. Improvement of SW calibration for drought-resistant plants may be achieved by quantifying GSI dynamics.

1 | INTRODUCTION

The Energy Independence and Security Act of 2007 called for US reductions in foreign oil dependence and greenhouse gas emissions by increased use of biofuels (US EPA, 2019). The act set Renewable Fuel Standard (RFS2) targets to produce 136 billion L of oil equivalent in 2022, and this target is reset annually (US EPA, 2019). Lignocellulosic biofuels, which are derived from plants with large cellulose, hemicellulose, and lignin concentrations, are classified as advanced

Abbreviations: ALMANAC, Agricultural Land Management Alternative with Numerical Assessment Criteria; BD, bulk density; CN2, curve number; EPIC, Erosion-Productivity Impact Calculator; ET, evapotranspiration; FC, field capacity, FFC, initial soil water; GSI, maximum stomatal conductance; IPAR, leaf area interception of photosynthetically active radiation; LAI, leaf area index; PKR, percolation beyond the rood zone; Q, surface runoff; SAN, sand content; SIL, silt content; SPAW, Soil-Plant-Air-Water model; SW, soil volumetric water content; U, permanent wilting point; WCR, water content reflectometer.

biofuels due to lifecycle reductions of greenhouse gas emissions by at least 60% compared with petroleum, attributable largely to low petroleum inputs for crop production.

Switchgrass has potential to contribute substantially to meeting the RFS2 goal as a perennial, herbaceous energy crop in conjunction with woody biomass, crop residues, and other herbaceous energy crops (Langholtz, Stokes, & Eaton, 2016). Switchgrass produces large biomass yields, has low requirements for water and nutrients, is compatible with conventional farming equipment, and is broadly adapted in the United States (McLaughlin & Walsh, 1998). The dense rooting and perennial growth habit of switchgrass contribute to mitigating soil erosion on erosion-prone soils (McLaughlin & Walsh, 1998) and restoring favorable hydraulic properties of topsoils that were eroded by annual cropping (Zaibon, Anderson, Kitchen, & Haruna, 2016).

Progress has been made recently in elucidating management practices for switchgrass establishment (Butler, Stein, Pittman, & Interrante, 2016), fertilization, and timing of harvest (Cahill et al., 2014; Lindsay et al., 2018). Further refinement of switchgrass management is needed to lower costs of feedstock production to meet year-round supply needs (Wetzstein, 2010). Lindsay et al. (2018) showed that single-pass harvesting (direct chopping) of senescent switchgrass could be economically more effective in meeting biorefinery needs than double-pass harvesting (swathing-curing-chopping). Harvest losses would be greater at the senescent stage; however, enhanced nutrient recycling would lower fertilizer replacement costs. Lindsay et al. (2018) concluded that refined prediction of switchgrass growth and nutrient removal using decision-making tools would aid in optimizing the allocation of time, labor, and fertilizers to maximize environment benefits and economic competitiveness of biomass as an energy source.

ALMANAC (Agricultural Land Management Alternative with Numerical Assessment Criteria) is a process-oriented, crop simulator designed to predict growth of various crops including switchgrass (Kiniry, Williams, Gassman, & Debaeke, 1992, 2005). It includes enhanced logic on plant growth, originally derived from the Erosion-Productivity Impact Calculator (EPIC) model (Williams, Jones, Kiniry, & Spanel, 1989). The first application of ALMANAC to simulating switchgrass yield was by Kiniry et al. (1996), mainly as a forage crop in fixing the response of leaf area index (LAI) development to heat unit accumulation, and in testing the relative sensitivity of parameters across wide ranges in precipitation and soil depth across Texas. The importance of accurately accounting for soil depth was highlighted to characterize water availability for deeply rooted crops. Interest in switchgrass as a lignocellulosic bioenergy crop stimulated efforts to further parameterize ALMANAC to simulate biomass yield over variable environments. Kiniry et al. (2005)

Core Ideas

- Calibrating ALMANAC for soil water improved its ability to predict switchgrass production.
- Model parameters were calibrated for accurate soil water simulation at a site in Arkansas.
- Soil water was overestimated during drought due to low ability to lower stomatal conductance.

tested the predictive ability of ALMANAC in three locations in Texas, one in southeast Louisiana, and one in southwest Arkansas. Mean biomass yields were acceptably simulated; however, yearly variations were not well simulated. Sensitive factors affecting simulations were USDA-NRCS (US Department of Agriculture National Resources Conservation Service) runoff curve number (CN2) and maximum stomatal conductance (GSI; parameter abbreviations are those used in ALMANAC as defined in Tables 1–3) which relate to soil and plant-water relations.

'Alamo' is a lowland type of switchgrass originating in south Texas and is a consistently high-yielding cultivar in the south-central United States (Cassida et al., 2005). Behrman, Keitt, and Kiniry (2014) adjusted plant growth parameters in ALMANAC to match temperature and day-length values of four common cultivars, including Alamo, to each cultivar's location of origin. ALMANAC simulated biomass yields well enough to construct meaningful yield-potential maps for each cultivar across the central and southern Great Plains of the United States. The same authors stated that spatial variations in simulated yields could be improved by further parameterization of drivers of growth. Tulbure, Wimberly, Boe, and Owens (2012) identified amounts and temporal distribution of precipitation as environmental factors having the greatest effects on switchgrass biomass yield and yield stability. These factors support a key role of soil water supply in driving yield, and are therefore important parameters for model accuracy. For example, erroneously low soil water simulation would underestimate biomass as a result of an overstated water stress factor, thereby compromising the calibration of the plant growth algorithm. The water stress factor is calculated by a subroutine from EPIC using water balance equations (Williams et al., 1989). The objective was to test a calibration of the simulation of soil water supply to improve the accuracy of the water logic because of its role in modulating the development of leaf area and thus, the conversion of solar radiation into biomass. This test contributes to a larger effort to accurately parameterize ALMANAC growth functions that apply to Arkansas growing conditions.

TABLE 1 ALMANAC management input file parameters. Parameter value selections were based on the field management applied from 2008–2012, Fayetteville, AR

Operation	Date	Parameter	Value	Description
Year 1: 2008				
Planting	3 July	COD (Operation)	17: PLANT DR	Planting with drill
		CRP (Crop input file)	27	Alamo switchgrass
		PHU (Potential heat units)	1750°C-d	–
		PLANTPO (plant population)	50 plants m^{-2}	–
Year 2: 2009				
Burning	1 Feb.	COD (Operation)	23: Burned	Burning without killing
Fertilization	1 Apr.	FN (Nitrogen fertilizer applied)	67 kg ha^{-1}	–
Year 3: 2010				
Harvesting	1 Mar.	COD (Operation)	47:HARHAY85	85% biomass harvested
Fertilization	1 Apr.	FN (Nitrogen fertilizer applied)	67 kg ha^{-1}	–
Year 4: 2011				
Harvesting	1 Mar.	COD (Operation)	47:HARHAY85	85% biomass harvested
Fertilization	1 Apr.	FN (Nitrogen fertilizer applied)	67 kg ha^{-1}	–
Year 5: 2012				
Harvesting	3 May	COD (Operation)	47:HARHAY85	85% biomass harvested
Fertilization	5 May	FN (Nitrogen fertilizer applied)	67 kg ha^{-1}	–

2 | MATERIALS AND METHODS

2.1 | Background on ALMANAC growth logic

ALMANAC (2014 Version 1.0.18; ARS, 2019) simulates daily dry biomass accumulation based on the development of LAI as a function of heat units, leaf area interception of photosynthetically active radiation (IPAR) with an appropriate light extinction coefficient, and conversion of IPAR to dry biomass yield via a radiation use efficiency ratio. Biomass growth is structured within limits of heat unit accumulation up to maturity and killing frost to cease IPAR. Growth rate is modulated by constraint coefficients which apply the influences of minimum and maximum air temperatures, soil and rooting conditions describing potential water availability, soil aeration, and N and P availability (Williams et al., 1989). The values of the constraint coefficients are 1 for non-stress conditions and 0–<1 for stress conditions. More description of the crop growth logic will be described in a companion publication, thus the soil water logic is emphasized here along with the approach to calibrating the associated parameters.

The model contains initial default parameter values for soil, management (e.g., establishment practices and fertilization), tillage, and crop traits. Soil profile characteristics are set in the soil input file derived from the SSURGO database (USDA-NRCS, 2019a) for a chosen field site. Site-specific soil profile descriptions are preferred when calibrating the model because the normal variability within a soil mapping unit causes errors. ALMANAC draws weather information from an independent weather input file, which can be imported from National Weather Service records or set up by the user for a specific site.

ALMANAC simulates daily, plant-available soil water contents in the rooting depth (SW, m m^{-1}; abbreviations shown here for parameters are consistent with their use in ALMANAC) based on the EPIC hydrology algorithm (Kiniry et al., 1992; Williams et al., 1989). The SW on a given day is the budget of surface runoff (Q, mm; modulated by runoff curve number, CN2), percolation below the root zone (PRK, mm), evapotranspiration (ET, mm), precipitation (RAIN, mm), and irrigation or precipitation of the previous day. The SW is an important variable for calculating most of the crop growth constraints such as plant-available soil water, aeration, N, and P. Consequently, the crop growth regulator factor (REG, the 0–1 fraction that constrains biomass growth) is sensitive to how soil-water status and hydrology are modeled.

2.2 | Field experiment description

Ashworth, Rocateli, West, Brye, and Popp (2017) describes the site, management, and experimental design in detail. In brief, a replicated field experiment was performed from 2009–2013 at the Arkansas Agricultural Research and Extension Center in Fayetteville (36°6′ N, 94°10′ W). The soil was mapped as Pickwick gravelly loam (fine-silty, mixed, semiactive, thermic Typic Paleudults; USDA, 2019). The study site

TABLE 2 ALMANAC soil input file parameters for soil attributes. Values are the parameters according to Pickwick gravelly loam, 3–8% slopes in the SSURGO database. Zero values are read as 'unknown value' by the ALMANAC model

Parameter	Description	Default value
NLAYER	Number of layers	5
HSG	Hydrologic soil group	B
SALB	Soil albedo	0.23
TSLA	Maximum number of soil layers	10
ZQT	Thickness layer, m	0
ZF	Minimum soil profile thickness, m	0
FFC	Initial soil water, m m^{-1}	0.75
WTMN	Maximum depth to water table, m	0
WTMX	Minimum depth to water table, m	0
WTBL	Initial depth to water table, m	0
XIDS	Soil weathering code	0
RFTT	Subsurface flow, days	0

Soil layer attributes		Soil layers				
LAYER	Layer number	1	2	3	4	5
Z	Depth of layer, m	0.10	0.20	0.38	0.61	0.80
BD	Soil bulk density, g cm^{-3}	1.40	1.40	1.40	1.53	1.55
U	Permanent wilt point, m m^{-1}	0.12	0.12	0.11	0.18	0.22
FC	Field capacity, m m^{-1}	0.27	0.27	0.26	0.31	0.32
SAN	Sand content, %	13.7	13.7	13.7	7.0	8.4
SIL	Silt content, %	69.3	69.3	69.3	64.5	53.1
WN	Organic N concentration, mg kg^{-1}	0	0	0	0	0
pH	Soil pH	5.0	5.0	5.0	5.0	5.0
SMB	Sum bases, cmol kg^{-1}	2.5	2.5	2.5	2.5	2.5
CBN	Organic carbon, %	1.03	1.03	0.60	0.18	0.18
CAC	Calcium carbonate, %	0	0	0	0	0
CEC	Cation exchange, cmol kg^{-1}	0	0	0	0	0
ROK	Coarse fragment, %	0	0	0	0	3
WNO3	Nitrate, mg kg^{-1}	0	0	0	0	0
AP	Labile P, mg kg^{-1}	0	0	0	0	0
RSD	Crop residue, Mg ha^{-1}	0	0	0	0	0
BDD	Bulk density dry, g cm^{-3}	1.46	1.46	1.46	1.60	1.63
PSP	P sorption ratio	0	0	0	0	0
SC	Saturated conductivity, mm h^{-1}	32.4	32.4	32.4	32.4	32.4
RT	Subsurface flow, d	0	0	0	0	0
WP	Organic P, g Mg^{-1}	0	0	0	0	0

was located in the Ozark Highlands ecoregion with an average annual precipitation of 1155 mm, average daily high and low temperatures of 20.2°C and 8.7°C, respectively (US Climate Data, 2019).

'Alamo' switchgrass was tested under 10 sequential clipping dates from May to February from 2009–2011 which comprised switchgrass in- and post-season to capture the complete growth and senescence phases. Sequential clipping was performed only from October to February in 2011–2013.

The data used to calibrate ALMANAC's soil water simulation were initial soil characteristics and nutrient concentrations, daily volumetric water content, and daily weather data. Initial characteristics, such as water pH (1:2 soil/water w/v ratio), extractable plant-available nutrients (P, K, Na, Fe, and Mg), and soil texture (sand, silt, and clay) were collected in 15-cm depth increments from the surface to 80 cm (Ashworth et al., 2017).

Soil volumetric water content profiles were measured throughout the experimental period from May 2009 to

TABLE 3 ALMANAC soil input file parameters for Trials 1 and 2 (Fayetteville, AR). Standard values are the parameters according to the ALMANAC database and the modified values are the parameters values according to initial soil analysis measured in field

Parameter	Description	Standard value					Modified value				
FFC	Initial soil water, m m^{-1}	0.75					1				
GSI[a]	Maximum stomatal conductance, m s^{-1}	7.4					3.3				
LAYER	**Layer number**	**1**	**2**	**3**	**4**	**5**	**1**	**2**	**3**	**4**	**5**
Z	Depth of layer, m	0.10	0.20	0.38	0.61	1.63	0.15	0.30	0.45	0.60	0.80
BD	Bulk density, g cm^{-3}	1.40	1.40	1.40	1.53	1.55	1.57	1.50	1.44	1.33	1.21
U	Permanent wilting point, m m^{-1}	0.12	0.12	0.11	0.18	0.22	0.04	0.07	0.14	0.19	0.24
FC	Field capacity, m m^{-1}	0.27	0.27	0.26	0.31	0.32	0.35	0.33	0.45	0.50	0.55
SAN	Sand content, %	13.7	13.7	13.7	7.0	8.4	40.9	35.3	30.1	21.0	12.0
SIL	Silt content, %	69.3	69.3	69.3	64.5	53.1	41.2	33.1	31.0	25	19
pH	Soil pH	5.0	5.0	5.0	5.0	5.0	5.8	6.1	6.1	5.5	4.8

[a]GSI, Crop input file parameter.

December 2012 using CS616 water content reflectometers (WCR; Campbell Scientific, Logan, UT) at depths of 15, 30, 45, and 80 cm. Eight WCRs were installed in each of two locations at opposite ends of the trial site for a total of 16 water content measurements. Sensors were connected to a CR10X datalogger (Campbell Scientific, Inc.) to record volumetric water contents at 4-h intervals (Ashworth et al., 2017).

Daily weather, such as total solar radiation, maximum and minimum air temperatures, relative humidity, and wind speed were acquired from the Arkansas Agricultural Research and Extension Center micro-meteorological weather station located less than 500 m from the trial site. Precipitation was recorded on-site daily using volumetric rain gauges.

2.3 | Model adjustments

The daily weather input file was generated using total solar radiation, precipitation, maximum and minimum air temperatures, relative humidity, and wind speed collected as previously described. The ALMANAC management input file was generated according to management described by Ashworth et al. (2017). All ALMANAC management input parameters are described in Table 1. Soil input was automatically generated by ALMANAC (2012 Version 1.0.3 Beta 2, ARS, 2019) based on the USDA-NRCS SSURGO database (Kiniry, Arnold, & Xie, 2002) according to longitude and latitude inputs (Table 2). The soil automatically selected by ALMANAC was Pickwick gravelly loam, 3–8% slopes, eroded. Finally, the crop input file parameters were the default 'Alamo' switchgrass values available in the ALMANAC crop file. The crop file also estimated potential evapotranspiration using the Penman–Monteith equation.

Pertinent soil inputs automatically generated by ALMANAC were modified according to the data collected prior to establishment. The values of SAN (sand in soil, % w/w) and SIL (silt in soil, % w/w) were modified according to in situ soil description for each soil depth. Bulk density values (BD, g cm^{-3}) for each depth were estimated based on clay and sand measurements using the Soil-Plant-Air-Water (SPAW) model (Saxton, 2007). According to Saxton and Rawls (2006), the SPAW model provides sufficiently accurate estimates for soil water infiltration, conductivity, storage, and plant-water relationships using statistical correlations between soil texture, soil water potential, and hydraulic conductivity.

The CN2 input parameter was used directly to estimate Q (mm), and used indirectly to calculate PRK. The two intermediate variables, Q and PRK, strongly affect SW, ET, and biomass simulations. Furthermore, the CN2 value was determined based on cover type (e.g., row crops, pasture, etc.), cover treatment (e.g., bare soil, residue cover, etc.), hydrologic condition (poor, fair, or good drainage), and hydrologic soil groups (A, B, C, or D). Hydrologic condition was based on specific on-site soil infiltration and runoff conditions, and the hydrologic groups were based on soil subsurface permeability and surface intake rates (Mockus, 2009). Furthermore, changes in SAN and SIL prompted us to test the suitability of CN2 default value based on changes caused by Q, PRK, and ET.

Other input parameters investigated were FFC (initial soil water, m m^{-1}), FC (soil field capacity, m m^{-1}), U (permanent wilting point, m m^{-1}), and GSI (m s^{-1}). The soil input parameters FFC, FC, and U were modified based on the observed SW at different soil depths. Finally, the value of GSI was modified to accurately simulate SW. According to Kiniry et al. (2005), finding an appropriate GSI parameter value for a specific location is critical for realistic SW simulation, especially in areas where soil moisture is limiting. Excessively large GSI values simulate greater ET, lower SW, and, consequently, lower biomass. Underestimation of SW triggers a lower value for the ALMANAC water stress factor, which reduces simulated biomass yield.

2.4 | Statistical analysis

Different model evaluation statistics were used to assess the goodness of fit of the simulated data with observed values. The first method was the Willmott agreement index (*d*-index) (Willmott et al., 1985) which quantifies the agreement between general trends in simulated and observed values. The *d*-index was estimated using Eq. (1):

$$d\text{-index} = 1 - \left[\frac{\sum_{i=1}^{n}\left(P_i - O_i\right)^2}{\sum_{i=1}^{n}\left(\left|P_i'\right| + \left|O_i'\right|\right)^2}\right] \quad 0 \le d \le 1 \qquad (1)$$

where n was the number of observations, P_i was the model-predicted value for the ith measurement, O_i was the observed value for the ith measurement, and $\bar{O}$ is the overall mean of the observed values. P_i' was $P_i - \bar{O}$, and O_i' was $O_i - \bar{O}$. The *d*-index varies between 0–1, with a value of 1 indicating perfect agreement between predicted and observed data. In all years, *d*-index values were calculated for contrasting default and calibrated SW simulations (P_i) with observed SW (O_i). Also, separate *d*-indexes were calculated for the calibrated model in 2011 and 2012 to analyze SW discrepancies. A separate $d\text{-index}_{senesce}$ accounting for the switchgrass senescence period (i.e., days from peak yield to dormancy), and a separate $d\text{-index}_{other}$ accounting for all other remaining days in both years, were calculated.

Another evaluation method used was the RMSE, estimated using Eq. (2):

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

Root mean square errors were calculated for all contrasting default (RMSE_{def}) and calibrated (RMSE_{cal}) SW simulations (P_i) with observed SW (O_i).

3 | RESULTS AND DISCUSSION

3.1 | Soil water content calibration

The measured values of BD, U, FC, SAN, SIL, and pH differed from the standard values from USDA-NRCS SSURGO data for 'Pickwick gravelly loam, 3–8% slopes' (Table 3). Therefore, measured data were used in the soil input file.

The curve number (CN2) crop parameters CN2A, CN2B, CN2C, and CN2D are the suggested runoff curve numbers for the hydrologic soil groups A, B, C, and D for switchgrass; and their values are 31, 59, 72, and 79, respectively. ALMANAC's preset runoff curve number for the Pickwick soil series was 59, which described this soil as in hydrologic soil group B.

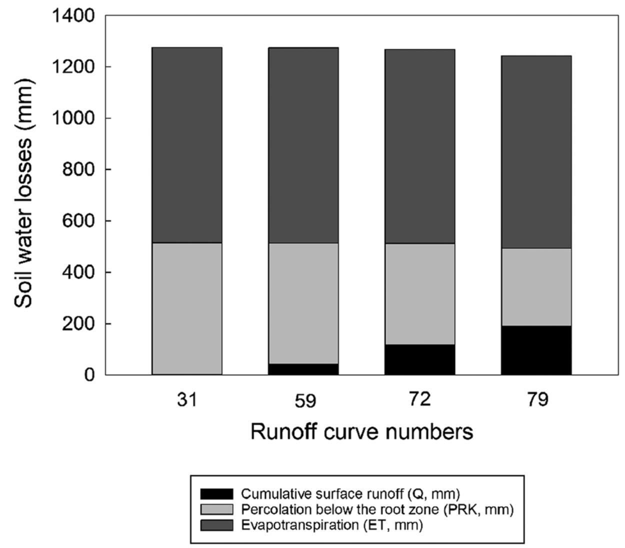

FIGURE 1 ALMANAC simulated soil water losses by runoff, percolation, and evapotranspiration for different runoff curve numbers at Fayetteville, AR

The soil description performed on site before planting showed that the actual soil texture, that is, SAN and SIL values, was different from the preset texture (Table 3). The soil texture for all pre-set soil layers was gravelly loam, whereas the actual soil texture of all soil layers were, on average, loam, clay loam, clay loam, clay loam, and clay, for the 0.15-, 0.30-, 0.45-, 0.60-, and 0.80-m soil depths. Soils in hydrologic group C typically contain between 20–40% clay and can have silt loam or loam textures. In contrast, soils in hydrologic group D have greater than 40% clay, less than 50% sand, and have clayey textures (Mockus, 2009). Therefore, the field-described soil fit as an intermediate between hydrologic groups C and D.

Analysis of the 2009 simulations for the different proposed switchgrass CN2 values showed cumulative Q outputs of 1, 41, 115, and 191 mm; and the cumulative PRK values were 514, 473, 397, 303 mm for CN2s 31, 59, 72, and 79, respectively (Figure 1). In addition, the 2009 cumulative ETs were 761, 760, 756, and 749 mm, respectively. Therefore, the total 2009 simulated soil water losses were 1276, 1274, 1269, and 1243 mm for CN2s 31, 59, 72, and 79, respectively. The different switchgrass CN2 values proposed for different hydrologic groups did not substantially change the total simulated soil water losses based on the analysis of 2009 simulations (Figure 1). There was an equivalent water-loss trade-off between Q and PRK along the range of CN2 values. Simulated ET values for the CN2 values were not substantially different which indicated that changes in CN2 values would not affect the soil-water-plant constraint factor. However, running ALMANAC with a large CN2 value of 79 reduced total simulated dry biomass to unrealistic values compared to Ashworth et al. (2017) results (data not shown). A large CN2 value leads to large Q, potentially large nitrate (NO_3^-) loss in surface runoff (YNO3, kg ha^{-1}), a large N-plant constraint factor, and consequently, low simulated total biomass accumulation. Therefore, the CN2 value of 72 was considered the most acceptable.

To improve the soil water simulation, values of U and FC were modified. Heavy rainfall was recorded on 22–30 May 2009 (347 mm) which likely resulted in field capacity or near soil saturation. The measured values were assumed to represent maximum SW and therefore were used as best estimates of field capacity. The maximum soil water contents were 0.35, 0.33, 0.45, 0.50 and 0.54 m^3 m^{-3}, for 0.15-, 0.30-, 0.45-, 0.60-, and 0.80-m depths, respectively, which were used to modify the FC parameter (Table 3). The minimum soil water contents were 0.04, 0.07, 0.14, 0.19, and 0.24 m^3 m^{-3} for the same soil depths, respectively. The low soil water contents occurred mostly in July 2010, owing to the lack of rainfall for 30 d and high plant water demand. During summer 2010, switchgrass started to show signs of stress such as chlorosis and senescence of lower leaves (Ashworth et al., 2017). According to Barney et al. (2009), lowland switchgrass cultivars such as Alamo start to exhibit severe reductions in biomass yield (75–80%) when soil water potential declines to −4.0 MPa. Biomass yield collected at its peak in 2011 was only 18% lower than the maximum achieved yield in 2010 (15.2 vs. 18.6 Mg ha^{-1}, data not shown); therefore, soil potentials, based on the minimum measured soil water contents, were likely greater than −4.0 MPa. For this reason, it was assumed that the U values for each layer were equal to the minimum observed SW readings. Therefore, the U values of 0.04, 0.07, 0.14, 0.19, and 0.24 m m^{-1} were selected for the 0.15-, 0.30-, 0.45-, 0.60-, and 0.80-m soil depths, respectively. The value of the FFC parameter was considered to be 1, which meant that the first simulated day had a SW set to field capacity.

The soil water simulation was partially improved after inputting actual weather data and modifying pertinent soil parameters listed above (partial results not shown). However, at this point, the simulated SW underestimated actual SW during July to September 2011 and 2012. The total default simulated ET for the 2009, 2010, 2011, and 2012 growing seasons were 532, 643, 420, and 454 mm, respectively. These simulated ET values were greater than those reported by McIsaac, David, and Mitchell (2010), wherein total annual ET from 'Cave-In-Rock' switchgrass during the growing season in Urbana, IL ranged from 258–359 mm across the 4-yr study.

The default GSI was 7.4 10^{-3} m s^{-1}, which was derived from the EPIC model. Large GSI values result in large ET and, consequently, increased plant water use (Kiniry et al., 2005). Testing different GSI values via trial and error yielded a value of 3.3 10^{-3} m s^{-1} as that which best improved SW simulations to levels shown in Figure 2. In addition, the reduction in the GSI parameter value decreased simulated ET during the growing season to 253, 331, 297, and 390 mm for 2009, 2010, 2011, and 2012, respectively.

3.2 | Soil water simulation: Calibrated vs. default model

The calibrated simulated daily SW output for 2009–2012 was based on all modified soil input parameters to the 0.8-m depth, modified GSI, and actual weather data and compared with the default ALMANAC model output. Overall, the calibrated model performed more accurate SW simulations than the default, in that the latter model consistently underestimated SW in all years (Figure 2). Improved SW simulations were achieved with the calibrated model because key soil input parameter values were adjusted based on in situ soil sampling and measurements that better represented actual soil conditions than estimated conditions (Table 3). Even though calibration drastically improved SW simulation, the calibrated model accuracy varied among years. In 2009, the average observed, default, and calibrated SW contents were, respectively, 0.28, 0.07, and 0.27 m^3 m^{-3}. The corresponding *d*-indexes were 0.28 for default and 0.94 for the calibrated model. Similar results were observed in 2010 in which the average observed, default, and calibrated SW were 0.27, 0.08, and 0.29 m^3 m^{-3}, respectively. The 2010 default and calibrated models, respectively, underestimated and accurately simulated SW year-round. The *d*-index values for default and calibrated models in 2010 (0.30 and 0.89, respectively) were also similar to the values in 2009.

In subsequent years, the calibrated model was still more accurate than the default; however, its accuracy was lower than in 2009 and 2010. In 2011, the average observed, default, and calibrated SW contents were 0.28, 0.08, and 0.24 m^3 m^{-3}, respectively. The corresponding 2011 *d*-indexes were 0.40 for the default and 0.83 for the calibrated model. Finally, in 2012, the average observed, default, and calibrated SW contents were 0.26, 0.07, and 0.22 m^3 m^{-3}, respectively. The corresponding 2012 *d*-indexes were 0.41 for the default and 0.81 for the calibrated models. Even though SW averages and *d*-indexes calculated for the calibrated model still demonstrated a more accurate overall simulation than the default model in 2011 and 2012, the simulated values did not agree with observed SW during some specific periods. Calibrated SW simulation values were much lower than observed values during switchgrass senescence, that is, from peak yield to dormancy which occurred from July to October in 2011 and 2012 (Figure 2c,d). To quantify the SW discrepancies, separate *d*-indexes for the calibrated model were calculated for the senescence period (d-index$_{senesce}$) and for the combined remaining months (d-index$_{other}$) in 2011 and 2012. The corresponding separate d-index$_{senesce}$ for 2011 and 2012 were 0.48

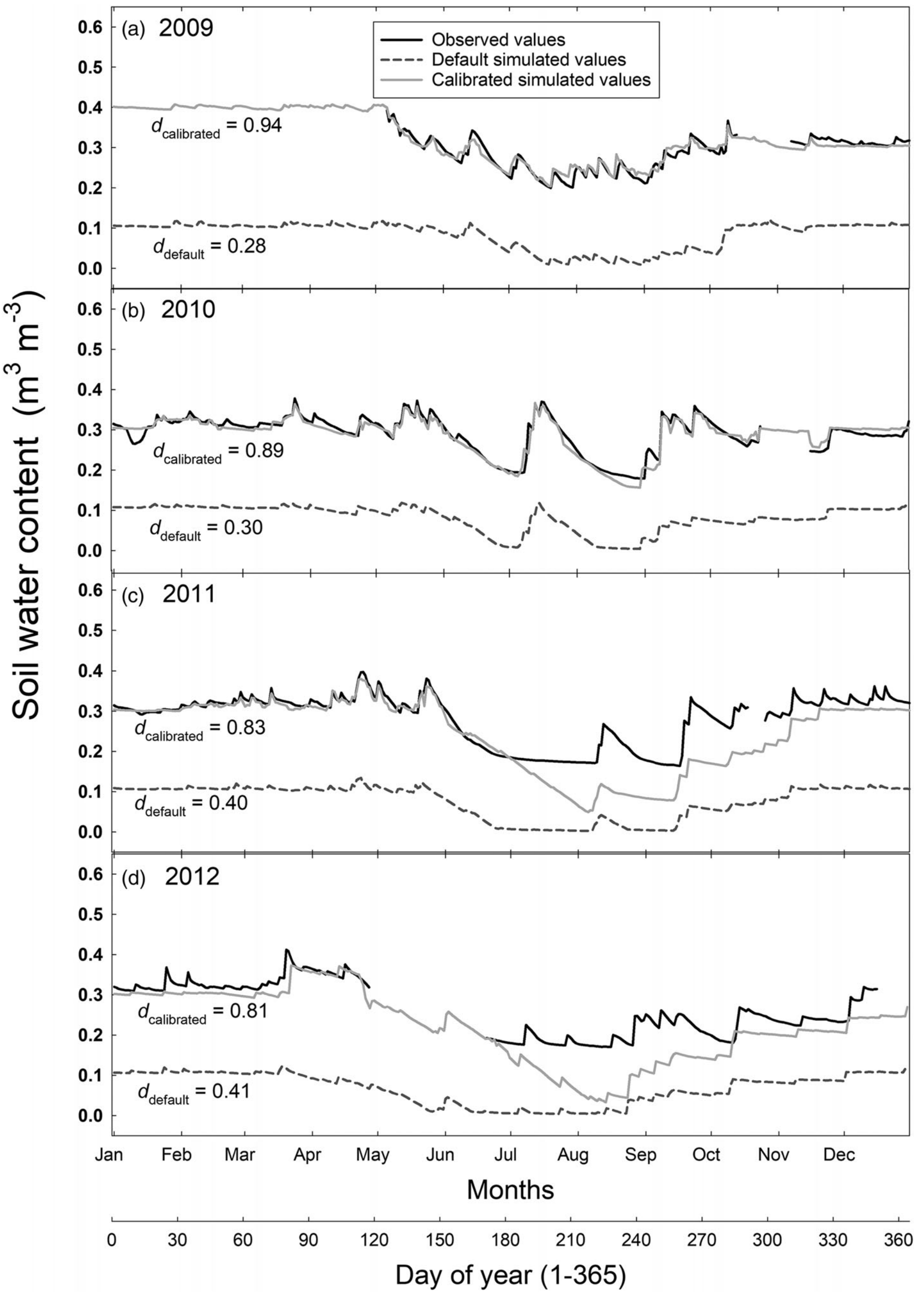

FIGURE 2 Observed, default, and calibrated soil volumetric water content simulated by ALMANAC in 2009 (a), 2010 (b), 2011 (c), and 2012 (d) seasons for a switchgrass field located at Fayetteville, AR. The *d* values are Willmott agreement indices

and 0.35, respectively. Furthermore, the separate d-index$_{other}$ values were 0.87 and 0.91 in 2011 and 2012, respectively, which were equivalent to the accurate 2009 and 2010 d-index values. Therefore, it was conclusive that model modifications during the senescence period were less effective than during the rest of the season which was likely the primary cause of lower overall 2011 and 2012 d-index values.

Relatively ineffective calibration during senescence also explained the larger RMSE values calculated for the calibrated model ($RMSE_{cal}$) in 2011 and 2012 (Figure 3). The $RMSE_{cal}$ values were 0.014 m^3 m^{-3} in 2009 and 2010, and 0.059 and 0.065 m^3 m^{-3} in 2011 and 2012, respectively (Figure 3). Even though the inaccurate, low-simulated SW values during senescence increased the error between the calibrated model and the observed values in 2011 and 2012, the calibrated model still had an improved relationship with the observed values compared to the default model. The RMSE for the default model ($RMSE_{def}$) were 0.219, 0.210, 0.208, and 0.198 in 2009, 2010, 2011, and 2012, respectively.

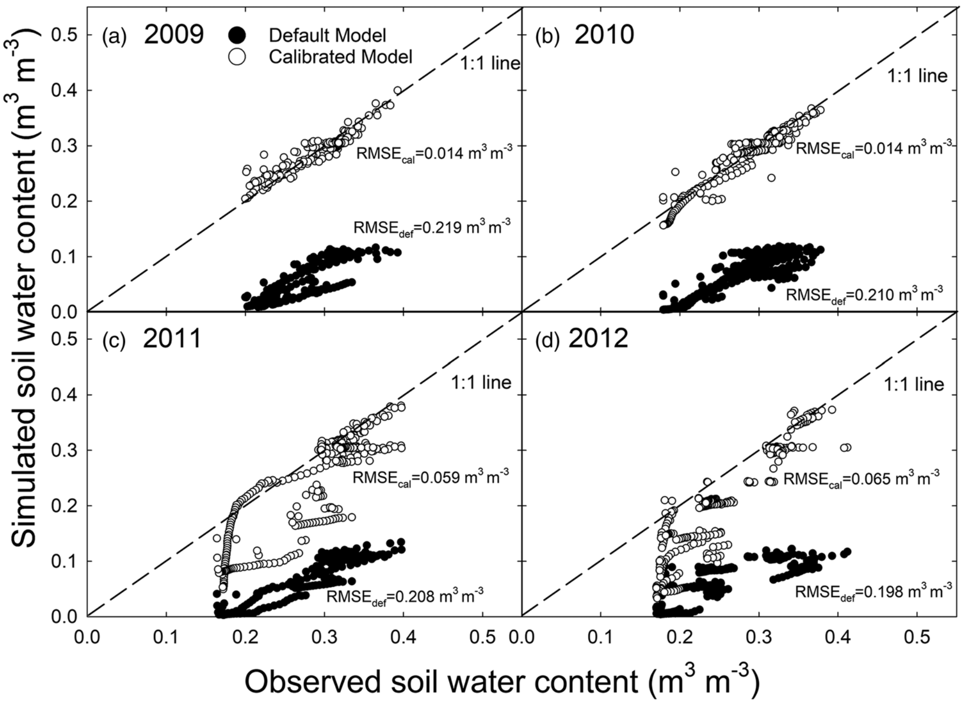

FIGURE 3 A comparison of simulated vs. observed soil water contents values for the default and calibrated ALMANAC model in 2009 (a), 2010 (b), 2011 (c), and 2012 (d). Statistic shown is root mean square error for default ($RMSE_{def}$) and calibrated ($RMSE_{cal}$) models

3.3 | Model performance and limitations

The default model underestimated SW for all years which demonstrated the inaccuracy of the SSURGO database when used for a specific site. The SSURGO database was developed for parcel, township, or county levels, which contain map scales ranging from 1:12,000 to 1:63,360 (USDA-NRCS, 2019b); therefore the SSURGO database is recommended for uses such as developing erosion practices and land use potential at a watershed scale rather than site-specific crop-growth-model calibrations. However, the ALMANAC model was able to accurately predict SW after site-specific soil parameter values for FFC, BD, U, FC, SAN, and SIL were used. Efforts must focus on collecting site-specific data that improve model parameters to refine ALMANAC SW simulations. Even though calibration of the listed parameters greatly improved overall SW simulation, the 2011 and 2012 simulated values from day of year 183–283 underestimated actual SW. One plausible explanation was the greater total precipitation during the growing season (May–Oct.) in 2009 (906 mm) and 2010 (782 mm) compared with that in 2011 (516 mm) and 2012 (422 mm). Furthermore, the 2009 and 2010 rainfall was evenly distributed during the growing seasons. Conversely, low precipitation, such as 37 and 12 mm, was measured from 28 May to 9 August in 2011 (74 d) and from 28 June to 13 August in 2012, respectively. The SW underestimation coincided during these two short drought periods and carried forward through October. Switchgrass can decrease its evapotranspiration during drought periods, which decreases soil water losses (McIsaac et al., 2010). The dynamic of switchgrass attenuating its evapotranspiration during periods of differential soil water availability is not currently modeled by ALMANAC. Conversely, the GSI parameter is a fixed value irrespective of changes in soil water availability to the modeled crop, which limits the simulation of ET during dry periods. Nevertheless, the modified parameters resulted in overall improved soil water simulation, as shown by close matching of observed and simulated values.

3.4 | Conclusions and recommendations

Simulation of soil water content in ALMANAC can be improved by using site-specific soil input, where FFC, BD, U, FC, SAN, and SIL were considered the most influential soil parameters. The model was limited in simulating accurate soil water content during extended drought periods. This limitation was related to the GSI crop parameter, which demands a more representative value, especially for drought-resistant plants such as switchgrass. Therefore, efforts should focus on quantifying stomatal conductance dynamics of drought-resistant plants to further improve soil-plant simulations.

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REFERENCES

Agricultural Research Service. (2019). ALMANAC simulation model. Release 1.0.18. Agricultural Research Service, Temple, TX. Retrieved from https://www.ars.usda.gov/plains-area/temple-tx/grassland-soil-and-water-research-laboratory/docs/193226/ (accessed 10 Oct. 2019).

Ashworth, A. J., Rocateli, A. C., West, C. P., Brye, K. R., & Popp, M. P. (2017). Switchgrass growth and effects on biomass accumulation, moisture content, and nutrient removal. *Agronomy Journal*, *109*, 1359–1367. https://doi.org/10.2134/agronj2017.01.0030

Barney, N. B., Mann, J. J., Kyser, G. B., Blumwald, E., Deynze, A. V., & DiTomazo, J. M. (2009). Tolerance of switchgrass to extreme soil moisture stress: Ecological implications. *Plant Science*, *177*, 724–732. https://doi.org/10.1016/j.plantsci.2009.09.003

Behrman, K. D., Keitt, T. H., & Kiniry, J. R. (2014). Modeling differential growth in switchgrass cultivars across the central and southern Great Plains. *BioEnergy Research*, *7*, 1165–1173. https://doi.org/10.1007/s12155-014-9450-8

Butler, T. J., Stein, J. D., Pittman, J. J., & Interrante, S. M. (2016). Seedbed preparation and planting depth affect switchgrass establishment and yield. *Crop, Forage Turfgrass Manage*, *2*, 1–6. https://doi.org/10.2134/cftm2016.0012

Cahill, N., Popp, M., West, C., Rocateli, A., Ashworth, A., Farris, R., Sr., & Dixon, B. (2014). Switchgrass harvest time effects on nutrient use and yield: An economic analysis. *Journal of Agricultural and Applied Economics*, *46*, 487–507. https://doi.org/10.1017/S1074070800029060

Cassida, K. A., Muir, J. P., Hussey, M. A., Read, J. C., Venuto, B. C., & Ocumpaugh, W. R. (2005). Biofuel component concentrations and yields of switchgrass in south central US environments. *Crop Science*, *45*, 682–692. https://doi.org/10.2135/cropsci2005.0682

Kiniry, J. R., Arnold, J. G., & Xie, Y. (2002). Applications of models with different spatial scales. In L. R. Ahuja, L. Ma, & T. A. Howell (Eds.), *Agricultural system models in field research and technology transfer* (pp. 207–227). Boca Raton, FL: Lewis Publishers.

Kiniry, J. R., Cassida, K. A., Hussey, M. A., Muir, J. P., Ocumpaugh, W. R., Read, J. C., … Williams, J. R. (2005). Switchgrass simulation by the ALMANAC model at diverse sites in the southern US. *Biomass Bioenergy*, *29*, 419–425. https://doi.org/10.1016/j.biombioe.2005.06.003

Kiniry, J. R., Sanderson, M. A., Williams, J. R., Tischler, C. R., Hussey, M. A., Ocumpaugh, W. R., … Reed, R. L. (1996). Simulating Alamo switchgrass with the ALMANAC model. *Agronomy Journal*, *88*, 602–606. https://doi.org/10.2134/agronj1996.00021962008800040018x

Kiniry, J. R., Williams, J. R., Gassman, P. W., & Debaeke, P. (1992). A general, process-oriented model for two competing plant species. *Transactions of the ASAE*, *35*, 801–810. https://doi.org/10.13031/2013.28665

Langholtz, M. H., Stokes, B. J., & Eaton, L. M. (2016). 2016 Billion-Ton Report: Advancing domestic resources for a thriving bioeconomy, ORNL/TM-2016/160. US Department of Energy, Washington DC. https://doi.org/10.2172/1271651

Lindsay, K. R., Popp, M. P., West, C. P., Ashworth, A. J., Rocateli, A. C., Farris, R., … Acosta-Gamboa, L. (2018). Predict harvest time effects on switchgrass moisture content, nutrient concentration, yield, and profitability. *Biomass Bioenergy*, *108*, 74–89. https://doi.org/10.1016/j.biombioe.2017.09.017

McIsaac, G. F., David, M. B., & Mitchell, C. A. (2010). Miscanthus and switchgrass production in central Illinois: Impacts on hydrology and inorganic nitrogen leaching. *Journal of Environment Quality*, *39*, 1790–1799. https://doi.org/10.2134/jeq2009.0497

McLaughlin, S. B., & Walsh, M. E. (1998). Evaluating environmental consequences of producing herbaceous crops for bioenergy. *Biomass Bioenergy*, *14*, 317–324. https://doi.org/10.1016/S0961-9534(97)10066-6

Mockus, V. (2009). Hydrologic soil groups. In J. Werner, D. E. Woodward, R. Nielsen, R. Dobos, A. Hjelmfelt, & C. C. Hoeft (Eds.), *NRCS national engineering hanbook part 630* (pp. 7-i–7-5). Washington, DC: United States Department of Agriculture.

Saxton, K. E. (2007). SPAW Soil – Plant – Atmosphere – Water Field & Pond Hydrology field and pond hydrology. Release 6.02.75. Agricultural Research Service in cooperation with Department of Biological System Engineering at Washington State University, Pullman, WA. Retrieved from https://hrsl.ba.ars.usda.gov/SPAW/Index.htm (accessed 2 Oct. 2019).

Saxton, K. E., & Rawls, W. J. (2006). Soil water characteristics estimates by texture and organic matter for hydrologic solutions. *Soil Science Society of America Journal*, *70*, 1569–1578. https://doi.org/10.2136/sssaj2005.0117

Tulbure, M. G., Wimberly, M. C., Boe, A., & Owens, V. N. (2012). Climatic and genetic controls of yields of switchgrass, a model bioenergy species. *Agriculture, Ecosystems & Environment*, *146*, 121–129. https://doi.org/https://doi.org/10.1016/j.agee.2011.10.017

US Climate Data. (2019). Climate Fayetteville– Arkansas. Retrieved from https://www.usclimatedata.com/climate/fayetteville/arkansas/united-states/usar0189 (accessed 7 Feb. 2019).

USDA. (2019). Pickwick gravelly loam (n.d.). Official Series Description (OSD). Retrieved from https://soilseries.sc.egov.usda.gov/osdname.aspx (accessed 7 Feb. 2019).

US EPA. (2019). Renewable fuel standard program. Retrieved from https://www.epa.gov/renewable-fuel-standard-program (accessed 7 Feb. 2019).

USDA-NRCS. (2019a). County Levels Soil Surveys in Digital Format–SSURGO. Retrieved from https://www.nrcs.usda.gov/wps/portal/nrcs/detail/soils/survey/office/ssr12/tr/?cid=nrcs142p2_010596 (accessed 2 Oct. 2019).

USDA-NRCS. (2019b). Description of SSURGO Database. Retrieved from https://www.nrcs.usda.gov/wps/portal/nrcs/detail/soils/survey/?cid=nrcs142p2_053627 (accessed 2 Oct. 2019).

Wetzstein, M. E. (2010). Should we invest in biofuel? *Journal of Agricultural and Applied Economics*, *42*, 395–401. https://doi.org/10.1017/S1074070800003576

Williams, J. R., Jones, C. A., Kiniry, J. R., & Spanel, D. A. (1989). The EPIC crop growth model. *Transactions of the ASAE*, *32*, 497–511. https://doi.org/10.13031/2013.31032

Willmott, C. J., Ackleson, S. G., Davis, R. E., Feddema, J. J., Klink, K. M., Legates, D. R., … Rowe, C. M. (1985). Statistics for the evaluation and comparison of models. *Journal of Geophysical Research, Oceans*, *90*, 8995–9005. https://doi.org/10.1029/JC090iC05p08995

Zaibon, S., Anderson, S. H., Kitchen, N. R., & Haruna, S. I. (2016). Hydraulic properties affected by topsoil thickness in switchgrass and corn-soybean cropping systems. *Soil Science Society of America Journal*, *80*, 1365–1376. https://doi.org/10.2136/sssaj2016.04.0111

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