PROGRESS TOWARD EVALUATING THE SUSTAINABILITY OF SWITCHGRASS AS A BIOENERGY CROP USING THE SWAT MODEL

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ABSTRACT. Adding bioenergy to the U.S. energy portfolio requires long-term profitability for bioenergy producers and long-term protection of affected ecosystems. In this study, we present steps along the path toward evaluating both sides of the sustainability equation (production and environmental) for switchgrass (Panicum virgatum) using the Soil and Water Assessment Tool (SWAT). We modeled production of switchgrass and river flow using SWAT for current landscapes at a regional scale. To quantify feedstock production, we compared lowland switchgrass yields simulated by SWAT with estimates from a model based on empirical data for the eastern U.S. The two produced similar geographic patterns. Average yields reported in field trials tended to be higher than average SWAT-predicted yields, which may nevertheless be more representative of production-scale yields. As a preliminary step toward quantifying bioenergy-related changes in water quality, we evaluated flow predictions by the SWAT model for the Arkansas-White-Red river basin. We compared monthly SWAT flow predictions to USGS measurements from 86 subbasins across the region. Although agreement was good, we conducted an analysis of residuals (functional validation) seeking patterns to guide future model improvements. The analysis indicated that differences between SWAT flow predictions and field data increased in downstream subbasins and in subbasins with higher percentage of water. Together, these analyses have moved us closer to our ultimate goal of identifying areas with high economic and environmental potential for sustainable feedstock production.

Keywords. Bioenergy, Functional validation, River flow, Sensitivity analysis, Sustainability, Switchgrass, Water quality.

Long-term sustainability of the nascent bioenergy industry is influenced by several factors. These include economic feasibility and concerns over environmental impacts (Simpson et al., 2008; Simpson, 2009). Switchgrass (Panicum virgatum L.) is a native grass that has high potential as a sustainable dedicated energy crop (Sanderson et al., 1996; McLaughlin and Kszos, 2005). According to Hall (1997), biomass productivity is an important aspect determining the long-term economic feasibility of bioenergy. Unfortunately, there are only a limited number of field sites where dedicated energy-crop production has been measured. Estimates of production for a wide range of regions and a variety of growing conditions are essential to provide more accurate spatial estimates of bioenergy resource potential. Because they are capable of extrapolating to new locations, mechanistic plant growth models are well-suited for this purpose (Williams et al., 1989; McMaster et al., 2005; Johnson et al., 2009).

A second aspect of long-term sustainability of bioenergy is the protection of soil, water, and biodiversity associated with emerging bioenergy landscapes (Graham et al., 1996). The widespread degradation of water quality associated with agriculture is well documented (e.g., Carpenter et al., 1998; USEPA, 2009). It is therefore likely that cultivation of switchgrass, a deep-rooted perennial grass, on agricultural lands previously supporting row crops can improve water quality by reducing sediment and nutrient loadings to streams (Graham et al., 1996). Projecting how changes in the agricultural landscape will influence water quality is a complex issue that requires an appropriate modeling tool capable of representing important aspects of the question.

Quantifying energy crop production and ecological effects on aquatic ecosystems at large regional spatial extents requires crop and watershed modeling in response to geographic variation in climate. Our choice of a model depended on two factors: (1) its ability to predict both the yields of bioenergy crops and crop residues, and (2) its ability to represent watershed influences on water quality at regional spatial scales. Working at a regional scale placed a number of constraints on our choices. First, although bioenergy land covers are the focus of our research, other land covers also influence water quality. Therefore, we required a model that could simulate watershed influences of natural, agricultural, and urban land as well as bioenergy crops. Second, we
required a model capable of using spatially explicit input data that are generally available throughout the conterminous U.S. Third, we required a model capable of representing watershed influences on water quality at relatively coarse spatial scales consistent with the resolution of national GIS input datasets. The size of subwatersheds used in the modeling was limited by the ability to process high-resolution digital elevation models and in the inherent resolution of satellite-derived spatial data. Fourth, tile drainage can adversely impact water quality in rivers draining agricultural lands by providing a preferential flow pathway for nitrates (Zhao et al., 2001). The ability to represent tile drains has been shown to improve flow predictions in agricultural regions (Green et al., 2006). These four requirements for a tool to quantify yields of bioenergy crops and water quality effects at regional to national scales were addressed by the Soil and Water Assessment Tool (SWAT). The large user community and widespread application and testing is another advantage of the SWAT model (Gassman et al., 2007). Although applications of SWAT to large, regional river basins are much less common than those for smaller spatial areas (e.g., Vache et al., 2002; Nelson et al., 2006), the model has been used to represent larger areas (e.g., the Upper Mississippi River basin; Arnold et al., 2000).

This article describes our efforts to advance research from two directions, addressing aspects of sustainability related to energy and environment. These advances are part of a larger framework of sustainability research designed to understand how much bioenergy is likely to be added to agricultural landscapes (top of fig. 1) and how these changes will affect water quality (bottom of fig. 1). Two goals of this research effort were (1) geographic modeling of potential production of a bioenergy crop and (2) producing and validating SWAT predictions of water quantity (flow). To address our first goal, we implemented switchgrass as a perennial crop and used the SWAT model to quantify potential growth of switchgrass in the U.S. The results provide valuable information toward understanding switchgrass growth potential and resource availability over a large spatial extent. In addition, our yield estimates can be used to predict where growing switchgrass will be economically feasible and to forecast where switchgrass is likely to replace other crops in future agricultural landscapes (top right in fig. 1). We focused our analysis on Alamo, a lowland variety of switchgrass, in its natural range, the eastern U.S. (Parrish and Fike, 2005).

A critical aspect of validating water quality predictions is to ensure that the processes controlling stream flow are represented adequately. In the second part of this article, we describe our efforts to implement, calibrate, and validate stream flow predictions of the SWAT model for the Arkansas-White-Red (AWR) River basin. We conducted a functional validation of SWAT flow predictions. The philosophy of functional validation is not to “validate” or pass judgment on a model but rather to analyze residual patterns to gain constructive guidance for further model improvement (Jager et al., 2000). Future research will build on these efforts to simulate and compare water quality in current landscapes and future landscapes that include switchgrass where it is economically feasible (fig. 1). Using future bioenergy landscapes projected by the economic model (top right of fig. 1) as input, we will simulate future water quality from the calibrated and validated SWAT model for each region. Ultimately, this approach will help to quantify changes in water quality in surface waters as energy crops are added to the landscape (bottom middle of fig. 1). Only by evaluating both the energy and environmental implications of landscape changes can informed decisions about bioenergy policy be made, leading toward a sustainable energy future.

**METHODS**

We used the ArcSWAT version of SWAT2005 for our analyses (Neitsch et al., 2005). Although the SWAT model was used in both our characterization of potential feedstock production and our validation of water quantity, methods for the two components of our larger research effort differ substantially. For example, whereas the assessment of potential production was easily accomplished for most of the conterminous U.S., evaluation of SWAT-predicted water quantity required smaller geographic regions. Therefore, this article focuses on water quantity predictions for one large river basin. Methods for each of these components are described in two sections below.

**BIOENERGY FEEDSTOCK PRODUCTION**

Predicting the amount of switchgrass produced requires knowing two things: (1) where lands will be converted to grow switchgrass, and (2) how much switchgrass will be produced on those lands. The goal of this analysis was to address the second question for the conterminous U.S. based on soil, slope, and climate.

To implement the SWAT model, we delineated subbasins for each major river basin in the eastern U.S. (New England, Mid-Atlantic, South Atlantic-Gulf, Great Lakes, Ohio, Lower Mississippi, Texas-Gulf, Arkansas-White-Red, Missouri, Upper Mississippi, Souris-Red-Rainy, and Rio-Grande) using a 1 km resolution digital elevation model (DEM) based on shuttle radar topography mission (SRTM) data (Farr et al., 2007). We identified larger, mainstem reaches from the National Hydrologic Dataset (NHDPlus) (thinnered in NHDPlus, 2009) and superimposed this stream network on the DEM before delineating subbasins with an average size of 500,000 ha.
Switchgrass yields were simulated using SWAT for hydrologic response units (HRUs) within each subbasin. An HRU is a unique combination of subbasin, land cover, soil, and slope class. For the purpose of obtaining regional estimates of switchgrass yield, we created two land-cover classes within each subregion by reclassifying all land-cover classes other than water in the 30 m resolution 2001 National Land Cover Dataset (Homer et al., 2004) to Alamo switchgrass. The reclassified land cover had two classes (switchgrass and water), which helped create a national-scale map of potential yield of switchgrass within its natural range. Soil characteristics were defined by the STATSGO dataset (Soil Survey Staff, 1994). We defined three slope classes, slopes of 0% to 3%, 3% to 5%, and greater than 5%, based on the 1 km resolution SRTM data. All HRUs created using the above described land cover, soil, and slope data were used in the SWAT runs, regardless of area.

The default parameters for Alamo switchgrass (lowland ecotype) were used in our simulations, with a few modifications. Because switchgrass is a perennial grass, lands planted in switchgrass were initialized as mature stands with a leaf area index of 0.5, initial biomass of 500 kg ha\(^{-1}\), and 3 m rooting depth (Parrish and Fike, 2005). Each year, we assumed that switchgrass required 1,100 physiological heat units (degree-days °C above a base temperature) to reach maturity. This value is at the low end of values reported in the literature for switchgrass. Growth parameters included radiation use efficiency of 47 kg MJ\(^{-1}\), base temperature of 12°C, and an optimal temperature for growth of 25°C (Kiniry et al., 2005). Growth is simulated by increasing the leaf area index over the growing season from the initial value of 0.5 to a maximum potential value, BLAI = 6.0 (if there is no water or nutrient stress), followed by a decrease during senescence. To allow for crop drying, we delayed harvesting until reaching 120% of heat units required to reach maturity and harvested 80% of above-ground biomass each year.

Switchgrass is known to have low nutrient requirements, but variability among studies and site-to-site variation has prevented a consensus from emerging on best management practices for nutrients (Parrish and Fike, 2005). We allowed SWAT to automatically apply nitrogen fertilizer whenever plants experienced nutrient stress that reduced growth by more than 0.85 of its potential. Use of the automatic fertilizer routine allowed us to account for geographic and site-specific differences in nutrient requirements, which are currently unknown.

We simulated mature, lowland switchgrass yields using SWAT for 21 years using simulated climate. We treated the first two years of the model run as spin-up years and averaged predicted switchgrass yields over the remaining 19 years. The average switchgrass yield for each hydrologic response unit was then mapped. To evaluate SWAT predictions of switchgrass yield, we compared geographic patterns with those of an empirical model developed by Jager et al. (2010) to describe yields from published field trials (Davis, 2007; Gunderson et al., 2008). For the lowland ecotype, field trials were available from studies over many years at 28 locations ranging from Texas to New Jersey. The empirical model used to predict yield included climate variables (average and minimum annual temperature, average annual precipitation, an interaction between average temperature and precipitation, all in the year of harvest) as well as management variables (harvest frequency and stand age), as described by Jager et al. (2010). A mixed modeling approach was used to account for spatial correlation among yields measured in the same geographic area.

**WATER QUANTITY (FLOW)**

We followed a series of steps to set the SWAT modeling environment validated toward reaching our eventual goal of projecting changes in water quantity and quality associated with a bioenergy landscape. These include (1) SWAT model implementation, (2) sensitivity analysis and calibration of stream flow on SWAT parameters in smaller subbasins, and (3) functional validation at a regional scale. Each of these steps is described below.

**SWAT Model Implementation**

We used USGS-defined 8-digit hydrologic units (HUC8) obtained from NHDPlus as subbasins instead of SWAT-delineated subbasins. Because SWAT requires one major stream reach per subbasin, we used the following procedure to derive main reaches from NHDPlus data. Within each subbasin, we identified the collection of reaches sharing the largest stream order to produce one stream feature per subbasin, as required by SWAT. To identify the main channel, we selected the collection of reaches sharing the smallest value of an NHDPlus code (levelpathi) identifying the mouth of each stream network. Finally, we combined the final set of reaches in each subbasin to produce a single stream feature.

HRUs were defined by unique combinations of land-cover categories, STATSGO map units, and slope categories, where only those land cover and soil units comprising more than 10% of a subbasin were included. The 2008 crop data layer (CDL-08) was used to define land cover, substituting 2001 NLCD for one state (New Mexico) lacking CDL-08 data. We assigned CDL land-cover categories to SWAT land cover. Because of the large spatial extent of the AWR basin, we reclassified a 30 m digital elevation model (DEM) to 56 m, which also matched the resolution of the CDL land-cover data. Using the 56 m DEM, we categorized slope into three categories: <2%, 2% to 5%, and >5%. Because even small areas of steep exposed soils can lead to considerable erosion, we included all three slope categories in the definition of HRUs, regardless of area.

Tile drainage is common in agricultural areas of the Midwestern U.S., including the AWR basin. The presence of tile drains can have important effects on water quality. To model the geographic distribution of tile drains, we assumed that tile drainage was present in cropland areas with poorly drained soils and with less than 2% slope. We identified the poorly drained soils using the dominant hydrologic group of the STATSGO map units. Soils with a hydrologic group of C or D are known to have slow infiltration rates (USDA, 1994) and were selected to apply tile drainage parameters. For HRUs with tile drainage, we assumed that tiles were located at a depth of 1.1 m and drained over a period of 36 h.

Because flow prediction is sensitive to local variations in precipitation, we assembled climate data from DAYMET (Thornton et al., 1997) to estimate climate for the center of each subbasin over the period 1980 to 2003. Daily climate drivers for the SWAT model included were total precipitation (mm), minimum and maximum temperatures (°C), and solar radiation (MJ m\(^{-2}\) d\(^{-1}\)). Wind speed, relative humidity, and potential evaporation were simulated by SWAT.
Table 1. Results from sensitivity analysis and autocalibration of stream flow parameters for two subbasins.

| Parameter Code | Parameter Description                                      | Sensitivity Analysis Ranking | Parameter Variation Method[a] | Parameter Changes for Basin 1 | parameter Changes for Basin 2 | Average
<table>
<thead>
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<tbody>
<tr>
<td>Alpha_B0[b]</td>
<td>Baseflow alpha factor (d⁻¹)</td>
<td>1</td>
<td>1</td>
<td>0.06</td>
<td>0.06</td>
<td>0.06</td>
</tr>
<tr>
<td>Blai</td>
<td>Maximum potential leaf area index</td>
<td>6</td>
<td>8</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>Canmx[b]</td>
<td>Maximum canopy storage (mm)</td>
<td>4</td>
<td>10</td>
<td>0.14</td>
<td>0.00</td>
<td>0.07</td>
</tr>
<tr>
<td>Ch_K2[b]</td>
<td>Channel effective hydraulic conductivity (mm h⁻¹)</td>
<td>7</td>
<td>7</td>
<td>6.86</td>
<td>8.06</td>
<td>7.46</td>
</tr>
<tr>
<td>Cn2</td>
<td>Initial SCS CN II value</td>
<td>8</td>
<td>1</td>
<td>-0.34</td>
<td>4.73</td>
<td></td>
</tr>
<tr>
<td>Epco</td>
<td>Plant uptake compensation factor</td>
<td>11</td>
<td>1</td>
<td>0.44</td>
<td>NA</td>
<td></td>
</tr>
<tr>
<td>Gw_Delay</td>
<td>Groundwater delay (d)</td>
<td>12</td>
<td>2</td>
<td>NA</td>
<td>9.84</td>
<td></td>
</tr>
<tr>
<td>Esc0[b]</td>
<td>Soil evaporation compensation factor</td>
<td>2</td>
<td>2</td>
<td>0.80</td>
<td>0.01</td>
<td>0.41</td>
</tr>
<tr>
<td>Gwqmm</td>
<td>Threshold water depth in the shallow aquifer for (mm)</td>
<td>5</td>
<td>9</td>
<td>503.76</td>
<td>-868.14</td>
<td></td>
</tr>
<tr>
<td>Revapmm</td>
<td>Threshold water depth in the shallow aquifer for “revap” (mm)</td>
<td>3</td>
<td>12</td>
<td>-95.58</td>
<td>99.81</td>
<td></td>
</tr>
<tr>
<td>Sol_Awc</td>
<td>Available water capacity (mm H2O mm⁻¹ soil)</td>
<td>11</td>
<td>3</td>
<td>2.03</td>
<td>-21.03</td>
<td></td>
</tr>
<tr>
<td>Sol_Z</td>
<td>Soil depth (mm)</td>
<td>10</td>
<td>6</td>
<td>-3.18</td>
<td>24.95</td>
<td></td>
</tr>
<tr>
<td>Surlag[b]</td>
<td>Surface runoff lag time (d)</td>
<td>9</td>
<td>5</td>
<td>1.79</td>
<td>1.00</td>
<td>1.40</td>
</tr>
</tbody>
</table>

[a] 1 = replacement of initial parameter by value, 2 = adding value to initial parameter, and 3 = multiplying initial parameter by 1 + value.
[b] Parameters chosen for calibrating across the whole region.

**Sensitivity Analysis and Calibration**

We performed a sensitivity analysis to identify parameters with the largest influence on stream flow (van Griensven et al., 2006). The analysis was conducted for each of two subbasins that were headwater subbasins selected to have different land-cover distributions and located in different parts of the study region. The Current River watershed (HUC 11010008) has an upstream drainage area of 6817 km² and is predominantly forested (75.5% of total drainage area). The Southern Beaver watershed (HUC 11130207) has an upstream drainage area of 1780 km² and has grassland and pasture (47.6%), dominantly forested (75.5% of total drainage area). The Southern Beaver watershed (HUC 11130207) has an upstream drainage area of 1780 km² and has grassland and pasture (47.6%), shrubland (30.5%), and agriculture (17.3%) as the dominant land-cover types. The results of the sensitivity analysis helped to identify a subset of SWAT parameters with the highest influence on flow.

We calibrated SWAT-simulated monthly flows against monthly stream flow records from USGS gauging stations near the outlets of the two subbasins of interest. We selected parameters that had the most influence on stream flow from the sensitivity analysis and entered them into SWAT’s autocalibration routine. SWAT-simulated monthly flows were automatically calibrated against monthly flows between 1985 and 1996. We measured the quality of calibration results using the Nash-Sutcliffe efficiency (NSE).

To apply the calibration results to the whole region, we selected parameters from the two calibrated subbasins with similar final calibrated values (baseflow alpha factor, maximum canopy storage, channel effective hydraulic conductivity, soil evaporation compensation factor, and surface runoff lag time; table 1). We averaged the optimal parameter values from the two subbasins and used these averages for simulations of the AWR region. For other parameters, such as the curve number, calibrated results for the two subbasins were different, and default values were retained.

**Functional Validation**

After calibrating the SWAT model at a finer scale, we conducted a functional validation of flow predictions for the AWR basin. We see this as a first step toward validating water quality predictions for the current landscape. We used a constructive approach of validation that seeks to analyze patterns in residuals to better understand discrepancies between model-simulated values and field measurements (Jager et al., 2000).

Flows were simulated by SWAT with calibrated parameter values described above for the AWR region from 1980 to 2003 for the current pre-bioenergy landscape. Predictions from the first five years (1980 and 1984) were excluded from the comparison. We identified USGS gauges closest to the outlets of 88 of 173 eight-digit hydrologic unit (HUC8) subbasins in the AWR and obtained daily stream flow data from 1985 to 2003. Because USGS gauges were not all located exactly at the outlet of the subbasins, we estimated flow at the outlets by assuming that the additional, ungauged drainage area would produce the same amount of flow per unit drainage area as the gauged drainage area. The percentage of drainage area gauged ranged from 33% to 100% (median = 80%) for subbasins included in our final analysis. We excluded two subbasins with fewer than 20 months of flow data and an incomplete representation of different seasons. For each of the remaining 86 USGS gauges, we compared monthly average flows against those predicted by SWAT for the same month and year.

To identify possible factors distinguishing watersheds with better fit from those with poorer fit, we fitted a linear model for the absolute values of residuals (monthly averages of SWAT-predicted minus area-adjusted USGS flows at HUC8 outlets). HUC8 attributes used as predictors included (1) the number of upstream HUCs, (2) the proportion of water as a “land” cover, (3) the proportion of agricultural cropland, (4) the proportion of wetland, (5) average elevation, (6) the product of annual precipitation (mm) from DAYMET and watershed area (km²), and (7) month. Standardized coefficients are reported, where large coefficients identify watershed attributes associated with poorer flow predictions. In addition, we displayed correlations between measured and predicted flows and Studentized residuals on maps with mainstem rivers and reservoirs depicted, allowing us to visually identify geographic patterns. To address the question of whether simulated and empirical flows are controlled by similar factors, we compared linear models for modeled and measured flows and compared standardized coefficients for the suite of predictors listed above.
RESULTS

BIOENERGY FEEDSTOCK PRODUCTION

Lowland switchgrass yields simulated by SWAT varied from zero in the northern U.S. to over 16 Mg ha$^{-1}$ in southern Illinois, Arkansas, western Kentucky, and Tennessee (fig. 2). In addition to the latitudinal gradient, predicted yields increased from very low values west of the 100th meridian to higher values farther east (fig. 2). Yields predicted across the southern extremes of the eastern U.S. were typically between 6 and 12 Mg ha$^{-1}$ (fig. 2). The SWAT-simulated values in figure 2 were compared to those derived from an empirical model, which are based on published field trials in the eastern U.S. (Jager et al., 2010).

The geographic patterns produced by SWAT and by the empirical data at a regional scale were qualitatively similar, with the highest yields extending from west to east across the mid-latitudes, from Missouri, Illinois, Kentucky, and Tennessee to Virginia and North Carolina. Yields decreased away from the center. The average county yields predicted by empirical model and the SWAT model were correlated with an $R^2$ of 0.51 (fig. 3). However there was a bias, with the SWAT model yields being lower than the empirical model yields. The differences between the average county yields predicted by the empirical model and by SWAT in the counties that shared the prediction range of both models indicated that the average SWAT model yields tended to be lower in most of the regions (counties shaded in teal in fig. 4). In less than 6% of the counties, the SWAT model predicted higher yields than the empirical model (counties shaded in brown in fig. 4). The differences between the empirical model and SWAT model results were within ±4 Mg ha$^{-1}$ in 52% of the counties, and the mean difference was 4.4. The largest differences (>6 Mg ha$^{-1}$), indicated by the dark teal shaded counties and comprising about 28% of the counties, were in the northeastern states, in counties along the Appalachian mountain range, and in counties along the western end of the prediction range in the Rocky Mountains (fig. 4). The large differences in the counties along the mountain ranges were caused by very low SWAT-predicted yield, which was due to reduced growth under lower temperatures and high slopes. Such unfavorable conditions were probably not represented among field trials, which are typically conducted near land-grant universities in flat areas suitable for agriculture. The SWAT model did not predict switchgrass yield in the northern latitudes because of the inability of plants to accumulate the requisite physiological heat units to maturity (1,100 physiological heat units - degree-days °C above a base temperature). This caused the empirical model yields to far exceed SWAT-simulated yields in the northeastern U.S. We conclude that the differences should not necessarily be attributed to problems in the model, as the empirical data and empirical model fitted to them are also imperfect (Jager et al., 2010), but this comparison adds to our understanding of geographic patterns.

WATER QUANTITY (FLOW)

Results are presented below for each step of the process, which began with sensitivity analysis and calibration performed in smaller subbasins and ended with functional validation on a regional scale. This analysis was conducted for the Arkansas-White-Red River basin, which is outlined in figure 4.

Sensitivity Analysis

We found that monthly flows were most sensitive to the baseflow alpha factor (Alpha_Bf in table 1) in one subbasin and to the curve number (Cn2) in the other. In both subbasins, the soil evaporation compensation factor (Esco) ranked second.
Figure 3. Correlation between average county switchgrass yield predictions from the SWAT model and the empirical model of lowland switchgrass yields.

Calibration

Nash–Sutcliffe efficiencies for the two calibrated subbasins with their own individual calibrated parameter values were 0.74 and 0.78 for the calibration time period. We then validated SWAT-predicted monthly stream flow using data from 1997 to 2003 for each calibrated subbasin. Validation results measured goodness-of-fit as NSE = 0.75 and 0.65. Using the five-parameter calibration averages reduced the NSE values to 0.63 and 0.45. Values exceeding 0.65 are considered to be good, and those greater than 0.75 are considered to be very good (Moriasi et al., 2007).

Flow Validation

The correlation between SWAT predictions and USGS estimates for 86 HUC8s was high (0.91). A strong relationship between area-weighted USGS-measured and SWAT-predicted monthly average flow was found (adjusted $R^2 = 0.8277$, RMSE = 90.48 m$^3$ s$^{-1}$, 16,589 df), with a slope near one (standardized slope = 0.91).

Functional validation is a methodology for analyzing residuals (model - field data) to expose and understand patterns where the model (SWAT) fits field data and where fit can potentially be improved (Jager et al., 2000). To this end, we fitted a linear model of absolute residuals (SWAT outflow minus area-adjusted USGS outlet flow) with attributes such as number of dams, upstream-downstream HUC position, percent of land cover area within an HUC, elevation, etc. The model explained 43% of the variation in absolute discrepancies between SWAT and USGS-measured flow. Not surprisingly, model-data deviations increased with downstream position (fig. 5). To a smaller extent, the percentage of water (reservoir area) increased absolute deviation, although the number of dams was not important (fig. 5). Other variables (increasing percentage of wetland, month) had smaller adverse influences on SWAT model fit (fig. 5). Deviations were smaller in HUC8s with a higher percentage of cropland (fig. 5).

These results suggest that SWAT-predicted flows for upstream, headwater HUC8s are more accurate than those in

Figure 4. Difference between average county switchgrass yield predictions from empirical model of lowland switchgrass yields and those predicted by the SWAT model. The Arkansas-White-Red river basin is outlined in black.
mainstem rivers. Spatially, the poorest correlations between SWAT and USGS flows occurred in HUC8s along the mainstem of the Canadian River, the upper portion of the mainstem Arkansas River, and in one high-elevation headwater HUC8 on the Arkansas River, approximately 25% of which was ungauged (fig. 6). This is apparent when looking at the lowest correlations (light shading in fig. 6) and highest magnitude Studentized residuals. Visually, the presence of large reservoirs did not seem to correspond with larger-magnitude deviations. Note that in all cases, SWAT-simulated flows fell within 1.6 SD of those estimated from USGS data.

To further explore seasonal patterns, we examined the distribution of residuals for each month (including multiple years and HUC8 watersheds). The Studentized residuals generally bracketed zero but showed a seasonal pattern, with higher deviations (overprediction of flow) in summer than at other times (fig. 7). One possible explanation for this would be underprediction of evapotranspiration. Another explanation might be water storage in reservoirs during summer months.

Our comparison of HUC8 influences on SWAT-predicted and USGS-measured outlet flows suggests that similar factors influence both (fig. 8), although simulated upstream influences on SWAT-predicted flows are greater than those reflected in measured flows.
DISCUSSION

In this article, we compared regional-scale empirical data with SWAT predictions for switchgrass production and river flow with the goal of quantifying two important aspects of bioenergy sustainability (energy production and water quality). Our productivity estimates suggested that the highest yields of this perennial energy crop are possible in the middle latitudes of the eastern U.S. Low yields simulated for higher latitudes reflect the fact that this analysis is for a lowland ecotype. Geographic patterns in SWAT-simulated yields and those predicted by a model fitted to empirical data by Jager et al. (2010) were similar, but SWAT-simulated switchgrass yields tended to be lower, especially in the northern states and also mountainous regions. SWAT-simulated yields could be increased to match those of empirical data by calibrating growth parameters, such as the maximum potential LAI. However, it is important to note that yields obtained in field-scale trials are often higher than those achieved at production scales.

We see several future directions for this research on the production of switchgrass as a bioenergy crop. First, future efforts will examine yields for the upland ecotype, which is grown successfully at higher latitudes. Changes in plant growth parameters will be needed to accomplish this, and subsequent comparisons with field-trial data will be useful. Second, a functional validation of SWAT-simulated yields for both ecotypes would be useful to help understand model-data discrepancies, keeping in mind that field data are also fraught with uncertainty. Third, modeling the uncertainties in the empirical estimates, for example by mapping prediction errors, and evaluating SWAT model fit in the context of uncertainty in empirical data are needed to provide context.

One future role of SWAT-simulated potential switchgrass yields such as those presented here can be as input to economic models of the agricultural and bioenergy sector (fig. 1). Adequate yield is a necessary, but not sufficient, condition for the economic viability of switchgrass as a bioenergy crop. Clearly, producing switchgrass is not profitable in areas where yields are inadequate. If yields are adequate, then other factors not addressed here come into play, such as the cost of producing switchgrass and the relative profitability of alternative crops. For example, economic studies have suggested that switchgrass would require a crop prices between $43 per dry Mg (in 1989 dollars; Turhollow, 1994) and $88 per dry Mg (Jain et al., 2010). The availability of geographic distribution of potential yields in all regions can help in the economic analysis of resource potential for bioenergy crop production (Walsh et al., 2003). The potential yields predicted by SWAT in this study can be used in economic models such as POLYSYS to estimate where switchgrass could replace other land uses based on relative economic profit. POLYSYS allocates land in 305 agricultural statistical districts and contains major crops, livestock, food, and feed markets, with initial conditions anchored to USDA baseline economic projections (Hellwinckel et al., 2010). To demon-

![Figure 8. Comparison of influences on estimated monthly flows at HUC8 outlets (USGS flow) and those predicted by the SWAT model.](image)

![Figure 9. Preliminary estimates of agricultural areas where cultivation of switchgrass may become economically feasible by 2030 in the Arkansas-White-Red River basin.](image)
strate, mapped results from preliminary economic simulations suggest where the conversion to switchgrass would be feasible for a crop price of $60 per dry tonne and 5% annual increase in yield of new plantings (fig. 9). Such projections can be input to the SWAT model to simulate future water quality under a bioenergy landscape. These results, when compared to the water quality in the current landscape, will help us understand potential implications on water quality owing to a bioenergy future (fig. 1).

The second goal of this study was to validate SWAT-predicted river flow. Overall, we were encouraged by the validation results, which showed good agreement across the Arkansas-White-Red River basin. In our future research, we will implement the SWAT model and conduct functional validation in other major river basins of the eastern U.S.

Our functional validation provided constructive feedback that can be used to improve region-wide prediction, if it is deemed necessary. The increase in deviation downstream, as measured by the number of upstream HUC8s, may simply result from compounding errors in flows simulated in upstream HUC8s. The increased deviation in HUC8s with higher percentages of water, suggesting substantial reservoir area, suggests that including reservoirs (losses to irrigation and evaporation) might improve simulation of seasonal flow patterns, although HUC8s above and below larger reservoirs showed good agreement (fig. 6). We are encouraged by the fact that flow prediction in HUC8s with a higher percentage of agricultural cropland were good, suggesting that representation of tile drains has improved our prediction of monthly flows. Other studies have shown that representing tile drains using SWAT improves flow prediction for agricultural watersheds (e.g., Green et al., 2006).

Although the model could be fine-tuned along particular mainstem drainages, the current model structure and parameters may be adequate for the purpose of regional-scale research focused on water quality. Our next step will be to evaluate the availability of water quality data to compare against SWAT water quality (nutrients and sediment concentrations) on a regional scale. Previous studies have suggested that water quality, and nitrate in particular, can be better predicted with higher-resolution data, up to a point (Jha et al., 2004; Chaubey et al., 2005). The USGS maintains the National Water Information System (NWIS), an extensive database for surface water data including time-series data that describe stream flow and surface-water quality (USGS, 2001). To compare SWAT water quality output against empirical data, we queried the NWIS for suitable records from gauges at the most downstream position within watersheds. However, our validation efforts were severely constrained by the limited availability of appropriate time-series data because gauge location within a watershed, water quality parameters measured by the USGS, the number of data records for individual parameters of interest, or the period of data collection were rarely compatible in terms of overlap with our model predictions. We plan to pursue validation of water quality data by comparing the distribution of measurements at the level of subregions within the AWR.

This study demonstrated the use of the SWAT model as a step toward exploring the productivity and environmental sustainability of switchgrass as a bioenergy crop at regional scales. As our work with modeling bioenergy landscapes continues, we can improve our understanding of which areas provide the highest economic and environmental potential for biomass feedstock production. The approach we have outlined can be applied to other major river basins to produce guidance at a national scale.

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REFERENCES


