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**Modeling to Evaluate and Manage Water and Environmental Sustainability of Bioenergy
Crops in the U.S.**

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ABSTRACT

Decisions are being made that will determine the path to be taken for biofuel production and use. The objectives of this chapter are to describe some simulation modeling tools as they have been applied to issues related to biofuel production and to describe how to use the ALMANAC model for these applications. In order to verify that the biomass yields are realistic, we compared mean simulated yields for four sites in the Central Great Plains to reported yields of maize and switchgrass. We were successful in getting mean simulated values close to the mean measured values in each case. The model was then used to simulate water use efficiency of different production systems and biomass yield stability of these systems. This study demonstrated the usefulness of this process-based model for these portions of life cycle analyses. Further work developing parameters to simulate other candidate plant species will prove useful to extend this type of approach. Likewise, further validation of the plant yields on various soils in various rainfall zones will be invaluable as a proof of concept for this approach.

Biofuel Production is Currently at a Critical Crossroads

Decisions are being made that will determine the path to be taken for biofuel production and use. Maize (*Zea mays* L.) has recently been the crop of choice, and the impacts of its use have been dramatic. Widespread expansion of biofuel maize acreage has been reported to impact the economics of feed production, soil erosion, and water quality downstream. Other options such as perennial grasses for cellulose, oilseed crops, biofuel sorghum (*Sorghum bicolor* L. Moench), energy cane (*Saccharum spontaneum*), or sugarcane (*Saccharum officinarum* L.) each have their own advantages as well as negative aspects.

Many of the basic questions and issues concerning biofuel production and use in the U.S. have been the same for at least the last 20 years. A background paper for the U.S. Congress by the Office of Technology Assessment (1993, Potential Environmental Impacts of Bioenergy Crop Production) outlines several of the issues we are still facing today. Impacts of expanded biofuel production on “soil quality and soil erosion, water quality, air quality, habitat for a variety of species, and the global environment” are all discussed in this publication. Growing bioenergy crops on set-aside or conservation reserve program (CRP) lands and degraded lands were and still are important concerns. The ability of herbaceous environmental crops like switchgrass (*Panicum virgatum*) or short rotation woody crops such as hybrid poplar (*Populus spp.*), “to stabilize erosive soils or perhaps filter agricultural chemicals and sediments before they reach water supplies” are discussed in this publication. Even economic impacts, especially on the rural economies, are also discussed. With the current concern over expanded maize production and the negative economic impacts of its use for biofuel, it is interesting to note that this 20-year-old publication discusses positive impacts, with the hope that expanded biofuel production might provide “alternative crops for rural agricultural communities: to provide

employment, to stabilize rural incomes, and to maintain the rural infrastructure of equipment and supplies distribution and service”.

Likewise, with the current rush to convert CRP lands back into production agriculture, it might be wise to consider one of the main reasons this program was originally established: to protect highly erodible soils. In the 1993 report, when discussing herbaceous environmental crops like switchgrass, authors propose that “Bioenergy crops are a potential alternative cash crop that could protect fragile soils or could be grown on lands previously idled in order to strengthen commodity crop prices. This could result in a win-win scenario, allowing economic production on these lands while maintaining the soil and water environmental benefits of a permanent plant cover”. The report goes on to discuss impacts of bioenergy crop production on soil organic matter, nutrient cycling, soil erosion, water quality, air quality, riparian zones and wetlands, wildlife habitat, greenhouse gases (GHGs), and atmospheric concentration of CO₂, all important and frequently discussed issues today.

To address these issues, process-based models have offered and continue to offer promise as valuable tools to rapidly and efficiently assess the benefits and negative impacts of these various biofuel plant species as they are considered for large-scale production. Such crop models, once parameterized for the various plants and validated across diverse landscapes and production scenarios, are useful for calculating water requirements, impacts of limited water availability on production capacity, stability of production over years and over climatic conditions such as periodic drought, and impacts on soil erosion and water quality downstream. Before the first acre is dedicated to such production, effects on water use, soil erosion, water quality downstream, and acreage lost for crop production for food or for livestock production through grazing can be assessed. Such models can assess tradeoffs between the use of smaller acreage of

prime farmland to meet biofuel production goals vs. more marginal soils or rangeland, but increased acreage to reach the same goals. Local, regional, and even national assessments are possible with these models in an efficient and scientifically defensible manner.

There has been much progress in development of such process-based models and their parameterization, validation, and application in the last 20 years since publication of the congressional report. The first objective of this chapter is to describe some of these modeling tools as they have been applied to issues related to biofuel production. Secondly, we will describe one such single field scale simulation tool, the ALMANAC model (Kiniry et al., 1992), as an effective means to address some of the current issues concerning biofuel production. We will describe the basic processes simulated by the model, present examples that demonstrate its usefulness, and show some applications in typical regions that can be considered for biofuel production in the future.

MATERIALS AND METHODS

Applications of Simulation Models to Address Questions Related to Biofuel Production

Crop modeling. As discussed by Behrman et al. (2014) simulation models of biomass production by plants such as switchgrass are being used to address many of the above-mentioned issues. One type of model for bioenergy crops are the statistical approaches that rely on relationships between environmental variables and empirical biomass estimates. Statistical models have been used to estimate yields across large spatial extents (Wullschleger et al., 2010). Another type of model relies on the process-based approach that simulates the actual processes governing plant growth. For this chapter, we will concentrate only on the process-based modeling approach.

Process-based simulations include detailed information on plant growth and development, climate, soil dynamics, and management (Williams et al., 1989; Kiniry et al., 1992; Kiniry et al., 1996; Arnold et al., 1998; Del Grosso et al., 2005; Di Vittorio et al., 2010; Miguez et al., 2011; Gelfand et al., 2013). These models have been used to not only estimate yields but also to analyze water use efficiency, impacts of management practices, long-term effects on soil properties, and the impact of climate change (Kiniry et al., 1996; Kiniry et al., 2008; Brown et al., 2000).

Process-based models of plant growth that have been used to simulate switchgrass production include Agro-BGC, ALMANAC, BIOCRO, DAYCENT, EPIC, and SWAT (Williams et al., 1989; Kiniry et al., 1992; Kiniry et al., 1996; Arnold et al., 1998; Del Grosso et al., 2005; Di Vittorio et al., 2010; Miguez et al., 2011; Gelfand et al., 2013). These models have been used to track GHG emissions, soil erosion, nutrient cycling, and plant productivity. Because of the variability in modeling objectives, these models vary in their functions and amount of detail incorporated to simulate plant growth. However each model shares the following basic functionality. First, they simulate biomass production by specifying light interception, conversion of sunlight to biomass, and partitioning of biomass into structural components. Second, they simulate soil water dynamics, which depends on precipitation, run-off, and evapotranspiration. Third, they simulate soil carbon and nitrogen dynamics. Lastly, each model simulates the effect of drought stress on plant growth. Models with more complex functions for the effects of environmental stress on plant growth, such as ALMANAC and EPIC, incorporate additional stress effects including stresses due to extreme temperatures, nutrient deficiency, salinity, low pH, aluminum toxicity, and poor soil aeration.

Recent Modeling Applications

Modeling Biomass Production

Simulating switchgrass growth. The following sections will mainly concern switchgrass simulation, due to its prevalence in discussions of potential biofuel plant species. The concepts discussed herein are directly relevant for other plant species potentially useful for biofuel.

As described by Behrman et al. (2014) Agro-BGC, ALMANAC, BIOCRO, DAYCENT, EPIC, and SWAT are process-based models that have been used to simulate switchgrass productivity (Williams et al., 1989; Kiniry et al., 1992; Kiniry et al., 1996; Arnold et al., 1998; Del Grosso et al., 2005; Di Vittorio et al., 2010; Miguez et al., 2011). Each model keeps track of the number of growing degree days to specify the developmental rate or phenological stage. The number of growing degree days is determined by the average of the daily maximum and minimum temperature above the specified baseline temperature (Williams et al., 1984). ALMANAC, EPIC, and SWAT use a function relating radiation use efficiency to biomass based on the leaf area and the amount of light intercepted (Williams et al., 1989). For switchgrass, plant development is initiated when temperatures exceed 12°C (ALMANAC, EPIC, and SWAT). Senescence begins when plants exceed the maximum number of growing degree days (Williams et al., 1989; Kiniry et al., 1992). Biomass is partitioned into roots and shoots. The DAYCENT model uses a constant energy biomass conversion factor (Parton et al., 1998). BIOCRO was developed from WIMOAC and uses an empirical derivation of the relationship between photosynthesis, stomatal conductance, and biomass production (Humphries and Long, 1995; Miguez et al., 2011). Agro-BGC simulates carbon uptake and assimilation (Di Vittorio et al., 2010).

Modeling Water Use Efficiency

Water use efficiency (WUE) can be vitally important for predicting areas suitable for switchgrass biofuel production. To avoid competition with farmland already used for food, fiber, and feed production, the areas most likely for switchgrass production are the less productive soils where soil water and nutrients often limit production (Perlack et al., 2005). In dryland production systems, limited rainfall and/or limited capacity of soils to store moisture are important issues for switchgrass production. Plant water use and WUE also are major concerns in irrigated regions, where competition between agriculture and other water users arises. Direct measurements of WUE are important but require labor intensive procedures involving soil water measurement with soil moisture sensors, gravimetric measurements of soil moisture from soil cores, or use of weighing lysimeters. Likewise, determinations of WUE require harvesting to quantify plant dry weights. To adequately define WUE for a range of soils, plant species, and climatic conditions requires considerable resources and time.

Water Use Efficiency of Four Switchgrass Types

Behrman et al. (2014) parameterized the ALMANAC model and used the model to simulate WUE for the four major switchgrass types: northern upland (NU), northern lowland (NL), southern upland (SU), and southern lowland (SL) in multiple locations across the Great Plains. This was an extension of the work with these four types by Kiniry et al. (2008a) in the northern U.S. and Woli et al. (2012) in Mississippi. These locations are representative sites in the region anticipated to be the primary production area for biofuel crops in the U.S. The data for comparing simulated WUE among switchgrass types and among locations using ALMANAC came from two studies (Table 1). The first study (Kiniry et al., 2008) simulated plant

transpiration and biomass for four sites: Stephenville, TX; Mead, NE; Columbia, MO and Ames, IA. The second study (Kiniry et al., 2012; Behrman et al., in review) involved 10 sites in the central and southern Great Plains. These ranged from northern MO at Elsberry to subtropical southern TX at Weslaco. The model was used, with appropriate soil parameters for each site and with actual measured weather for the growing season, to calculate plant transpiration (EP). For the first study, crop parameters were adjusted to get reasonable simulated yields of each switchgrass type, as compared to the mean of the two years of measured yields. For the second study, rainfall was severely limiting due to a drought throughout much of the region. Therefore, the crop parameters were adjusted to match LAI values measured early in the growing season in an effort to minimize the impact of severe drought stress on results (Behrman et al., in review).

The simulated WUE of all four switchgrass types showed values generally ranging from 3 to 6 mg g⁻¹, with a few exceptions. These values are within the range of empirical data that range widely and depend on the environmental conditions and switchgrass ecotype. Byrd and May (2000) calculated the WUE of many different potted switchgrass cultivars and reported that WUE ranges from 4.3 to 8.5 mg dry weight per g of water used. In germplasm nurseries in TN and OK, WUE of switchgrass accessions were 3.5 to 6.3 mg CH₂O g⁻¹ of water transpired (McLaughlin et al., 2006). In the field in NE, switchgrass WUE values were 1.0 to 5.5 mg g⁻¹ (Eggemeyer et al., 2006), values similar to those demonstrated by switchgrass seedlings in a growth chamber (1.45 to 5.5 mg g⁻¹) (Xu et al., 2006).

The greatest simulated WUE values were most often for the lowland types. The southern lowland types had the highest WUE values in most of TX and the northern lowland types generally had the greatest WUE values at locations further north (Table 1). The northern lowland type had the highest WUE in more than half the cases, being greatest for 8 of the 14 locations.

The southern upland's values for WUE were greatest at 2 sites: Booneville, AR and Mead, NE. The northern upland types only had the greatest value at Stillwater, OK. High WUE of lowland varieties allows for increases in yield in southern locations where water is often limiting.

Long-term Environmental Impacts of Bioenergy Production Systems

Mechanistic models will be useful for comparing bioenergy production systems to more conventional agricultural crops. Meki et al. (2012) applied a version of the EPIC model, APEX, to assess the sustainability of maize stover removal from the Upper Mississippi River Basin (UMRB), based on a set of 'acceptable planning criteria' used in the CEAP analysis (USDA-NRCS, 2010) to judge whether or not a farm field needed additional conservation treatment. The 'acceptable criteria' included; (a) N in surface runoff $< 16.8 \text{ kg ha}^{-1} \text{ y}^{-1}$ ($15.0 \text{ lb ac}^{-1} \text{ yr}^{-1}$), (b) N in sub-surface runoff $< 28.0 \text{ kg ha}^{-1} \text{ y}^{-1}$ ($25.0 \text{ lb ac}^{-1} \text{ yr}^{-1}$), (c) total P losses $< 4.5 \text{ kg ha}^{-1} \text{ y}^{-1}$ ($4.0 \text{ lb ac}^{-1} \text{ yr}^{-1}$), (d) Sediment loss $< 4.5 \text{ Mg ha}^{-1} \text{ y}^{-1}$ ($2.0 \text{ ton ac}^{-1} \text{ yr}^{-1}$), and (e) soil organic carbon (SOC) with a more 'stringent' restriction that the annual rate of change be positive. Given the critical functions of SOC in maintaining soil quality and productivity, biomass removal can only be justified if it does not deplete the SOC pool. These 'acceptable' levels represent field-level losses that are feasible to attain using traditional conservation treatment (nutrient management and soil erosion control), are agronomically feasible, and can equally be adapted to most bioenergy production systems. Scientific literature on field research and edge-of-field monitoring in the U.S. Midwest, coupled with model simulations of conservation practices effects, provided guidance for identifying these thresholds (USDA-NRCS, 2010).

Examples of ALMANAC Applications

General description of the model. The ALMANAC model has been described numerous times as it has been used to simulate crops (Kiniry et al., 1997; Kiniry and Bockholt, 1998; Yun Xie et al., 2001) and warm season grasses (Kiniry et al., 1996; Kiniry et al., 2002; Kiniry et al., 2005; McLaughlin et al., 2006; Kiniry et al., 2007; Schilling and Kiniry, 2007; Kiniry et al., 2008; Kiniry et al., 2013; Kiniry et al., 2014; Behrman et al., 2014). Parameters to simulate different plants continue to be refined as new research results are reported. Basically, the model simulates the soil water balance, the soil and plant nutrient balance, and the interception of solar radiation. This model includes subroutines and functions from the EPIC model (Williams et al., 1984, 1990) with added details for plant growth. The model has a daily time step. It simulates plant growth for a wide range of species and is implemented easily.

Light Interception

ALMANAC simulates light interception by the leaf canopy with Beer's law (Monsi and Saeki, 1953) and the leaf area index (LAI). The LAI is the amount of leaf area per unit ground area, a unitless variable. With greater extinction coefficient values (k), a given LAI intercepts more light. The fraction of incoming solar radiation intercepted by the leaf canopy is

$$\text{FRACTION} = 1.0 - \exp(-k \times \text{LAI}) \quad [1]$$

Leaf Area Development

Accurate prediction of light interception depends on realistic simulation of leaf area. The model estimates leaf area production up to the point of maximum leaf area for the growing season using Eq. [2]. The sigmoid-curve function for potential LAI production takes the form:

$$F = \text{SYP} / [\text{SYP} + \exp(Y1 - Y2 \times \text{SYP})] \quad [2]$$

Where F is the factor for relative LAI, SYP is the fraction of the degree days from planting to maturity, and Y1 and Y2 are the sigmoid-curve coefficients generated by ALMANAC. This curve passes through the origin and through two points, asymptotically approaching $F = 1.0$.

The model calculates SYP each day. The sum of degree days is zero at planting in the establishment year and at tiller emergence in subsequent years, and reaches its maximum value at maturity.

The model describes the loss of leaf area late in the season with the LAI decline factor. The LAI begins to decrease after a defined fraction of the seasonal degree days have accumulated.

Biomass Production and Partitioning

The model simulates biomass with an RUE value for each plant species (Kiniry et al., 1989). Values for RUE have a wide range for different crops and grasses (Kiniry et al., 1989; Kiniry et al., 1992; Kiniry et al., 1999; Kiniry et al., 2007). ALMANAC describes declining RUE in later growth stages with an identical function to the one for the decrease in LAI.

The maximum rooting depth defines the potential depth in the absence of a root-restricting soil layer. Soil cores at Temple, TX in 1994 showed that switchgrass roots extend to depths of at least 2.2 m.

Simulating water uptake with ALMANAC. The ALMANAC model is the only process-based plant model that has been used to analyze switchgrass WUE (Kiniry et al., 2008a; Behrman et al., 2014). ALMANAC simulates the water balance by determining plant water use while taking into account soil properties, weather, and plant species cover. ALMANAC calculates the effects of soil water availability on plant growth by calculating the potential

evaporation, potential soil water evaporation, and potential plant water transpiration based on the leaf area index (LAI). Potential evaporation is estimated by the Penman-Monteith method (Ritchie, 1972). Potential soil evaporation and plant transpiration is estimated by:

$$EP = E_0(LAI/3) \quad 0 \leq LAI \leq 3.0 \quad [1]$$

$$EP = E_0 \quad LAI > 3.0 \quad [2]$$

$$ES = \text{minimum of } (E_0 \exp(-0.1BIO), E_0 - EP) \quad [3]$$

Where EP and ES are potential plant transpiration and soil evaporation (mm), E₀ is potential evaporation (mm), and BIO is the sum of the above-ground biomass and plant residue (Mg ha⁻¹). Simulated plant leaf area and biomass is reduced when available soil water is depleted. Water use depends on soil water availability and plant water demand. Water demand is based on potential evapotranspiration and the leaf area index. The water stress factor is estimated and decreases daily leaf area and consequently biomass growth if current available soil water is insufficient to meet demands.

Water and Nutrient Uptake

Critical for yield and biomass simulation in water-limited conditions is the simulated water demand, as discussed above. The ALMANAC model calculates effects of soil water on crop growth and yield with similar functions. Potential evaporation is calculated first, then potential soil water evaporation and potential plant water transpiration are derived from potential evaporation and leaf area index. Based on the soil water supply and crop water demand, the water stress factor is estimated to decrease daily crop growth and yield. Water stress factor (WSF) is the ratio of water use to water demand (potential plant transpiration) in ALMANAC, and water use (WU) is a function of plant extractable water and root depth.

The nutrient balance (N and P) also allows plants to acquire sufficient nutrients to meet the demands if adequate quantities are available in the current rooting zone. Nutrient values for switchgrass were refined with N concentration data collected at Stephenville during 5 years (Sanderson, unpublished data).

Base Temperature, Optimum Temperature, and Total Degree Days

Base temperature in ALMANAC is constant for all growth stages of any plant species. Base temperature constrains the initiation of leaf area growth and thus dry matter accumulation. Higher optimum temperature can allow increased plant development rate later in the season when temperatures are greater. The sum of degree days to maturity controls the duration of growth. Heat units are reset to zero after maturity each year. Heat units are calculated from daily maximum and minimum temperatures, assuming the maximum equals the optimum if it exceeds the optimum.

Plant parameters can be adjusted to get reasonable simulated yields of each switchgrass type, as compared to the mean of multiple-year measured yield data, as discussed above. Using parameters developed for Alamo switchgrass in Texas (Kiniry et al., 1996; Kiniry et al., 1999; Kiniry et al., 2007), adjusting only two parameters: degree days to maturity (base 12 C) and the potential leaf area index (PotLAI), can often lead to realistic simulations for other switchgrass ecotypes. The light extinction coefficient for Beer's Law (Monsi and Saeki, 1953) can be set to 0.51, the average of the two means from Kiniry et al. (1999) and Kiniry et al. (2007).

The values of PotLAI and degree days varies with latitude and switchgrass types. Other parameters that can be used for a wide range of locations and switchgrass types are:

1. 3.9 g per MJ intercepted photosynthetically active radiation for the RUE at low vapor pressure deficits (VPD)
2. 0.65 unit decrease in RUE for each 1 kPa increase in VPD above 1 kPa
3. Base temperature of 12°C and optimum temperature of 25 °C
4. Linear decreases in LAI and in RUE from 70% of total degree day accumulation until maturity
5. Maximum potential rooting depth of 2.2 m
6. Optimum nitrogen concentrations of 2.57% for plants early in the spring, 1.1% for plants near mid season, and 0.28% for plants near maturity each year
7. Optimum phosphorus concentrations of 0.14% for plants early in the spring, 0.10% for plants near mid season, and 0.07% for plants near maturity each year.

Four Study Locations with Simulated Yields of Switchgrass and Maize

Verification results. Prior to conducting comparisons among crops and soils, it is imperative to verify that the biomass yields are realistic. This was accomplished by comparing the mean simulated yields for four sites (Table 2) over 17 years (we simulated 20 years, but ignored the first three to allow various model components to stabilize). The soils in each case were the “good soil” described below. The measured yield values were derived by various ways, either the NRCS values of maize given for that soil in that county on USDA NRCS Web Soil Survey, the mean for the county reported by USDA NASS (1991), published values for the site (esp. for South Dakota, Zilverberg et al., 2014), or, especially for switchgrass, yields derived from NRCS values using the regressions of Johnson et al. (2010).

We were successful in getting mean simulated values close to the mean measured values in each case (Table 3). This was accomplished after determining the appropriate degree days or

potential heat units (PHUs) for duration of growth for the crops in each region and with reasonable input annual fertilizer amounts. Potential LAI (DMLA) was the primary variable adjusted to get simulated yields close to measured values.

Biomass yields and water use results. Decisions on which crops to use and which site to use depends not only on biomass yields, but also on yield stability. To be economically viable, producers must have the assurance that even dry years will have adequate biomass production.

As production is moved to poorer marginal soils (Tables 4 to 7), not only are mean yields consistently lower as expected, but also yield variability, as shown by the CV's, usually increased. Thus not only will it take more area of these poorer marginal soils to meet yield goals, but the increased yield variability will increase risk. Thus this type of simulation model can be readily used to assess such risk.

For South Dakota (Table 4), maize yields were less stable, with greater variability in yields than switchgrass or the native seed mix as expected. In addition, mean maize yields for the two soils at this site were greater than for switchgrass or the mixture of warm season grasses on the better soil, however lower than switchgrass for the poorer soil.

Somewhat similar trends occurred for the three more southern sites (Tables 5, 6, and 7). Yields for switchgrass were much greater than for maize in each case. Yield stability, as indicated by the CV's, were lower for switchgrass than for maize with the two soils in MO and for the poorer soil in TX. For the better soil in TX and for both soils in OK, yield stability for maize was higher than for switchgrass.

Water use efficiency is reported in three ways: yield divided by seasonal precipitation (WUE_1), yield divided by seasonal evapotranspiration (water loss from soil evapotranspiration and plant transpiration, WUE_2), and yield divided by plant transpiration (WUE_3). Thus WUE_1 is

a general measure of water use efficiency for a particular rainfall zone. WUE_2 has water loss to deep infiltration and runoff taken out of the calculation. It therefore is more indicative of how efficient the production system is in terms of actual water in the soil profile. Finally, WUE_3 has soil evaporation taken out of the calculation also. As plants develop their LAI over the course of the season, and as evaporative demand changes, plant transpiration increases and eventually decreases to zero by the day of total leaf senescence. Thus this final WUE value is useful for comparing production systems in terms of actual plant use of water.

There are different trends for WUE depending on the way it was calculated. In terms of total precipitation (WUE_1) for the SD site (Table 4), values for maize were highest for the better soil, while values for switchgrass were highest for the poorer soil. WUE_1 values for switchgrass were higher for both soils at the other three sites (Tables 5, 6, and 7). In terms of total ET (WUE_2), maize was higher than switchgrass in SD for the better soil, however switchgrass was higher for the poorer soil. Again for the three other sites, switchgrass had the higher WUE when calculated in this manner. Finally, when WUE was calculated in terms of plant transpiration (WUE_3), results consistently showed the higher values for switchgrass than for maize in all cases.

Comparing better versus poorer soil, WUE results were highly variable. For SD switchgrass and the mixture, all three WUE values were nearly the same on the two soils or slightly higher on the poorer soil. For maize, WUE values were noticeably higher on the better soil. These trends varied for the other three sites. At MO, switchgrass WUE values were higher on the better soil for WUE_1 , higher on the poorer soil for WUE_3 , and nearly the same for the two soils for WUE_2 . Maize at the MO site had the higher WUE for the better soil for the first two WUE values and nearly the same for the two soils for WUE_3 . In OK, switchgrass WUE values were higher for the better soil for WUE_1 and for the poorer soil for WUE_2 and WUE_3 . Maize in OK

had the highest values on the better soil for all three WUE values. Switchgrass in TX had the WUE₁ values on the better soil, the higher WUE₃ value on the poorer soil, and nearly identical values for WUE₂ on the two soils. Maize in TX had the highest WUE₁ and WUE₃ on the better soil and nearly identically WUE₂ values on the two soils.

It should be noted that these comparisons between maize and switchgrass WUE values would be different if total biomass of maize was considered instead of just grain. With a harvest index of near 0.5, such whole biomass WUE values of maize would be approximately twice as large. Similar comparisons were reported by Kiniry et al. (2008a).

Water runoff, soil erosion, and N and P simulation. The permanent cover of perennial switchgrass (and the native grass mixture in SD) as compared to maize had the expected effects of reducing water runoff (Q) and reducing water-induced soil erosion (MUSL) often quite dramatically, as expected (Tables 8, 9, 10, and 11). At the SD site, the mean Q values for maize were

6 and 78% greater than for switchgrass. The mixture had 1-2% lower Q than for switchgrass. Soil erosion (MUSL) was dramatically greater for maize, than for switchgrass or for the mixture.

The other three sites showed how the increased Q of maize and reduced soil cover relative to switchgrass dramatically increased soil erosion of maize. Thus this type of model provides quantitative values for the expected trends for the two crops. These values can show which soils should be in row crop production if reduced soil erosion is the goal.

The N and P results were highly dependent on the Q and MUSL values and on the nutrient uptake by the particular crop simulated. Fertilizer applications within the model were aimed at preventing nutrient deficiencies with the continuous long-term annual harvests simulated.

Annually, applied N values simulated on the two soils were 100 kg N ha⁻¹ and 50 kg P ha⁻¹ in

SD, 200 and zero in MO, and 100 and zero in OK and TX. This allowed direct comparisons of the various production systems within each site. Variables YON and YP are the organic N and P loss in the sediment each year. YNO_3 and YP are the NO_3 and P loss in the surface runoff each year. The two sediment values, YON and YP, showed dramatically greater values for maize than for switchgrass in each case, as expected. Similarly, the two runoff nutrient values (YNO_3 and YAP) were higher for maize than for switchgrass in all cases. Again, as discussed above, these values give quantitative estimates for known phenomena, providing useful quantitative assessments for known environmental impacts on various soils and with various crops.

Concluding remarks:

Development of bioenergy systems needs thorough, scientifically defensible analyses on areas required, production stability across wet and dry years, water requirements, nutrient requirements, and impacts on soils and water quality downstream. Process-based models such as the ALMANAC model described herein offer a means to effectively evaluate these complex interacting facets of such systems. This study demonstrated the usefulness of this process-based model for these portions of life cycle analyses. Further work developing parameters to simulate other candidate plant species will prove useful to extend this type of approach. Likewise, further validation of the plant yields on various soils in various rainfall zones will be invaluable as a proof of concept for this approach.

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Table 1. Simulated water use efficiency in mg g^{-1} (WUE) for four switchgrass ecotypes: Southern Lowland (SL), Northern Lowland (NL), Southern Upland (SU), and Northern Upland (NU) from Kingsville, TX to Ames, IA. The greatest WUE value at each location is bold. This table is from Behrman et al. (2014).

Location	Latitude	Soil Type	WUE	WUE	WUE	WUE
			SL	NL	SU	NU
Weslaco, TX**	26.22	Hidalgo sandy clay				
		loam	4.2	4.3	3.7	4.2
Kingsville, TX**	27.54	Cranell sandy clay				
		loam	5.3	3.1	2.6	2.8
Temple, TX**	31.04	Houston black clay	11.3	4.9	3.5	3.3
Nacogdoches, TX**	31.5	Atoyac sandy loam	5.8	3.6	2.2	2.1
Stephenville, TX*	32.22	Brackett clay loam	3.5	3.3	3.2	3.2
Booneville, AR**	35.09	Leadvale silty loam	3.3	3.5	3.5	4.7
Fayetteville, AR**	36.09	Pinckwick gravelly				
		loam	5.0	5.2	4.9	4.9
Stillwater, OK**	36.12	Kirkland silt loam	3.1	2.2	2.5	3.7
Mt. Vernon, MO**	37.03	Gerald silt loam	5.4	5.6	4.4	3.5
Columbia, MO*	38.89	Keswich silt loam	4.5	4.6	4.1	3.9
Columbia, MO**	38.89	Mexico silt loam	2.3	3.1	1.6	2.4
Elsberry, MO**	39.16	Menfro silt loam	3.7	5.1	3.2	3.2
Mead, NE*	41.23	Yutan silty clay loam	4.1	4.0	4.5	3.3
Ames, IA*	42.03	Clarion loam	5.3	5.4	3.9	3.6
Average			4.8	4.1	3.4	3.5

*Reproduced from Kiniry et al. 2008, ** Reproduced from Behrman et al. *in review*.

Table 2. Four sites simulated with the ALMANAC model for maize and switchgrass. All slopes were assumed to be 1% with the exception of the better soil in SD, with a slope of 4%.

Location	County	Lat., Long	Years run	Better soil	Poorer soil
Temple, TX	Bell	31.0508N, -97.354W	1983-2002	Houston Black Clay	Austin Silty Clay
Chickasha, OK	Grady	35.082N, -97.8853W	1990-2009	Zaneis Loam	Nash-Lucien Complex
Columbia, MO	Boone	38.9008N, -92.2087W	1949-1968	Mexico Silt Loam	Armstrong Loam
Colman, SD	Moody	4.0824N,-96.7381W	1988-2007	Wentworth-Egan Silty Clay Loam	Baltic Silty Clay Loam

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Table 3. Yield verification; simulated yields (on the “abetter” soils, see text) and reported yields (Mg/ha) of ALMANAC (last 17 years of 20 simulated) for switchgrass (above-ground biomass) and maize (grain only) at four different locations. Switchgrass potential LAI (DMLA) values were 1.3, 12, 6, and 12 for the four sites in order. Maize input DMLA values were 3.2, 4.1, 2.0, and 3.2 for the four sites in order.

	Switchgrass		Maize	
	Simulated	Measured	Simulated	Measured
Colman, SD ¹				
Mean Yields	5.9	5.3	6.7	6.8
Warm season grass mixture	3.6	3.7		
Columbia, MO ²				
Mean Yields	17.4	18.1	4.9	4.7
Chickasha, OK ³				
Mean Yields	5.9	6.6	4.0	2.3(5.1)
Temple, TX ²				
Mean Yield	14.2	14.5	4.8	4.7

¹ Measured data from Zilverberg et al. (2014).

² Measured data derived from NRCS values for the soils near the site.

³ Measured data derived from NRCS values for the soils near the site and, in parentheses, the NASS mean reported yield for four years.

Table 4. At Colman, SD, ALMANAC model simulated yields and water use efficiency (WUE) of switchgrass, native plant mixture (Mix) (both above-ground biomass) and maize (grain only). Simulations were conducted for 17 years on two soils. WUE₁ is the ratio of yield divided by rain, WUE₂ is yield divided by evapotranspiration (ET; water loss from soil evapotranspiration and plant transpiration), and WUE₃ is yield divided by plant transpiration (Transp.). Mean annual precipitation was 1433±300 mm. Switchgrass is upland switchgrass, Mixture is a mixture of warm season, native grasses, and maize is a locally adapted hybrid.

	Yield Mg ha ⁻¹	ET -----mm y ⁻¹ -----	EP	WUE ₁	WUE ₂ -----mg g ⁻¹ -----	WUE ₃
<u>Switchgrass</u>						
Better soil						
Mean ± SD	5.86±0.96	432±22	158±22	0.42±0.13	1.35±0.20	3.70±0.30
CV(%)	16	5	14	32	14	8
Poorer soil						
Mean ± SD	5.85±0.95	394±19	157±22	0.42±0.14	1.48±0.22	3.72±0.31
CV(%)	16	5	14	32	15	8
<u>Mixture</u>						
Better soil						
Mean ± SD	3.57±0.57	551±44	306±47	0.26±0.08	0.64±0.09	1.18±0.21
CV(%)	16	8	15	30	14	18
Poorer soil						
Mean ± SD	3.55±0.59	486±56	259±54	0.25±0.08	0.74±0.13	1.41±0.29
CV(%)	17	12	21	30	18	21
<u>Maize</u>						
Better soil						
Mean ± SD	8.53±0.16	554±41	354±36	0.60±0.15	1.54±0.26	2.42±0.44
CV(%)	18	7	10	25	17	18
Poorer soil						
Mean ± SD	5.69±2.51	496±51	287±44	0.39±0.11	1.12±0.38	1.93±0.65
CV(%)	44	10	15	37	34	33

Table 5. For Columbia, MO for 17 simulated years; simulated yields (Mg/ha) of ALMANAC for switchgrass and native plant mixture (both above-ground biomass) and maize (grain only) at four different locations with two soils at each location. WUE values are all mg per g. WUE₁ is the ratio of yield divided by rain, WUE₂ is yield divided by evapotranspiration (ET; water loss from soil evapotranspiration and plant transpiration), and WUE₃ is yield divided by plant transpiration (Transp.). Mean annual precipitation was 1222±312 mm. Switchgrass is a lowland switchgrass and maize is a locally adapted hybrid.

	Yield Mg ha ⁻¹	ET -----mm y ⁻¹ -----	EP	WUE ₁	WUE ₂ -----mg g ⁻¹ -----	WUE ₃
<u>Switchgrass</u>						
Better soil						
Mean ± SD	13.39±3.33	673±101	470±89	1.13±0.34	1.96±0.33	2.82±0.45
CV(%)	25	15	19	30	19	16
Poorer soil						
Mean ± SD	11.26±3.36	578±101	360±88	0.97±0.34	1.94±0.46	3.15±0.72
CV(%)	30	17	24	35	24	23
<u>Maize</u>						
Better soil						
Mean ± SD	5.14±1.81	607±53	344±41	0.43±0.13	0.84±0.25	1.48±0.42
CV(%)	35	9	12	30	29	29
Poorer soil						
Mean ± SD	3.72±1.72	543±74	253±60	0.31±0.10	0.67±0.22	1.43±0.38
CV(%)	46	15	24	33	34	26

Table 6. For Chickasha, OK for 17 simulated years; simulated yields (Mg/ha) of ALMANAC for switchgrass and native plant mixture (both above-ground biomass) and maize (grain only) at four different locations with two soils at each location. WUE values are all mg per g. WUE₁ is the ratio of yield divided by rain, WUE₂ is yield divided by evapotranspiration (ET; water loss from soil evapotranspiration and plant transpiration), and WUE₃ is yield divided by plant transpiration (Transp.). Mean annual precipitation was 899±227 mm. Switchgrass is a lowland switchgrass and maize is a locally adapted hybrid.

	Yield Mg ha ⁻¹	ET -----mm y ⁻¹ -----	EP	WUE ₁	WUE ₂ -----mg g ⁻¹ -----	WUE ₃
<u>Switchgrass</u>						
Better soil						
Mean ± SD	7.21±3.36	590±79	545±65	0.82±0.37	1.20±0.47	2.04±0.74
CV(%)	47	13	19	45	39	36
Poorer soil						
Mean ± SD	6.39±3.01	513±118	281±57	0.74±0.37	1.43±1.29	2.23±0.88
CV(%)	47	23	20	51	90	39
<u>Maize</u>						
Better soil						
Mean ± SD	3.97±1.39	583±79	265±52	0.47±0.22	0.67±0.21	1.47±0.40
CV(%)	35	14	20	47	32	27
Poorer soil						
Mean ± SD	2.42±1.09	524±79	205±51	0.29±0.18	0.46±0.21	1.17±0.45
CV(%)	45	15	25	62	45	38

Table 7. For Temple, TX for 17 simulated years; simulated yields (Mg/ha) of ALMANAC for switchgrass and native plant mixture (both above-ground biomass) and maize (grain only) at four different locations with two soils at each location. WUE values are all mg per g. WUE₁ is the ratio of yield divided by rain, WUE₂ is yield divided by evapotranspiration (ET; water loss from soil evapotranspiration and plant transpiration), and WUE₃ is yield divided by plant transpiration (Transp.). Mean annual precipitation was 841±193 mm. Switchgrass is a lowland switchgrass and maize is a locally adapted hybrid.

	Yield Mg ha ⁻¹	ET -----mm y ⁻¹ -----	EP	WUE ₁	WUE ₂ -----mg g ⁻¹ -----	WUE ₃
<u>Switchgrass</u>						
Better soil						
Mean ± SD	13.64±3.52	841±193	669±93	1.69±0.55	2.04±0.48	2.86±0.59
CV(%)	26	23	14	33	23	21
Poorer soil						
Mean ± SD	9.94±2.78	493±63	340±64	1.26±0.53	2.03±0.53	2.97±0.74
CV(%)	28	13	19	42	26	25
<u>Maize</u>						
Better soil						
Mean ± SD	4.82±1.15	620±67	358±75	0.60±0.22	0.77±0.16	1.33±0.18
CV(%)	24	11	21	36	21	13
Poorer soil						
Mean ± SD	4.05±1.27	515±49	323±59	0.51±0.21	0.78±0.21	1.23±0.28
CV(%)	31	10	18	42	27	23

Table 8. For Colman, SD for 17 simulated years; environmental impacts, water quality, and soil erosion values simulated by the ALMANAC model. Switchgrass is upland switchgrass, Mixture is a mix of warm season, native grasses, and maize is a locally adapted hybrid. Variables are surface runoff (Q), soil loss from water erosion (MUSL), organic N loss with sediment (YON), P loss with sediment (YP), NO₃ loss in surface runoff (YNO3), and soluble P loss in runoff (YAP).

	Q mm y ⁻¹	MUSL Mg ha ⁻¹ y ⁻¹	YON -----kg ha ⁻¹ y ⁻¹ -----	YP	YNO3	YAP
<u>Switchgrass</u>						
Better soil						
Mean ± SD	386±186	0.32±0.16	1.3±0.6	0.2±0.1	3.4±1.6	0.2±0.14
CV(%)	49	49	43	43	48	60
Poorer soil						
Mean ± SD	596±248	0.07±0.03	0.4±0.1	0.05±0.02	5.1±2.0	0.05±0.03
CV(%)	42	39	24	33	38	49
<u>Mixture</u>						
Better soil						
Mean ± SD	381±188	0.35±0.16	1.4±0.6	0.2±0.1	3.2±1.6	0.26±0.14
CV(%)	49	47	43	44	49	30
Poorer soil						
Mean ± SD	583±248	0.08±0.04	0.5±0.2	0.1±0.0	5.0±2.0	0.07±0.03
CV(%)	42	45	42	42	40	44
<u>Maize</u>						
Better soil						
Mean ± SD	688±262	24.3±9.3	70.1±24.4	9.3±3.2	5.7±2.1	0.12±0.05
CV(%)	38	38	35	34	37	43
Poorer soil						
Mean ± SD	633±247	4.7±1.9	25.6±9.7	3.4±1.3	9.6±5.0	0.55±0.39
CV(%)	39	40	38	38	52	72

Table 9. For Columbia, MO for 17 simulated years; environmental impacts, water quality, and soil erosion values simulated by the ALMANAC model. Switchgrass is a lowland switchgrass and maize is a locally adapted hybrid. Variables are surface runoff (Q), soil loss from water erosion (MUSL), organic N loss with sediment (YON), P loss with sediment (YP), NO₃ loss in surface runoff (YNO₃), and soluble P loss in runoff (YAP).

	Q mm y ⁻¹	MUSL Mg ha ⁻¹ y ⁻¹	YON -----kg ha ⁻¹ y ⁻¹ -----	YP	YNO ₃	YAP
<u>Switchgrass</u>						
Better soil						
Mean ± SD	388±193	0.06±0.04	0.1±0.1	0.02±0.01	3.1±1.5	0.013±0.009
CV(%)	57	60	44	45	48	66
Poorer soil						
Mean ± SD	329±191	0.64±0.37	1.3±0.6	0.2±0.1	5.2±2.4	0.078±0.053
CV(%)	58	58	46	46	45	68
<u>Maize</u>						
Better soil						
Mean ± SD	395±206	4.7±2.4	11.8±5.2	1.8±0.8	13.6±3.9	0.60±0.30
CV(%)	52	51	44	43	29	51
Poorer soil						
Mean ± SD	471±237	68.5±33.6	109.7±49.9	18.6±8.7	21.7±12.4	0.84±0.43
CV(%)	50	49	45	47	57	51

Table 10. For Chickasha, OK for 17 simulated years; environmental impacts, water quality, and soil erosion values simulated by the ALMANAC model. Switchgrass is a lowland switchgrass and maize is a locally adapted hybrid. Variables are surface runoff (Q), soil loss from water erosion (MUSL), organic N loss with sediment (YON), P loss with sediment (YP), NO₃ loss in surface runoff (YNO₃), and soluble P loss in runoff (YAP).

	Q mm y ⁻¹	MUSL Mg ha ⁻¹ y ⁻¹	YON -----kg ha ⁻¹ y ⁻¹ -----	YP	YNO ₃	YAP
<u>Switchgrass</u>						
Better soil						
Mean ± SD	42±38	0.007±0.009	0.039±0.02	0.004±0.005	0.45±0.36	0.014±0.013
CV(%)	90	120	68	140	80	94
Poorer soil						
Mean ± SD	65±48	0.07±0.05	0.18±0.11	0.02±0.01	0.61±0.39	0.0088±0.007
CV(%)	74	73	59	62	64	79
<u>Maize</u>						
Better soil						
Mean ± SD	162±77	2.5±1.3	6.0±2.8	1.00±0.50	10.6±4.3	0.320±0.157
CV(%)	48	50	47	50	41	49
Poorer soil						
Mean ± SD	182±89	8.9±4.0	16.0±7.7	2.36±1.13	8.7±2.4	0.019±0.095
CV(%)	49	52	48	48	28	50

Table 11. For Temple, TX for 17 simulated years; environmental impacts, water quality, and soil erosion values simulated by the ALMANAC model. Switchgrass is a lowland switchgrass and maize is a locally adapted hybrid. Variables are surface runoff (Q), soil loss from water erosion (MUSL), organic N loss with sediment (YON), P loss with sediment (YP), NO₃ loss in surface runoff (YNO₃), and soluble P loss in runoff (YAP).

	Q mm y ⁻¹	MUSL Mg ha ⁻¹ y ⁻¹	YON -----kg ha ⁻¹ y ⁻¹ -----	YP	YNO ₃	YAP
<u>Switchgrass</u>						
Better soil						
Mean ± SD	138±78	0.02±0.01	0.10±0.05	0.012±0.007	1.7±0.9	0.006±0.006
CV(%)	56	59	47	54	50	105
Poorer soil						
Mean ± SD	116±64	0.14±0.08	0.34±0.16	0.04±0.02	1.0±0.5	0.004±0.006
CV(%)	55	57	46	47	54	150
<u>Maize</u>						
Better soil						
Mean ± SD	161±90	1.9±1.1	6.6±3.2	0.95±0.46	7.1±4.6	0.225±0.155
CV(%)	56	58	49	49	65	69
Poorer soil						
Mean ± SD	170±85	12.8±6.5	28.5±13.0	4.3±1.9	6.8±3.3	0.148±0.088
CV(%)	50	51	46	45	49	60