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A WATERSHED SCALE EVALUATION OF SELECTED SECOND GENERATION BIOFEEDSTOCKS ON WATER QUALITY

A WATERSHED SCALE EVALUATION OF SELECTED SECOND GENERATION BIOFEEDSTOCKS ON WATER QUALITY

A thesis submitted in partial fulfillment
of the requirements for the degree of
Master of Science in Biological Engineering

By

Gurdeep Singh
Punjab Agricultural University
Bachelor of Technology in Agricultural Engineering, 2010

December 2012
University of Arkansas

ABSTRACT

This study compares a novel simulation approach to the conventional Soil and Water Assessment Tool (SWAT) modeler's approach for targeting biofuel crop production on marginal lands. In conventional SWAT modeling approach, non-spatial definition of hydrological response units (HRUs) results in the simulation of biofuel crops on both marginal and non-marginal land. This study provides an alternative approach in which a marginal-land raster was integrated into the land use and land cover (LULC) raster in such a way that the land uses were divided into marginal and non-marginal components. This modified LULC was used for model setup which resulted in marginal and non-marginal HRUs. This approach was evaluated for the L'Anguille River watershed (LRW) by calibrating and validating for total flow, surface flow, base flow, sediment, total phosphorus, and nitrate-nitrogen followed by the simulation of biofuel crops only on marginal HRUs.

The results were analyzed for two cellulosic (second generation) biofuel crops: switchgrass (*Panicum virgatum* L.) and miscanthus (*Miscanthus* x *giganteus*). Compared to novel modeling approach, simulations using the conventional approach showed an increase in sediments by 20% and 61%, total phosphorus by 17% and 53%, and total nitrogen by 25% and 65% for the switchgrass and miscanthus, respectively. Compared to simulated pollutant losses from a mix of baseline row crops, switchgrass and miscanthus showed 94% and 78% decrease in sediment, 96% and 90% decrease in total phosphorus, and 80% and 67% decrease in total nitrogen, respectively. This study provided a novel approach to incorporate marginal land into the SWAT model and the model outputs suggest that producing perennial grass biofuel crops on marginal lands of the LRW resulted in lower sediment, total phosphorus, and total nitrogen losses than that obtained by conventional SWAT modeling. Pollutant losses from the non-

targeted marginal HRUs explained the differences in the sediment, total phosphorus, and total nitrogen losses. The simulation results also suggested that substantial reduction in pollutant losses could be achieved by replacing baseline row crops with perennial grass crops on marginal lands in the LRW.

The thesis is approved for recommendation
to the Graduate Council.

Thesis Director:

(Dr. Dharmendra Saraswat)

Thesis Committee:

(Dr. Marty D. Matlock)

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CHAPTER I

INTRODUCTION

1.1 PROBLEM STATEMENT

In order to meet increasing demand for fuel and reduced reliability on fossil fuels, the United States government encourages fuel production from sources other than petroleum. The Renewable Fuel Standard (RFS) program under the Energy Policy Act (EPAct) of 2005 required 7.5 billion gallons of renewable fuel to be blended into gasoline by 2012 (EPA, 2012). The Energy Independence and Security Act (EISA) of 2007 expanded the RFS program and increased the volume of renewable fuel required to be blended into transportation fuel to 36 billion gallons by 2022 (EISA, 2007). The Act identifies corn starch, cellulosic biofuels, and advanced biofuels as renewable fuel sources. Fuel requirement from corn starch ethanol is going to plateau at 15 billion gallons in 2015 (EISA, 2007). Corn, soybean, cotton, winter wheat, etc. falls under the category of first generation biofuel crops. Studies have reported eutrophication problems with the production of first generation biofuel crops. Increased uses of corn and soybeans have been reported to exacerbate eutrophication problems in Midwest US and Gulf of Mexico (Powers, 2007). Producing 15 billion gallons of corn based ethanol even by the year 2022 instead of 2015 will increase the average annual flux of dissolved inorganic nitrogen export by the Mississippi and Atchafalaya rivers to the Gulf of Mexico exceeding the hypoxia target by 95 per cent (Donner and Kucharik, 2008). Babcock et al. (2007) reported that the production of continuous corn, on all croplands (mostly corn and soybeans including lands that are already taken out of production), over a period of 20 years (1986 to 2005) in northeast Iowa's Maquoketa River watershed could have increased sediment, nitrate-nitrogen, total nitrogen, and total phosphorus loading at the outlet of the watershed by 23, 147, 150, and 138 per cent, respectively. Because of the fact that oil requirement from corn starch is projected to plateau in 2015 and increasing area under first generation biofuel crops has potential to exacerbate eutrophication as reported by other researchers, the research community has focused attention on second generation biofuel crops.

Second generation biofuel crops can be divided into two major categories: agricultural residues (e.g. corn stover), and dedicated energy crops (e.g. switchgrass and miscanthus) grown exclusively for fuel production. To meet the required target volume of 16 billion gallons mandated by EISA of 2007 for second generation biofuel crops, three production strategies can be implemented: displacement, intensification and expansion/targeting approach (Kloverpris et al., 2008). Displacement occurs when one crop displaces other, or when a field is cultivated for biofuel rather than food production. An increase in corn production as a biofuel rather than food crop because of high oil prices for corn ethanol (Harrison, 2009), is also an example of displacement approach. However, increase in corn production as a biofuel crop may result in the food vs. fuel debate (Harrison, 2009). The second strategy, intensification, involves an increase in the yield of biofuel crop production with increase in inputs like fertilizer application, pesticide application, irrigation level, and the cropping intensity; however increase in yield per unit of input is subjected to diminishing returns (Kloverpris et al., 2008). The third strategy, expansion/targeting, involves the conversion of marginal/degraded land to biofuel crop production.

Out of various strategies available for biofuel crop production, targeting marginal/degraded land is believed to have potential for second generation biofuel crops

(Campbell et al., 2008; Kort et al., 1998). Conversion of 10% of marginal lands along the Missouri and Mississippi rivers to energy crop production has been reported to result in annual production of around 8 billion gallons of advanced biofuels (Geiver, 2012). However, marginal land is not a static term and can be defined in many ways. Strijker (2005) defined marginal land as land with marginal economic viability. Tang et al. (2010) considered wasteland and paddy land fallowed in winter as marginal land. Indonesian government states that unproductive lands with high acidity should be considered marginal land. Marginal land can also be defined based on the land capability class (LCC) developed by the United States Department of Agriculture-Natural Resource Conservation Service (USGS-NRCS), as LCC separates different types of land per the soil's capability to support crops (NRCS, 2012). Marginal land can be defined with a single criterion (Strijker, 2005) or multiple criteria (Gopalakrishnan et al., 2011). In this study, land capability classes III and IV will be defined as marginal land.

Conducting field experiments to understand the long-term environmental impacts of biofuel crop production on marginal land can be very expensive. Therefore, use of hydrologic and water quality (H/WQ) watershed models have been suggested as an appropriate tool to predict sediment and nutrient loss under land use change, management, and climate conditions (Singh and Frevert, 2006). Among several H/WQ models, the soil and water assessment tool (SWAT) model was selected for the present study because of its abilities to model agriculture dominated watersheds (Babcock et al., 2007; Gu and Sahu, 2009; Love and Nejadhashemi, 2011). Relevant to this study, the SWAT model has been extensively used to analyze the impact of biofuel crops simulation on hydrology and water quality at the watershed and regional scale (ranging from 51.3 to 48.9×10^4 square kilometers) (Babcock et al., 2007; Folle, 2010; Gassman et al., 2008; Gu and Sahu, 2009; Love and Nejadhashemi, 2011; Nelson et al., 2006; Ng et al., 2010; Secchi et al., 2008). SWAT uses ArcSWAT as an interface to input the required data. ArcSWAT is an extension of ArcMap/ArcGIS - one of the Environmental Systems Research Institute/ESRI software products (ESRI, 2012). Based on user defined inputs, ArcSWAT divides a watershed into subwatersheds and subwatersheds into hydrological response units (HRUs) (Figure 1.1).

Biofuel crops can be simulated at the watershed, subwatershed, or HRU scale. In SWAT, watershed or subwatershed, in general, are large areas with various land uses, soils, and slopes. Conversely, HRUs are the unique combination of land use, soil, and slope, and are the lowest simulation level in SWAT with specific identification numbers (IDs). However, HRUs are discontinuous land masses in a subwatershed (Gassman et al., 2007; Pai et al., 2012). This poses a challenge in the simulation of biofuel crops on the location specific marginal land. For instance, assume that there is a typical model setup containing a rectangular subwatershed with four quadrants representing the arrangement of HRUs (Figure 1.2). Assume that marginal land is located in the first quadrant (Figure 1.3). Therefore, to simulate biofuel crop production on marginal land, quadrant no. 1 should only be the focus of simulation. However, in conventional model setup, if biofuel crop is simulated on HRU no. 1, then that crop will also get simulated in the fourth quadrant because of the presence of the same HRU in the fourth quadrant of the subwatershed. Thus, spatial discontinuity among HRUs will not allow simulation of biofuel crops on specific locations (i.e. marginal lands). Therefore, there is a need to develop a novel approach to simulate biofuel crops on HRUs representing marginal land for accurate spatial representation of land use in the watershed.

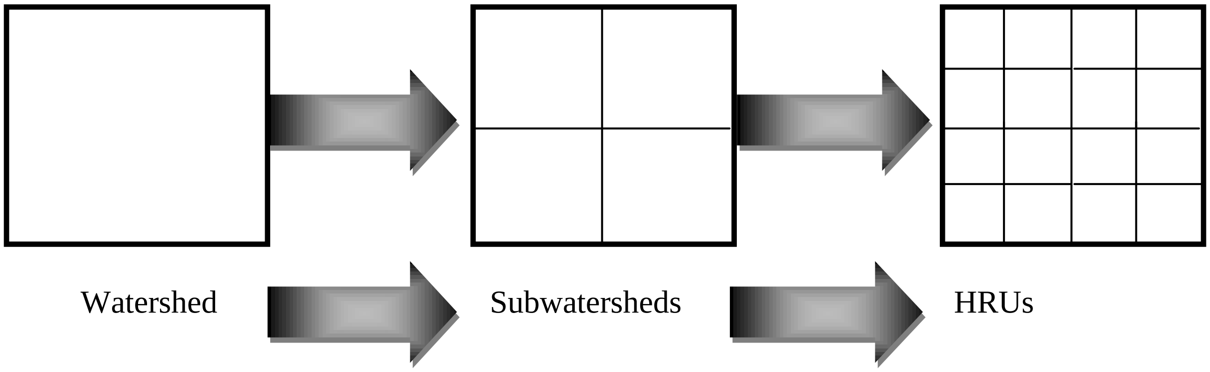
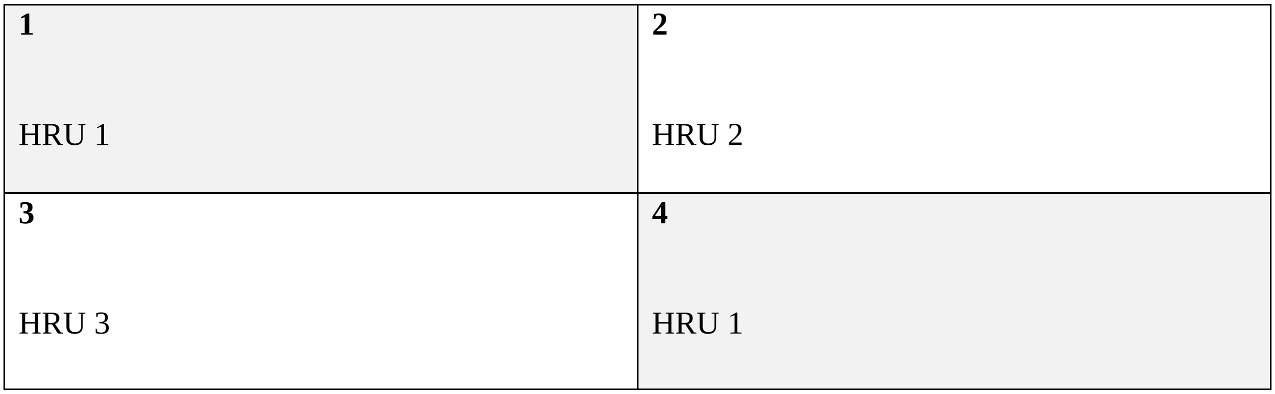


Figure 1.1: Hypothetical division of a watershed in the soil and water assessment tool (SWAT) model.



1 HRU 1	**2** HRU 2
3 HRU 3	**4** HRU 1

Figure 1.2: Hypothetical distribution of hydrological response units (HRUs) in a subwatershed.

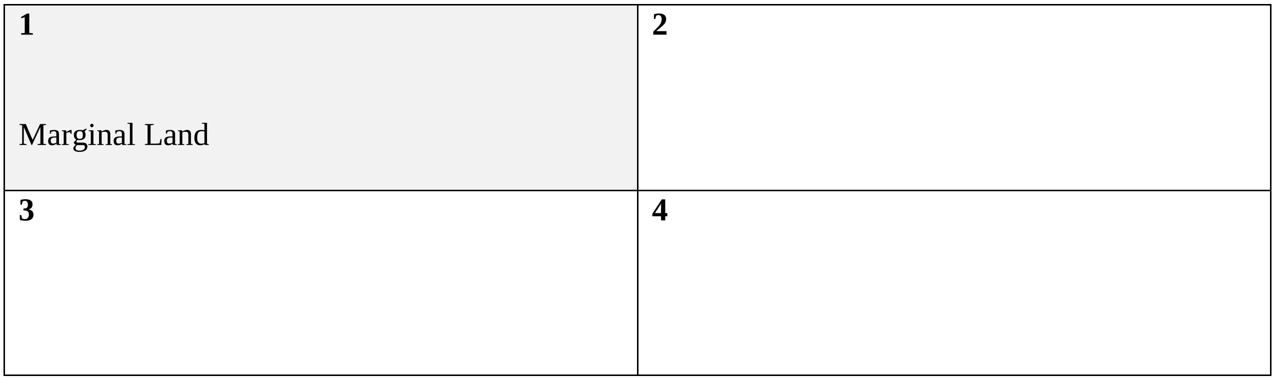


Figure 1.3: Hypothetical location of marginal land in a subwatershed.

Spatial discretization affects model outputs. Finer digital elevation model (DEM) resolutions increase the simulated flow (Chaubey et al., 2005; Cho and Lee, 2001), and targeting of spatial areas results in greater reductions in simulated pollutant loadings (Tuppad et al., 2010). Therefore, correct spatial representation of biofuel crops on marginal lands may help quantify their impacts on the water quality at the HRU scale. Analysis of pollutant losses from the HRUs to their respective subwatershed's reach includes the maximum possible spatial detail pertaining to land cover and soil combinations (White et al., 2009). In this study, the L'Anguille River watershed (LRW) was used as a study area. This is an agricultural dominated watershed located in Mississippi Delta ecoregion of east central Arkansas and is designated by the hydrological unit code (HUC) 08020205 (Seaber, 1994). The Arkansas Department of Environmental Quality (ADEQ) has included the L'Anguille River in the list of impaired water bodies (ADEQ, 2012). Marginal land on this watershed was simulated with the biofuel crops to analyze the water quality impacts of biofuel crop simulations at the HRU scale.

1.2 OBJECTIVES

This study was focused on developing a novel simulation approach for targeted simulation of biofuel crop production on marginal lands for quantifying impacts on water quality at the HRU scale. The following objectives were accomplished in this study:

1) Development of a novel simulation approach to incorporate marginal land in the SWAT model followed by calibration and validation of the model for the L'Anguille River watershed.
2) Comparison between the conventional and novel approach for water quality impacts of biofuel crop simulation on marginal land.

3) Analysis of the water quality impacts of biofuel crop simulation on the targeted marginal land (defined by the novel approach) at the HRU scale.

1.3 HYPOTHESIS

Null Hypothesis: Biofuel crop simulation on marginal land is not predicting reduced pollutant losses from marginal HRUs to their respective subwatersheds's reach.

Alternate Hypothesis: Biofuel crop simulation on marginal land is predicting reduced pollutant losses from marginal HRUs to their respective subwatersheds's reach.

1.4 SCOPE OF STUDY

This study will be helpful in targeted incorporation of marginal lands, based on user-defined criteria, in the SWAT model. The major benefit of this study is that marginal land can be spatially defined at the HRU scale. Simulating biofuel crops on marginal land may help in the quantification of its water quality impacts.

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CHAPTER II

BACKGROUND

The overall goal of this study was to develop a novel simulation approach for targeted incorporation of marginal lands in the soil and water assessment tool (SWAT) model at the hydrological response unit (HRU) level, and analyze water quality impacts of biofuel crop simulation on this land. Before proceeding to the methodology section, it was important to discuss types of biofuel crops and their corresponding fuel production share as mandated by the Energy Independence and Security Act of 2007 (Section 2.1). Moreover, simulation of biofuel crops with the SWAT model at the watershed/plot and regional scale (Section 2.2), calibration and validation of the SWAT model (Section 2.3), and the land cover/plant growth database present in the SWAT model (Section 2.4) were also discussed. Furthermore, impacts of spatial discretization on model outputs were discussed (Section 2.5). Towards the end, a brief review on yield analysis was presented (Section 2.6) followed by the summary of the entire chapter (Section 2.7) and, finally, the references (Section 2.8).

2.1 BIOFUEL CROPS

Biofuel crops can be classified as first, second, and third generation biofuels. An example of a first generation biofuel crop is corn. An example of a second generation biofuel crop is switchgrass. An example of a third generation biofuel crop is algae. Corn and soybeans have been reported to exacerbate the eutrophication problem in Midwest US and Gulf of Mexico (Powers, 2007). Increased demand for corn ethanol and the price inflation of food items that depend on corn are the reasons responsible for the food vs. fuel debate (Harrison, 2009).

However, Campbell et al. (2008) reported that the production of second generation biofuel crops on marginal land will eventually result in pacifying the food vs. fuel debate. Moreover, 26% to 55% of global fuel consumption can be met by planting second generation biofuel crops on the degraded or marginal land, and low-input high-diversity native perennials on marginal productivity grasslands (Cai et al., 2011). Switchgrass and miscanthus, can also play an important role in reducing erosion on marginal land (Lewandowski et al., 2003). Furthermore, switchgrass can act as a buffer for the field edges when grown on marginal land (Kort et al., 1998). As miscanthus has the ability to recycle nutrients at the end of the growing season, it can be grown successfully on poor soil/marginal land (Dohleman et al., 2010). In Arkansas, switchgrass is receiving continuous interest as a biofuel crop (Popp, 2007). Recently, the Biomass Crop Assistance Program (BCAP) launched a project, named Paragould, in the north east Arkansas. This project aims at producing 50,000 acres of miscanthus. As a result, it can be said that the research community has been increasingly focusing on second generation biofuel crops that mainly include switchgrass and miscanthus.

The first renewable fuel volume mandate in the United States was established by the Renewable Fuel Standard (RFS) under the Energy Policy Act (EPAct) of 2005 (EPA, 2012). Under this EPAct, 7.5 billion gallons of renewable fuel were required by the RFS program to be blended into gasoline by 2012. However, the RFS program was expanded under the Energy Independence and Security Act (EISA) of 2007. The EISA of 2007 mandated that 36 billion gallons of renewable fuel should be produced by 2022. The potential biofuel sources to contribute to this demand are corn starch (first generation biofuel), cellulosic (second generation biofuel), and other advanced biofuels (third generation biofuel) (EISA, 2007). Renewable fuel requirements in billions of gallons mandated by EISA of 2007 are shown in Table (2.1). As per

Table (2.1), 0.1 billion gallons of fuel from cellulosic feedstock was expected to be produced by 2010. However, the Environmental Protection Agency (EPA) revised the target volume of 0.1 billion gallons to 6.5 million gallons. The revised volume is significantly less than the earlier projected volume. As a result, it is imperative that cellulosic biofuel crop production will rise significantly in the near future in order to meet the 16 billion gallons of cellulosic biofuel demand by 2022. Conversely, fuel mandated from corn starch ethanol will plateau at 15 billion gallons in 2015 (EISA, 2007).

2.2 SIMULATION OF BIOFUEL CROPS WITH THE SWAT MODEL

Relevant to this study, the SWAT model has been used to simulate biofuel crops and analyze the impacts of biofuel crop simulation on water quality. Various past studies were organized as per the simulation of biofuel crops at the watershed/plot and regional scale, and are described in the following Sub-Sections 2.2.1 and 2.2.2.

2.2.1 WATERSHED/PLOT SCALE STUDIES

In one of the studies conducted at the watershed scale, Babcock et al. (2007) modeled corn and switchgrass in eastern Iowa's Maquoketa watershed (size 4799 square kilometers) from the year 1986 to 2005. On an average annual basis, they compared three scenarios with the baseline (current land uses): all cropland converted to switchgrass, all cropland converted to corn cultivation (50% biomass removal rate), and switchgrass placed on highly erodible land with continuous corn (50% biomass removal rate) on the less erodible land. They found that the first scenario resulted in 84%, 44%, 53%, and 83% reduction in sediments, nitrate-nitrogen (NO3-N), total nitrogen (TN), and total phosphorus (TP) respectively at the outlet of the watershed. The second scenario resulted in 23%, 147%, 150%, and 138% increase in sediments, NO3-N, TN, and TP respectively at the outlet of the watershed. The third scenario resulted in 19% and 43% reduction in sediments and TP respectively, and 48% and 32% increase in NO3-N and TP respectively at the outlet of the watershed.

Folle (2010) modeled corn and switchgrass in Minnesota's Le Sueur River watershed (size 2850 square kilometers) from the year 1990 to 2006. He considered three scenarios on an average annual basis: shift from a corn-soybean to a corn-corn-soybean rotation at 17% per year expansion, switchgrass planted on environmentally sensitive landscapes (less than 2% slope), and removal of crop residue for cellulosic biofuel production. He observed reductions in sediment yield (73%), phosphorus (39%), and NO3-N (9%) at the watershed outlet with the simulation of switchgrass on environmentally sensitive landscapes as compared to expanding corn-corn-soybean rotation or removing crop residues.

Gassman et al. (2008) modeled corn, switchgrass and fescue in north-central Iowa's Boone River watershed (size 2370 square kilometers) from 1986 to 2006. The first six scenarios considered conversion of different percentages of corn-soybean acreage (15%, 15%, 15%, 50%, 50%, and 100%) to continuous corn over a range of 172-224 kg-N/ha application rates. The next three scenarios considered conversion of different percentages of corn-soybean acreage (15%, 50%, and 75%) to switchgrass at 156.8 kg-N/ha application rates. The last three scenarios considered conversion of different percentages of corn-soybean acreage (15%, 50%, and 75%) to fescue at 156.8 kg-N/ha. They concluded that switchgrass and fescue were reducing more sediment (5% to 39% reduction) and NO3-N (3% to 26% reduction) at the outlet of the watershed when compared to corn (2% to 11% sediment reduction whereas 9% to 100% NO3-N increase).

Gu and Sahu (2009) modeled switchgrass in central Iowa's Walnut Creek watershed (size 51 square kilometers) from the year 1992 to 2000. They identified high impact subwatersheds based on the total NO3-N and per unit area NO3-N loadings. Four scenarios were considered: 10%, 20%, 30%, and 50% of the subwatershed area were simulated with switchgrass strips. They concluded that there was more reduction in NO3-N with the increase in the size of the area simulated with switchgrass strips. However, switchgrass strips with 10% to 20% subwatershed area were more efficient in reducing NO3-N compared to switchgrass strips with 30% to 50% subwatershed area. They also reported that on an average rainfall year, there was a reduction of 55% to 90% in NO3-N at the outlet of the watershed with contour strips occupying 10% to 50% of the subwatershed area.

Nelson et al. (2006) modeled switchgrass in northeast Kansas' Delaware basin (size 3000 square kilometers) from the year 1966 to 1989. They simulated switchgrass on conventional commodity crop rotations (corn, soybean, grain sorghum, and wheat) over a range of 0-224 kg-N/ha fertilizer application. They reported an average reduction of 99%, 55%, 34%, and 98% in sediment yield, surface runoff, NO3-N in surface runoff, and edge of field erosion respectively.

Ng et al. (2010) modeled miscanthus in the Salt Creek watershed, Illinois (size 303 square kilometers) from the year 1988 to 2003. First four scenarios: 0% (no land use change), 10%, 25%, and 50% land use change (corn-soybean 1:1 rotation) to miscanthus were analyzed each at a fertilizer application rate of 30, 60 and 90 kg-N/ha. The fifth scenario (all soybean scenario) was conversion of all croplands to soybean production at a fertilizer application rate of

90 kg-N/ha. They observed that the NO3-N load was decreased with the increase in the land use change to miscanthus. Moreover, at a fertilizer application rate of 30, 60, and 90 kg-N/ha, they reported a reduction of 34%, 32%, and 29% in the NO3-N at the outlet of the watershed when 50% land uses were changed to miscanthus. In addition, they also concluded that miscanthus was able to reduce more NO3-N as compared to the all soybean scenario.

Sarkar et al. (2011) modeled switchgrass plots (plot size 510 square meters) in the Pee Dee Research and Educational Center at Florence, South Carolina from the year 2007 to 2021. Initially cotton was simulated from the year 1985 to 2006. They observed that there was an average annual reduction of 87% in TN losses when switchgrass was simulated at a nitrogen fertilizer rate of 68 kg/ha compared to when cotton was simulated at a nitrogen fertilizer rate of 90 kg/ha.

2.2.2 REGIONAL SCALE STUDIES

Apart from modeling biofuel crops at the watershed/plot scale, SWAT was also used at the regional scale. Love and Nejadhashemi (2011) modeled corn, canola, cereal rye, sorghum, soybean, miscanthus, corn stover, switchgrass, and native grasses in four watersheds: Saginaw River (size 15262.8 square kilometers), St. Clair-Detroit (size 8182 square kilometers), southeastern Lake Michigan (size 18894 square kilometers), and St. Joseph (size 11018 square kilometers) located in the lower part of Michigan. The modeling period ranged from 1990 to 2008. They considered four land use change scenarios: row crops (corn, soybean, wheat, etc.) converted to bioenergy crops, other crops (sugarbeets, potatoes, dry beans, etc.) converted to bioenergy crops, marginal land (fallow cropland, pasture, wasteland, etc.) converted to bioenergy crops, and all of the above three land uses (row crops, other crops, and marginal land) converted to bioenergy crops. For scenario 1, they reported that the perennial grasses, except miscanthus, reduced the sediment, nitrogen, and phosphorus loadings at the outlet of the watershed. For scenario 2, 3 and 4, they recommended no land use change in areas with preexisting high nitrogen levels. However, miscanthus and native grasses were considered suitable on marginal land where nitrogen levels are of less concern.

Secchi et al. (2009) modeled switchgrass in the Upper Mississippi River Basin (UMRB) from the year 1981 to 2003. UMRB has an area of 489,508 square kilometers and include parts of Illinois, Indiana, Iowa, Michigan, Minnesota, Missouri, South Dakota and Wisconsin. They compared six scenarios with the baseline condition (current land uses) for analyzing water quality impacts of switchgrass simulation at the outlet of the watershed. The first three scenarios assumed prices recommended by Food and Agricultural Policy Research institute (FAPRI) with no switchgrass cultivation, with switchgrass cultivation, and with targeted switchgrass cultivation (switchgrass produced on most erodible land), respectively. The next three scenarios assumed prices recommended by Chicago Board of Trade (CBOT) with no switchgrass cultivation, with switchgrass cultivation, and with targeted switchgrass cultivation, respectively. They found that there was an increase in the sediment and phosphorus and a decrease in the NO3-N at the outlet of the watershed with the switchgrass and targeted swichgrass production scenario under both the FABRI and CBOT prices.

Two of the above land use change studies (Gassman et al., 2008; Ng et al., 2010) discussed conversion of different percentages of land uses for biofuel crop production without any information about the spatial distribution of these converted land uses. A common theme among land use change studies is targeting. Targeting refers to identification of critical areas and subsequently simulating suitable crops on these areas to reduce pollutant loadings. Marginal land is one of the targeting areas. For instance, two other land use change studies (Babcock et al., 2007; Folle, 2010) simulated biofuel crops on marginal land such as highly erodible land, and environmentally sensitive landscapes (low productivity land, critical contributing areas, and land with greater slopes). However, no studies have been conducted that discusses the challenges a modeler faces when deciding a mechanism to integrate existing marginal land delineation into a watershed model framework. For example, if the existing marginal land constitutes the upper half part of a subwatershed, then that upper half should only be simulated with the biofuel crops. This will result in no land use conversion in the lower half of a subwatershed. This type of simulation on existing marginal land is possible only at the HRU level (lowest simulation level) because of the fact that subwatersheds are large areas with various land uses, soils, and slopes. Hence, there is a need to discuss challenges that may encounter while integrating existing marginal land into the watershed model framework.

2.3 CALIBRATION AND VALIDATION OF THE SWAT MODEL

In general, many studies agreed that spatially variable hydrological processes can be more realistically simulated by using a multi-site and multi-variable calibration approach (Cao et al., 2006; El-Nasr et al., 2005; Li et al., 2010; Niraula et al., 2012; Schuol and Abbaspour, 2006; White and Chaubey, 2005; Zhang et al., 2008; Zhang et al., 2010). Multi-site calibrations are becoming common with the development of spatially distributed hydrologic models (Zhang et al., 2008). Moreover, better goodness of fit can be achieved from parameters estimated with the multi-site approach as compared to a single-site approach (Zhang et al., 2008). Migliaccio and Chaubey (2007) reported that all sites should be calibrated simultaneously to overcome any deviation in the parameterization process that arises because of calibrating one site at a time. Moriasi et al. (2007) reported that a multi-objective approach helps in minimizing the errors as it optimizes various statistics simultaneously. Multi-variable calibration involves sediment and nutrients calibrations along with flow. It is recommended to calibrate flow first; followed by sediment, TP and NO3-N (White and Chaubey, 2005). It is also recommended to calibrate the gauge furthest upstream first followed by calibration for downstream gauges, however calibrated parameters for the upstream drainage area should not change while calibrating the watershed at a downstream gauge (Arnold et al., 2011). Overall, it can be said that the multi-site, multi-objective, and multi-variable calibration and validation approach is the most robust method that should be used to increase the reliability of watershed models.

2.4 LAND COVER/PLANT GROWTH DATABASE IN THE SWAT MODEL

The land cover/plant growth parameters for most of the crops, including swichgrass, are available in the SWAT land cover/plant growth database. Miscanthus, being a relatively new second generation biofuel crop as compared to switchgrass, lacks its parameters in the land cover/plant growth database. In order to model miscanthus in the SWAT model, Ng et al. (2010) divided the plant growth parameters into three categories: optimal biomass growth under zero stress conditions, stress parameters for nitrogen and phosphorous, and miscellaneous parameters not included in the first two subsets. Love and Nejadhashemi (2011) defined four parameter values for miscanthus based on the literature reviews, expert opinions, and the existing parameter values defined for switchgrass in SWAT land cover/plant growth database.These four parameters were maximum potential leaf area index (BLAI), the fraction of growing season when leaf area begins to decline (DLAI), minimum temperature for plant growth (T_BASE), and maximum canopy height (CHTMX). Apart from the above four parameters, all other parameters were kept similar to that of switchgrass in the SWAT land cover/plant growth database. In summary, it can be said that the land cover/plant growth parameters should be selected with caution as per the condition of the watershed.

2.5 IMPACT OF SPATIAL DISCRETIZATION ON MODEL OUTPUTS

Spatial discretization may impact the output of models and the uncertainties associated with outputs. Studies have evaluated effects of various spatial discretizations on model outputs including digital elevation model (DEM) resolutions, land use resolutions, soil resolutions, land cover misclassifications, and weather. Model outputs have also been analyzed by targeting spatial areas based on simulated erosion rate and other field outputs. Chaubey et al. (2005) analyzed the effect of digital elevation model (DEM) resolutions on model outputs in the Moores Creek watershed, Arkansas. They analyzed seven different types of DEM resolutions: 30m, 100m, 150m, 200m, 300m, 500m, and 1000m. They reported that decreased DEM resolutions resulted in decreased simulated stream flow and NO3-N, whereas the simulated TP did not show continuously decreased pattern. Cho and Lee (2001) analyzed the effect of two different DEM resolutions (1:24000 and 1:250000) on the model output for runoff volume in the Broadhead watershed, New Jersey. They reported that the DEM with the finer resolution (1:24000) resulted in the increased runoff volume, which might be due to the simulation of increased average slope with the finer DEM resolution. Cotter et al. (2003) reported the effect of different resolutions of land use, soil, and DEM (each at 30m, 100m, 150m, 200m, 300m, 500m, and 1000m) on model outputs for flow, sediment, NO3-N, and TP in the Moores Creek watershed, Arkansas. Out of DEM, land use, and soil, DEM affected model outputs the most by increasing the slope length at courser DEM resolutions. Coarser land use resolutions affected the sediment, TP, and NO3-N by changing the distributions of pasture, forest and urban areas in the watershed. Different soil resolution affected the sediment and TP, whereas there was no significant effect on the flow and NO3-N. Miller et al. (2007) analyzed the effect of land cover misclassification on the model output uncertainty in the Upper San Pedro River basin, Arizona. Hundred different land covers were used for 40 different watershed sizes under two different rainfall events. They reported that the errors related with the land cover misclassification increased with the increase in watershed size, and decreased with the increase in rainfall magnitude. Regarding weather data, studies have reported that the model performance in simulating streamflow was improved by using the Next-Generation Radar (NEXRAD) derived rainfall data compared to the rain gauge data (Tobin and Bennett, 2009; Tuppad et al., 2010a). Beeson et al. (2011) reported that superior results for the streamflow simulation can be obtained by combining the rain gauge and NEXRAD data. Apart from analyzing the effect of spatial input data on model outputs, some studies have also targeted spatial areas. Tuppad et al. (2010b) analyzed the effect of targeting spatial areas on model outputs for sediment, TP, and TN in the Smoky Hill River watershed, Kansas. They classified the targeted areas based on the simulated erosion rate at the subwatershed level. They reported that simulating best management practices (BMPs) on half of the targeted land area as compared to the random land areas would result in a 10% reduction for the pollutant loads on an annual average basis at the subwatershed level. Daggupati et al. (2009) targeted field scale outputs for sediment, nitrogen, and phosphorus yields using different inputs for soil (STATSGO vs. SSURGO), land uses (Field vs. NLCD vs. NASS), and models (SWAT vs. RUSLE) in the Black Cattle Creek watershed, Kansas. Top 10% SWAT simulated fields by sediment yields changed by 37% with different soil inputs, 95% with different land use inputs, and 75% with different model types. Pai et al. (2012) mapped field outputs from the HRU outputs using the four different methods: mean, model, geometric mean, and area-weighted mean in the Second Creek watershed, Arkansas. They reported that the HRU outputs were best mapped to field outputs using the area-weighted mean approach, and can be used to identify and target critical source areas. In SWAT, HRUs are the lowest simulation level. However, as HRUs are not spatially defined in a subwatershed or are discontinuous land masses in a subwatershed (Gassman et al., 2007; Pai et al., 2012), simulation of biofuel crops on targeted HRUs is a challenge. This is because of the fact that if some targeted HRUs are simulated with biofuel crops, all HRUs having same identification numbers as that of targeted HRUs will also be simulated. Therefore, there is a need to simulate biofuel crops only on targeted HRUs.

2.6 YIELD ANALYSIS FOR THE BIOFUEL CROPS

Crop yield affects the water and nutrient balance in an agricultural watershed (Nair et al., 2011). Moreover, even to perform a realistic benefit cost analysis; there is a growing interest in evaluating the impact of conservation practices on both crop yield and water quality (Nair et al., 2011). Studies have compared the SWAT simulated yield values for the second generation biofuel crops with the reported literature values. Ng et al. (2010) compared the predicted miscanthus yield data with the field data in the Salt Creek watershed, Illinois. Wu and Liu (2012) compared the SWAT simulated switchgrass and miscanthus yield data with the values reported in literatures for the Iowa River basin, Iowa. Baskaran et al. (2010) evaluated the sustainability of switchgrass at the regional scale for the eastern U.S. by validating the SWAT simulated yield against the values reported by an empirical model based on the field trials. In summary, it can be said that an additional analysis performed for the simulated yield will increase the confidence in model simulations.

2.7 SUMMARY

Biofuel crops, mainly switchgrass and miscanthus, are getting increased attention from the research community. Biofuel crops have been simulated with the SWAT model both at the watershed/plot and regional scales. In order to successfully simulate biofuel crops, a robust calibration and validation approach is recommended namely multi-site, multi-objective, and multi-variable approach. While simulating biofuel crops, land cover/plant growth parameters for the considered crops should be selected with caution as to the condition of the watershed. Simulating biofuel crops on targeted HRUs representing marginal land is a challenge considering the fact that HRUs are not spatially defined in the SWAT model. Therefore, a novel simulation approach is required to first integrate marginal land into a watershed model in such a way that the HRUs get a spatial definition, and then simulate biofuel crops on targeted HRUs representing marginal land.

Table 2.1: Renewable fuel requirements mandated by the Energy Independence and Security Act (EISA) of 2007.

EISA Renewable Fuel Volume Requirements (billion gallons)				
	Cellulosic Biofuel	Biomass Based Diesel	Advanced Biofuel	Total Renewable Fuel
2010	0.1	0.65	0.95	**12.95**
2011	0.25	0.80	1.35	**13.95**
2012	0.5	1.0	2.0	**15.2**
2013	1.0	-	2.75	**16.55**
2014	1.75	-	3.75	**18.15**
2015	3.0	-	5.5	**20.5**
2016	4.25	-	7.25	**22.25**
2017	5.5	-	9.0	**24.0**
2018	7.0	-	11.0	**26.0**
2019	8.5	-	13.0	**28.0**
2020	10.5	-	15.0	**30.0**
2021	13.5	-	18.0	**33.0**
2022	16.0	-	21.0	**36.0**

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CHAPTER III

MATERIALS AND METHODS

Section 3.1 provides the description of the study area. Sections 3.2, 3.3, 3.4, and 3.5 include objective 1 (**development of a novel simulation approach to incorporate marginal land in the SWAT model followed by calibration and validation of the model for the L'Anguille River watershed**). The procedures for the development of novel approach, model setup, and model inputs are described in Sections 3.2, 3.3, 3.4, respectively. Section 3.5 details the procedure for sensitivity analysis, calibration, and validation of the model. Section 3.6 defines suitable marginal land for biofuel crop simulation and appropriate land cover/plant growth parameters and management practices for biofuel crops. Sections 3.7 and 3.8 describe the procedures for evaluating objective 2 (**comparison between the conventional and novel approach for water quality impacts of biofuel crop simulation on marginal land**) and objective 3 [**analysis of the water quality impacts of biofuel crop simulation on marginal land (defined by the novel approach) at the HRU scale]**. Section 3.9 details the procedure for analyzing biofuel crops yield and nitrogen uptake simulated by the model for evaluating the level of confidence in model simulations. Finally, Section 3.10 lists all the references that have been cited in this chapter.

3.1 STUDY AREA

The L'Anguille River watershed (LRW) is located in the Mississippi Delta ecoregion of east central Arkansas and is designated by the hydrological unit code (HUC) 08020205 (Seaber, 1994) (Figure 3.1). The total drainage area for this watershed is 2,474 square kilometers and covers a portion of Craighead, Cross, Lee, Poinsett, St. Francis, and Woodruff counties. The LRW is relatively a flat watershed with 90 percent slopes in the range of 0 to 3 percent. Crowley's Ridge, lying on the eastern part of the watershed, has slopes ranging from 8 to 38 percent (Saraswat et al., 2008). Land use and land cover in the LRW watershed consist of soybean (43.6 percent), forest (18.9 percent), rice (14.9 percent), cotton (6.9 percent), pasture (5.1 percent), corn (4.5 percent), urban (3.5 percent), water (1.4 percent), and generic agriculture (mixed land uses that are not statistically significant: tomatoes, watermelon, etc.) (1.2 percent) (CAST, 2007). Row crops dominate in the LRW occupying approximately 70 percent of its area. Hydrological soil groups C and D (high runoff potential) were identified as the dominant soil groups in the LRW (Saraswat et al., 2008). Arkansas Department of Environmental Quality (ADEQ) has included the L'Anguille River in the list of impaired water bodies (ADEQ, 2012). Moreover, Arkansas Natural Resources Commission (ANRC) designated the LRW as a priority watershed for the 2011-2016 NPS Pollution Management Plan with siltation, nutrients, low dissolved oxygen, total dissolved soils, chlorides, and sulfates as the pollutant of concern (ADEQ, 2011). As a result, this watershed was selected for conducting the land use change analysis relating to the simulation of biofuel crops so that the water quality impacts can be analyzed.

3.2 DEVELOPMENT OF A NOVEL SIMULATION APPROACH

In the novel approach, a modified land use and land cover layer was prepared and input into the model in place of the original land use and land cover layer. All other model inputs were the same as used for the conventional approach. Moreover, same procedure was followed for the sensitivity analysis, and calibration and validation of the model to determine the pollutant losses (sediment, total phosphorus/TP, and total nitrogen/TN). To conceptualize the difference in the novel approach from the conventional, an overview of both the approaches is shown in Figure (3.2).

In the conventional approach, typically adopted by SWAT modelers, when biofuel crops were simulated on identified marginal HRUs (highlighted with a boundary in Figure (3.2)), additional HRUs, that were not a part of the targeted land scape (i.e. marginal land), also got simulated because of the non-spatial nature of HRUs (Gassman et al., 2007; Pai et al., 2012). For this reason, a novel approach was developed in which the HRUs, located on marginal lands, were identified with the help of the modified land use and land cover layer that was prepared before the model setup. Appendix (A) contains step-by-step procedure for preparing the modified land use and land cover layer.

In the modified land use and land cover layer, the land uses that overlapped marginal land were labeled as a new category. While developing the new categories, SWAT procedure for identifying land uses using four letter codes was followed. As a result, if some portion of a land use, say soybean, overlapped marginal land, that portion of soybean (SOYB) was reclassified as a new land use category and named SOYM instead of SOYB. This resulted in two sub-categories for soybean: one on marginal land (SOYM) and the other on non-marginal land (SOYB). The new land use categories (e.g. SOYM) were incorporated in the “look up table” of the SWAT model. This look up table linked the numerical values of land uses in the attribute table of the modified land use and land cover layer with their respective land uses names. All reclassified marginal and non-marginal land use categories were included in the look up table (Figure 3.3). Moreover, SWAT has a default land cover/plant growth database (crop.dat) that include land cover/plant growth parameters for common land uses designated with four letter codes (e.g. SOYB). The new land use categories (e.g. SOYM) were defined in SWAT's land cover/plant growth database with same parameter values as that of original land use (e.g. SOYB) (Appendix B). As SOYB and SOYM differed only on the basis of marginal land criteria, their management practices were kept the same. Overall, nine land uses in the original land use and land cover layer for the LRW were reclassified into 18 land use categories in the modified land use and land cover layer (Figure 3.4).

3.3 SWAT MODEL INPUTS

The Soil and Water Assessment Tool (SWAT) model (SWAT2009, rev. 488) was used in this study. The SWAT model is a watershed scale model which operates on a daily basis to predict the impacts of management on hydrology, sediment, and agricultural chemical yields (Arnold et al., 1998). Hydrology, weather, sedimentation, soil temperature, crop growth, nutrients, pesticides, and agricultural management are the eight major subwatershed components in SWAT (Arnold et al., 1998). In this study, SWAT was used to simulate biofuel crops on marginal land in the LRW. Marginal land was defined based on the Soil Survey Geographic (SSURGO) Land Capability Class (LCC) developed by the United States Department of Agriculture – Natural Resource Conservation Service (USDA – NRCS). SSURGO is the most detailed soil database available for Arkansas. SSURGO LCC ranges from I to VIII, as per the soil's capability to support crops. LCC I to IV could be used for agricultural purposes (NRCS, 2012). However, Classes V to VIII are not meant for agriculture; rather, recreational activities, urban areas, etc. are common features of these classes. LCC I and II are the most favorable for agricultural crop production and are likely to be used for the production of food crops. Therefore, LCC III and IV were selected as marginal land for the simulation of second generation biofuel crops. A marginal land layer for the LRW was created in ArcMap/ArcGIS (version 9.3.1) based on the SSURGO LCC III and IV. This marginal land layer depicts the spatial distribution of marginal land in the LRW and covers 52 percent of its area (Figure 3.5).

SWAT inputs for the LRW were obtained from various state and national agencies (Table 3.1). All data layers were downloaded in the North American Datum 1983 (NAD83) Universal Transverse Mercator Zone 15N (UTM-Zone 15N) projection system. All inputs were the same for the conventional and novel approach except the land use and land cover layer. In the novel approach, the modified land use and land cover layer with 18 reclassified land uses was inputted into the SWAT model via ArcSWAT, an extension of ArcMap/ArcGIS. Processing of model inputs and other model related data are explained below:

Digital elevation model (DEM): The DEM for the LRW was downloaded from the GeoStor website. The z unit of this layer was kept same (meters) as the x-y units. Boundary of the DEM layer was matched with the LRW boundary by using a mask for the DEM layer. This DEM layer was used to calculate all subwatershed/reach topographic parameters.

Predefined subwatershed: The 12 digit watershed boundary dataset (HUC_12) for Arkansas was downloaded from the USDA Geospatial Data Gateway website. In ArcMap, the HUC_12 layer for the LRW was obtained by extracting the relevant HUC_8 id (08020205) from the attribute table. This obtained layer was saved twice as HUC_12 and HUC_8. All fields in the attribute table of HUC_12 layer were deleted except FID and shape. Two new fields were added: GRIDCODE and Subbasin with the field’s type set as long integer. GRIDCODE and Subbasin values were set equal to the subwatershed’s number. The obtained HUC_12 layer was the required predefined subwatershed layer used to generate subwatershed boundaries during the delineation of the LRW watershed.

Mask: For preparing the mask for the LRW, saved HUC_8 layer in the predefined subwatershed process was converted to a raster using “polygon to raster” command in ArcMap. The obtained raster layer, named as mask, was used to mask out a part of the DEM grid.

Burn-in streams: High resolution stream geodatabase for Arkansas was downloaded from the United States Geological Survey – National Hydrography Dataset (USGS – NHD) website. From this geodatabase, NHD flowline layer was exported as a shapefile, and clipped using HUC_12 boundary for the LRW in ArcMap. This completed the processing for the burn-in stream layer. This burn-in stream layer forced the SWAT subwatershed reaches to follow known stream locations, thereby improving the hydrographic segmentation.

User streams: A separate copy of the burn-in stream layer was processed further in ArcMap to generate the user stream layer. Only the major stream in various subwatersheds was retained by deleting all other streams. This resulted in one stream per subwatershed. This was followed by deletion of all fields in the attribute table except FID and shape. In addition, five new fields were added namely GRID_CODE, FROM_NODE, TO_NODE, Subbasin, and SubbasinR with the field’s type set as long integer. GRID_CODE, FROM_NODE, and Subbasin values were set equal to the subwatershed’s number, whereas TO_NODE and SubbasinR values were set equal to the downstream subwatershed’s number where water is flowing from the concerned subwatershed. This completed the processing for the user stream layer required to generate one major stream per subwatershed.

Land use: Land use and land cover (LULC) data for five years – 1992, 1999, 2001, 2004, and 2006 was available for the study watershed. The LULC data for 1999, 2004, and 2006 was obtained from the Center for Advanced Spatial Technologies (CAST) at the University of Arkansas. The LULC data for 1992 and 2001 was obtained from the National Land Cover Dataset (NLCD) website. CAST and NLCD were found to follow different classification schemes for various land use categories (Gorham and Tullis, 2007; Homer et al., 2004). Therefore, land use and land cover categories were merged to obtain a common land use classification for all the LULC data layers used within the model (Table 3.2). The "Value" field in the attribute table of each of the LULC data was related with the four letter SWAT codes for land uses via the look up table in ArcSWAT. This process allowed updating temporal land use information for the LRW during the model run. The land use change (LUC) module (SWAT2009_LUC) was used to update the HRU_FR in the SWAT model (Pai and Saraswat, 2011).

Soil: The SSURGO data was downloaded from the USDA Geospatial Data Gateway website for each county across which the LRW falls. In ArcMap, soil layer for all the counties were merged and extracted with the HUC_8 boundary for the LRW. This resulted in a single soil layer for the LRW. All fields were deleted except MUKEY, MUNAME, FID, and Shape. Missing MUNAME in the usersoil database were assigned neighboring soil names. The merged soil layer was rasterized using MUKEY as the primary field. "Value" was one of the fields in the attribute table of the rasterized soil layer. This field (value) had different values for different soils in the attribute table. These values were related with the soils database via the look up table for soil in ArcSWAT to identify the type of soil in the LRW.

Weather: Weather data was downloaded from the National Oceanic and Atmospheric Administration (NOAA) website for four rain gauge stations at Jonesboro, Beedeville, Wynne, and Mariana (Figure 3.6). Separate files were created for temperature and precipitation for each rain gauge. All .text and .dbf files were copied to the SWAT_compatible folder. STAT_Table.txt was used to populate the userwgn table in SWAT2009.mdb. In addition to the four weather stations, Next-Generation Radar (NEXRAD) data was also used in this study. Hourly NEXRAD data starting from April 1996 to December 2003 (data beyond 2003 was not available), was downloaded from the Lower Mississippi Basin River Forecasting Center (LMRFC) website. NEXRAD data was processed in a tool named NEXRAD-VC developed by Zhang and Srinivasan (2010). The PCP_SWAT tool was used to interpolate precipitation data using the inverse distance weighted method for each subwatershed from January 1986 to March 1996 and January 2004 to December 2008. SWAT's weather generator was used to generate other weather related data viz. relative humidity, solar radiation, and wind velocity from January 1986 to December 2008.

Point source data: Point source data at 18 major point pollution sources located within the watershed were obtained from the ADEQ. The location coordinates of point source facilities are given in Table (3.3). ADEQ collects information on various water quality constituents from the point source dischargers based on the permit requirements. Some of the commonly reported point source constituents are flow, sediment, TP, ammonia-nitrogen, pH, temperature, chemical oxygen demand, biochemical oxygen demand, and carbonaceous oxygen demand. Based on the availability of the point source constituents, flow, sediment, ammonia, and soluble phosphorus were converted into the SWAT compatible format on a monthly basis (Table 3.4).

As per the data received from ADEQ, a cubic feet per second was the measurement unit for flow, and milligram per liter was the measurement unit for sediment, ammonia, and soluble phosphorus. These measurement units for flow, sediment, ammonia, and soluble phosphorus were converted to its equivalent cubic meter per day, metric tons per day, kg per day, and kg per day, respectively.

Management data: Management practices for the crops grown in the LRW were obtained for each county from the research verification reports published by the University of Arkansas' Cooperative Extension Service. All of these management practices (Appendix C) were inputted into the model via the management operations table in the ArcSWAT interface for the SWAT model.

Measured water quality data: Measured data for flow, sediment, TP, and nitrate-nitrogen (NO3-N) were obtained for the Colt station from the USGS website. Sediment, TP, and NO3-N loads were calculated in mass per time according to the following equation (3.1):

$$Qs = Q * C \tag{3.1}$$

Where Qs is load in mass per time, Q is flow discharge in volume per time, and C is sediment concentration in mass per volume.

At Colt, while the flow data was continuous, the sediment, TP, and NO3-N data were irregular from 1990 to 2008. For sediment, TP, and NO3-N, there were 312, 70, and 74 available samples, respectively. In general, monthly water quality data is required for the calibration and validation of the SWAT model. As a result, the USGS LOAD ESTimator (LOADEST) tool was used to get continuous monthly load estimates for sediment, TP, and NO3-N loadings at Colt which was then used as a calibration target for SWAT. LOADEST provide three methods for the calculation of load estimates: maximum likelihood estimation (MLE), adjusted maximum likelihood estimation (AMLE), and least absolute deviation (LAD). AMLE assumes that the samples are normally distributed with a constant variance, and is the primary load estimation method used within LOADEST for generating a nearly unbiased estimates of instantaneous load even when the data is censored (data censoring occurs when one or more observations have constituent concentrations less than the laboratory detection limit) (Runkel et al., 2004). AMLE method incorporated in LOADEST was used in this study to estimate monthly loadings for sediment, TP, and NO3-N by building a regression model with the daily flow data available at Colt from January 1990 to December 2008. At Palestine, daily flow data, obtained from the USGS website, was available from October 1998 onwards. However, LOADEST was not used for obtaining monthly estimates at Palestine because an insufficient number of water quality samples (seven) were available from October 1998 to December 2008.

At Colt and Palestine, daily flows were split into surface runoff and base flow using a digital filter developed by Arnold and Allen (1999). This digital filter includes two equations (3.2 and 3.3) for calculating filtered surface runoff and baseflow:

$$q_t = \beta q_{t-1} + \frac{1+\beta}{2} * (Q_t - Q_{t-1}) \tag{3.2}$$

$$b_t = Q_t - q_t \tag{3.3}$$

Where q_t is the filtered surface runoff at the time step t (one day), β is the filter parameter (0.925), Q_t is the original streamflow (total flow) at the time step t (one day), and b_t is the filtered baseflow at the time step t (one day). Three passes can be made over the streamflow data, each pass resulting in less baseflow as a percentage of total flow. Third pass of baseflow filter over the streamflow was selected in this study to better match the simulated values. Surface runoff was obtained by subtracting the baseflow from the total flow.

3.4 SWAT MODEL SETUP

Based on the input data, ArcSWAT divides a watershed into subwatersheds and the subwatersheds into hydrological response units (HRUs). In SWAT, HRUs are the unique combination of land use, soil, and slope. Because of the presence of numerous HRUs in the watershed (might exceed 1000), HRUs are generally created using thresholds for land use, soil and slope. For example, a threshold of 5-0-0 (5 percent for land use, 0 percent for soil, and slope) indicates that any land use category that occupies less than 5 percent of a subwatershed area would not be simulated and merged into the nearby land use. Zero percent thresholds for the soil and slope would result in no change in the soil and slope categories. The thresholds are often set to save processing time. In this study, a threshold of 0-10-0 was used as a compromise between spatial resolution and computational time. The model was run from the year 1986 to 2008. The first four years (1986-1989) were set as a warm-up period and not used for calibration of the model. Warm-up period was used to estimate several parameters of the model, as the initial values of parameters were unknown (Bekiaris et al., 2005). Runoff, sediment and nutrient losses were calculated for each HRU. Surface runoff volume was calculated with the modified soil conservation service (SCS) curve number method (Neitsch et al., 2011). Modified Universal Soil Loss Equation (MUSLE) was used for calculating sediment losses for each HRU. Losses in the form of sediment and nutrients were integrated from all HRUs at the subwatershed level. These losses were then routed through streams to the watershed outlet.

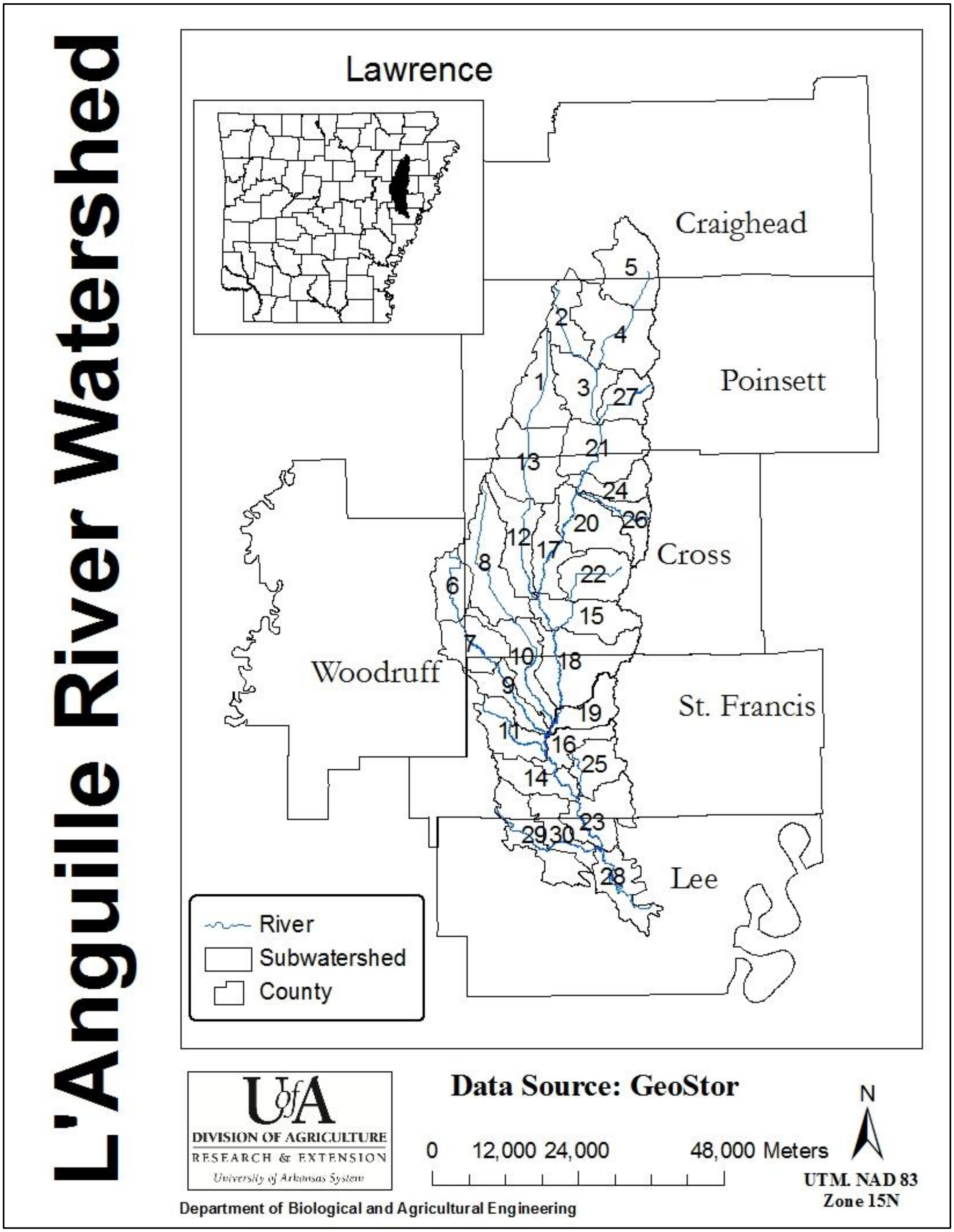


Figure 3.1: L'Anguille River Watershed.

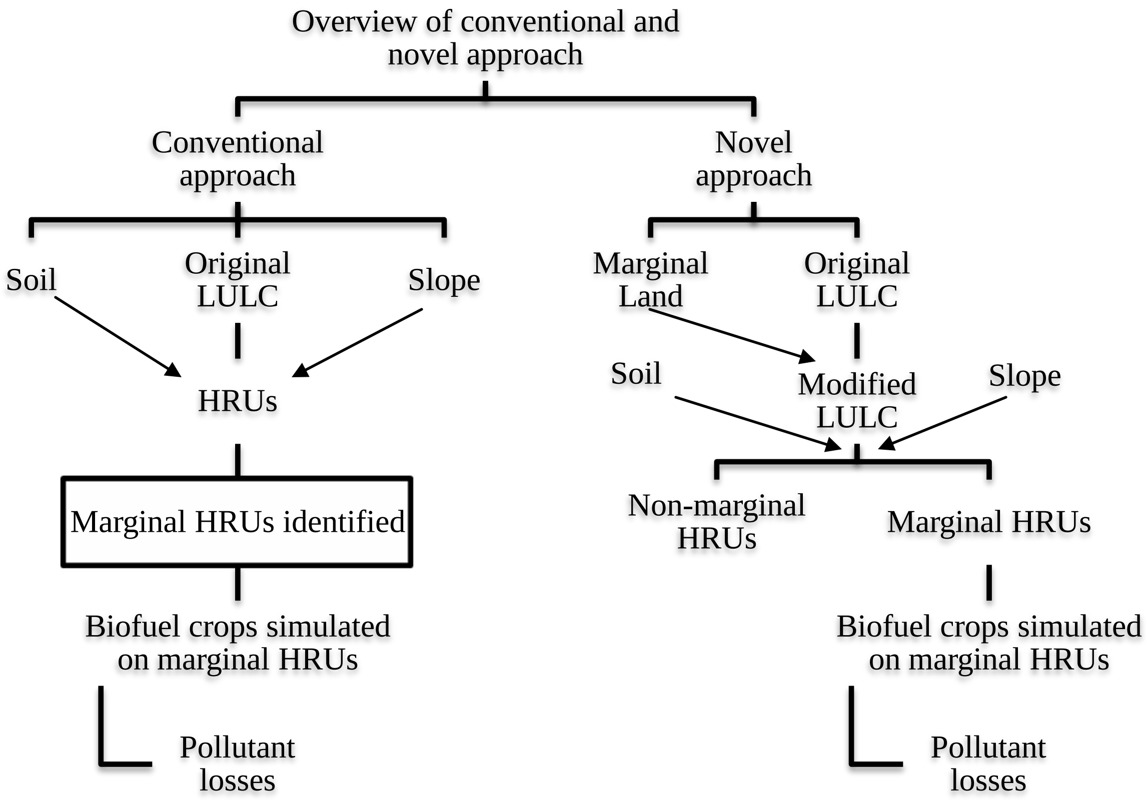
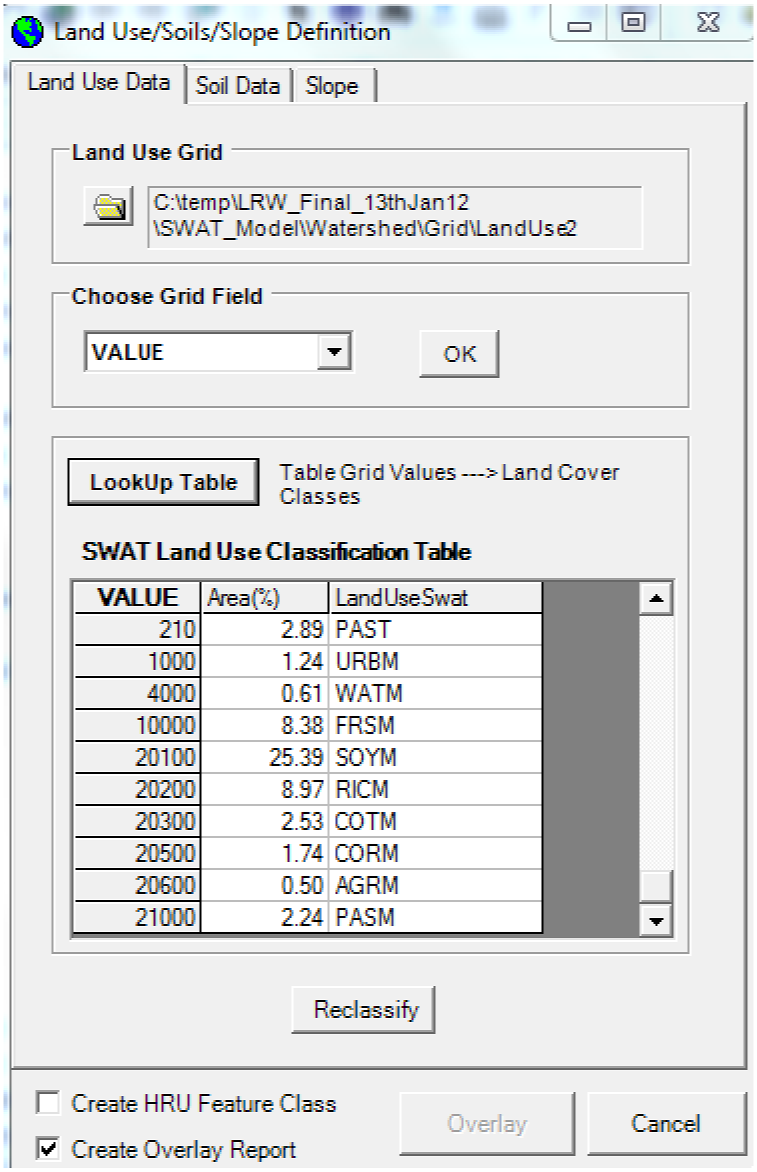


Figure 3.2: An overview of the conventional and novel approach.



Land Use Grid

C:\temp\LRW_Final_13thJan12
\SWAT_Model\Watershed\Grid\LandUse2

Choose Grid Field

VALUE

Table Grid Values ---> Land Cover Classes

SWAT Land Use Classification Table

VALUE	Area(%)	LandUseSwat
210	2.89	PAST
1000	1.24	URBM
4000	0.61	WATM
10000	8.38	FRSM
20100	25.39	SOYM
20200	8.97	RICM
20300	2.53	COTM
20500	1.74	CORM
20600	0.50	AGRM
21000	2.24	PASM

☐ Create HRU Feature Class

☑ Create Overlay Report

Figure 3.3: New land uses defined in the "look up table" for the SWAT model developed for the L'Anguille River watershed.

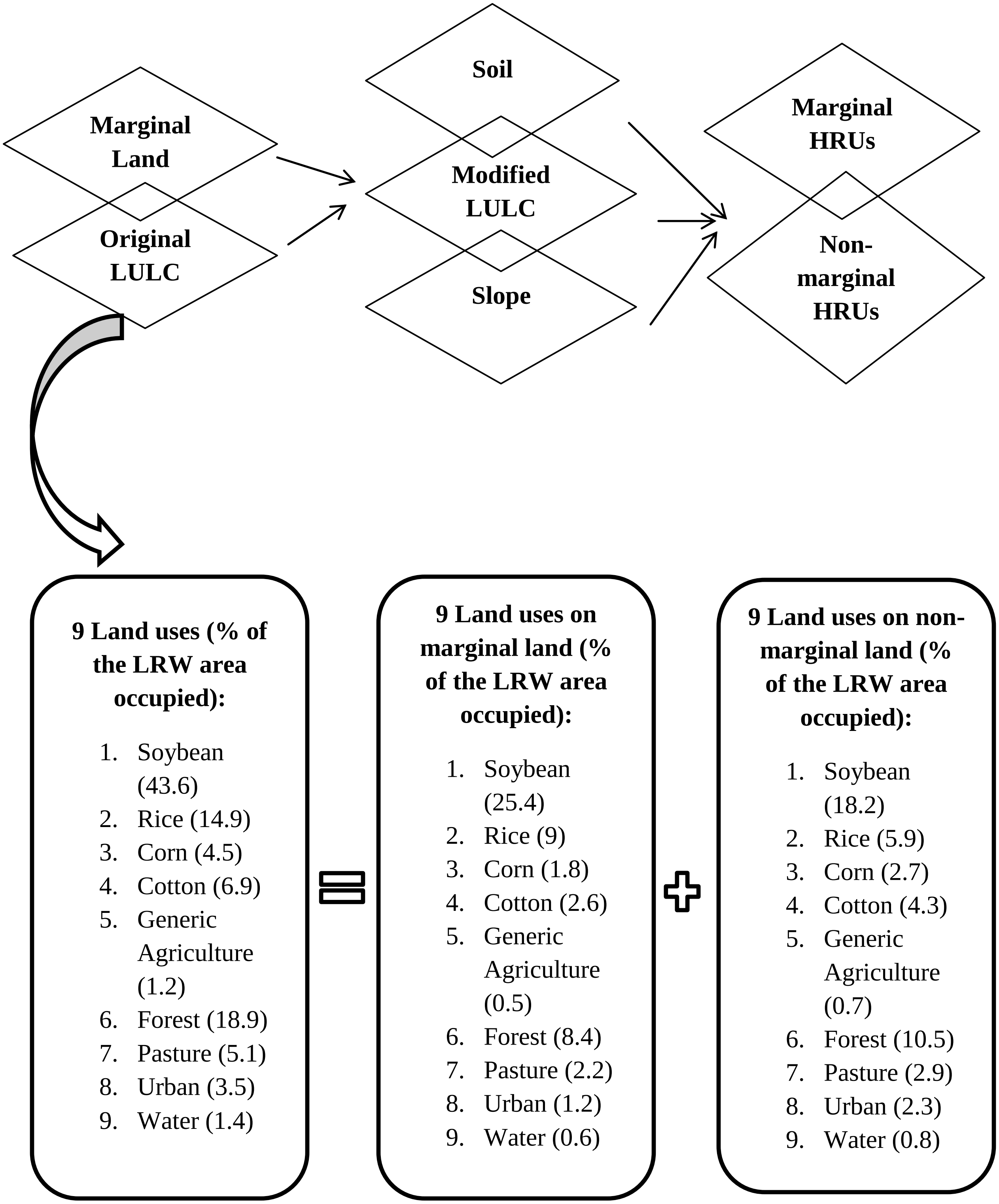


Figure 3.4: Reclassified land uses in the L'Anguille River watershed.

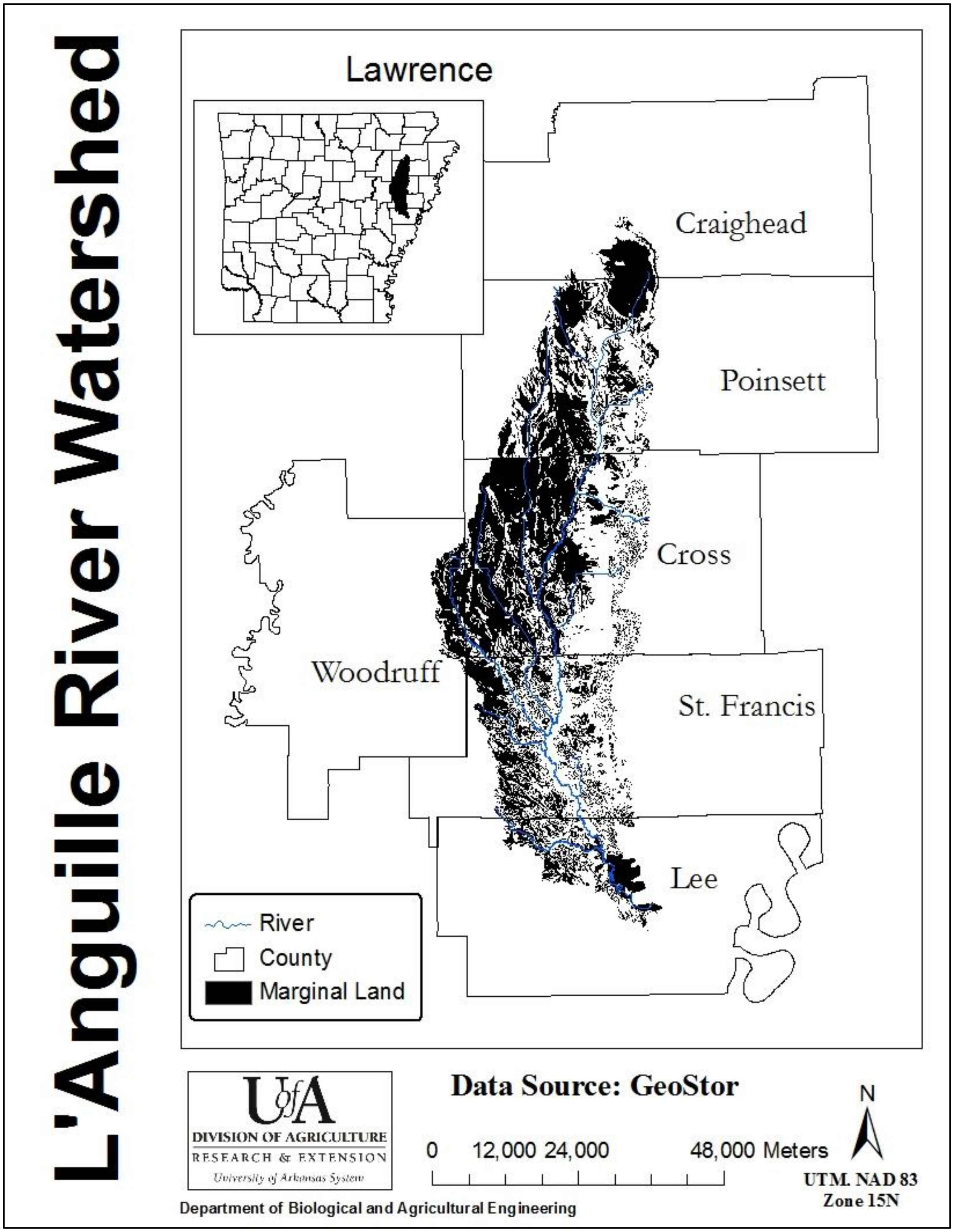


Figure 3.5: Marginal land based on the Soil Survey Geographic Land Capability Classes III and IV.

Table 3.1: Model inputs for the L'Anguille River watershed.

Data Type	Scale/Stations	Source	Description
Topography	5 m	Geostor Arkansas (http://www.geostor.arkansas.gov)	Digital Elevation Model
Land Use/Land Cover (LULC)	28.5 m and 30 m	Center for Advanced Spatial Technologies (CAST) (http://www.cast.uark.edu) National Land Cover Dataset (NLCD) (http://www.mrlc.gov)	1999, 2004, 2006 LULC 1992, 2001 LULC
Soil	150 m	United States Department of Agriculture-Natural Resources Conservation Service (USDA-NRCS) (http://www.nrcs.usda.gov)	Soil Survey Geographic (SSURGO) database
Watershed boundary	1:24000	United States Department of Agriculture-Natural Resources Conservation Service (USDA-NRCS) (http://www.nrcs.usda.gov)	12 digit watershed boundary dataset
Stream network	1:24000	National Hydrographic Dataset-USGS (NHD-USGS) (http://nhd.usgs.gov/)	High resolution stream reaches (February, 2008)
Weather	4 Stations NEXRAD	National Oceanographic and Atmospheric Administration (NOAA) (http://www.noaa.gov/) Lower Mississippi River Forecasting Center (LMRFC) (http://www.srh.noaa.gov/lmrfc/)	29 years (1980 to 2008) of daily temperature and precipitation NEXRAD dataset from 1996 to 2003
Point source pollution	18 stations	Arkansas Department of Environmental Quality (ADEQ) (http://www.adeq.state.ar.us/)	Monthly flow, sediment and nutrients (1990-2008)
Crop management information	County level	University of Arkansas Cooperative Extensive Service (UACES)	Fertilizer, pesticide and irrigation application rates and timings; tillage, planting and harvesting information

Table 3.2: Land use and land cover merged categories for the Center for Advanced Spatial Technologies (CAST) and National Land Cover Datasets (NLCD) layers.

Agency	Year	Categories	Category Name	Merged Name
CAST	1999, 2004, 2006	11, 14	Intensity 1 and Urban (other)	Urban low intensity
		12, 13	Intensity 2 and Intensity 3	Urban high intensity
		100, 101, 102, 103, 104, 105, 106, 107, 108, 109, 110, 111, 112, 113, 114, 115, 116, 117, 118, 119, 120, 121, 122, 123, 124, 125, 126, 127, 128	Various types of trees oak, pine, etc.)	Forest
		209, 210	Warm season and cool season grasses	Pasture
NLCD	1992, 2001	21, 22, 85	Low/High residential or recreational	Urban low intensity
		23, 24	Commercial, industrial, transportation	Urban high intensity
		41, 42, 43	Deciduous, evergreen, mixed	Forest

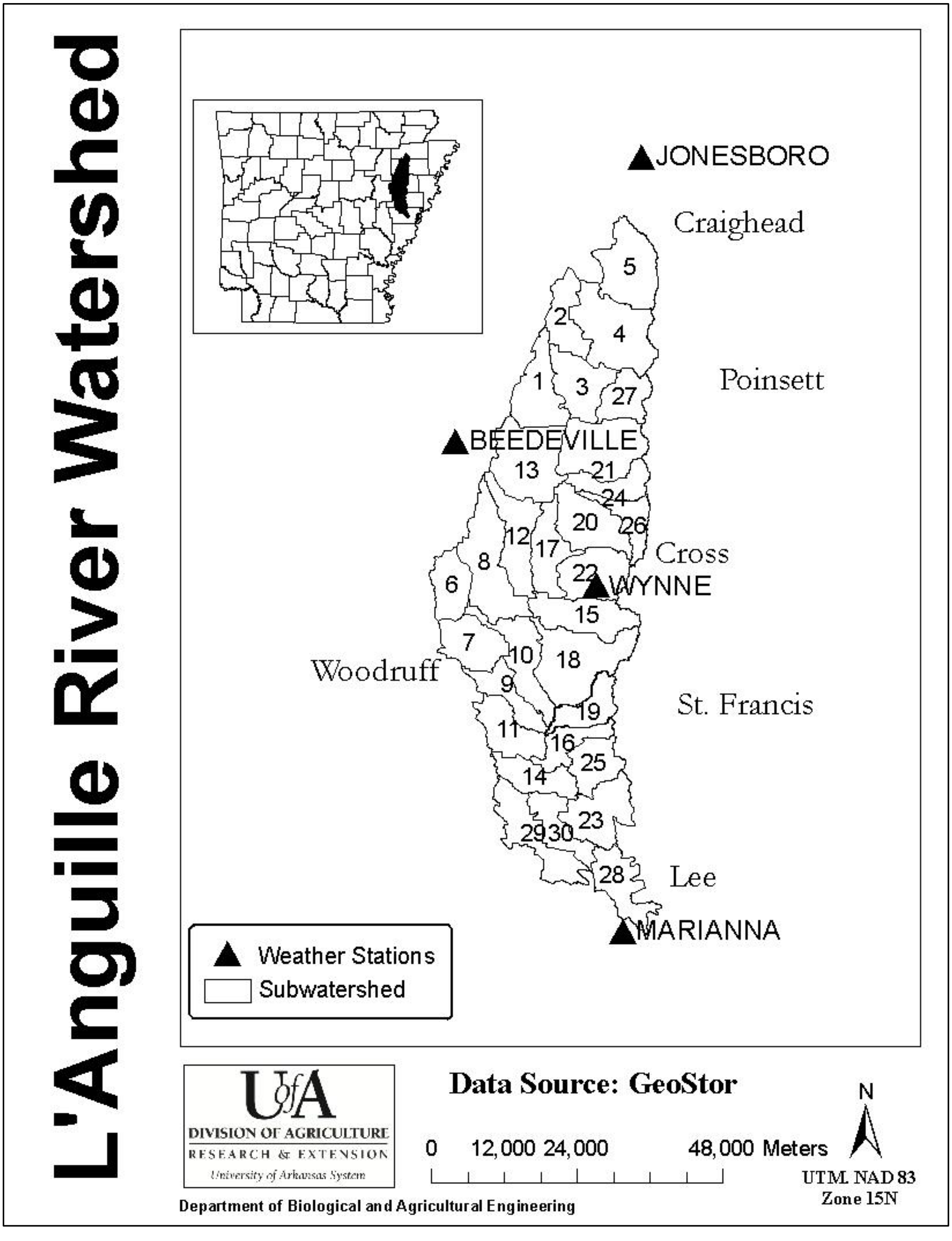


Figure 3.6: Location of weather stations in the L'Anguille River watershed.

Table 3.3: Point sources and their locations within the study area.

Facility Name	County	Nearest City	Latitude	Longitude
Hunters Glen Owners Assoc.	Craighead	Jonesboro	35.7375	-90.6916
City of Harrisburg	Poinsett	Harrisburg	35.5694	-90.7403
Crowley's Ridge Water Assoc.	Poinsett	Harrisburg	35.4853	-90.7331
Vannadale-Birdeye Water Assoc.	Cross	Cherry Valley	35.3775	-90.7056
City of Cherry Valley	Cross	Cherry Valley	35.4022	-90.7675
Cross County High School	Cross	Cherry Valley	35.4022	-90.8064
Polyone Corp.	Cross	Wynne	35.2556	-90.7833
Mueller Industries, Inc	Cross	Wynne	35.2292	-90.7847
Mueller Copper Tube Products	Cross	Wynne	35.2344	-90.785
City of Wynne	Cross	Wynne	35.2189	-90.8281
Andrews Trailer Park	Cross	Wynne	35.1917	-90.7917
Forrest City School - Caldwell	St. Francis	Forrest	35.0728	-90.8153
Entergy - Hamilton Moses Plant	St. Francis	Palestine	34.9775	-90.8764
City of Forrest	St. Francis	Forrest	34.9975	-90.8353
City of Palestine	St. Francis	Palestine	34.9625	-90.9136
City of Marriana - Pond B	Lee	Marianna	34.7911	-90.7628
Magna Lomason Inc.	Lee	Marianna	34.7844	-90.7728
City of Marriana - Pond A	Lee	Marianna	34.7769	-90.7442

Table 3.4: Conversion of point source constituents into SWAT compatible format.

Constituent	ADEQ* (units)	SWAT** (units)	Conversion Equation
Flow	Million gallon per day (MGD)	Cubic meter per day (CMD)	CMD = MGD * 3.79 * 10^3
Sediment	Milligram per liter (Mg/l)	Metric tons per day (Tons/day)	Tons/day = Mg/l * CMD * 10^{-6}
Ammonia	Milligram per liter (Mg/l)	Kilogram per day (Kg/day)	Kg/day = Mg/l * CMD * 10^{-3}
Soluble Phosphorus	Milligram per liter (Mg/l)	Kilogram per day (Kg/day)	Kg/day = Mg/l * CMD * 10^{-3}

*Arkansas Department of Environmental Quality

**Soil and Water Assessment Tool

3.5 SENSITIVITY ANALYSIS, CALIBRATION, AND VALIDATION OF THE SWAT MODEL

Sensitivity analysis is the procedure of identifying parameters having relatively greater influence on output variables. Latin hypercube sampling - one at a time (LH-OAT) incorporated in the ArcSWAT interface was used to perform the sensitivity analysis at the Colt station. LH method divided the range of parameters into 10 parts, and OAT method selected each parameter randomly one at a time varying it by 5 percent. Sensitivity analysis was carried out for 26 flow and 6 sediment related parameters resulting in 270 and 70 simulations, respectively. For TP and NO3-N, sensitivity analysis was carried out for 9 parameters resulting in 100 simulations.

Calibration is the procedure of adjusting model parameters within reasonable ranges to simulate the observed dataset as closely as possible. In general, the adjusted parameters are the sensitive parameters (Migliaccio and Chaubey, 2007). Validation is the procedure of comparing an independent dataset with the model outputs without any adjustment of model parameters. The study also includes validating the model performance at a station (namely Vannadale) that was not used for calibration. Thus, the SWAT model was calibrated and validated at Colt, Palestine, and Vannadale, respectively. Calibration and validation time periods along with the variables used for calibration and validation at Colt, Palestine, and Vannadale are shown in Table (3.5). Coefficient of determination (R^2), Nash-Sutcliffe efficiency (NSE), percent-bias (PBIAS) and root mean square error-standard deviations ratio (RSR) were the four objective functions optimized for simulating total flow, surface flow, base flow, sediment, TP and NO3-N (Equations 3.4 to 3.7).

$$R^2 = \left(\frac{\sum_{i=1}^{n} (O_i - O_{avg})(P_i - P_{avg})}{\left[\sum_{i=1}^{n} (O_i - O_{avg})^2 \sum_{i=1}^{n} (P_i - P_{avg})^2 \right]^2} \right)^2 \quad (3.4)$$

$$NSE = 1 - \frac{\sum_{i=1}^{n} (O_i - P_i)^2}{\sum_{i=1}^{n} (O_i - O_{avg})^2} \quad (3.5)$$

$$RSR = \frac{\sqrt{\sum_{i=1}^{n} (O_i - P_i)^2}}{\sqrt{\sum_{i=1}^{n} (O_i - O_{avg})^2}} \quad (3.6)$$

$$PBIAS = \left[\frac{\sum_{i=1}^{n} (O_i - P_i) * 100}{\sum_{i=1}^{n} P_i} \right] \quad (3.7)$$

Where O = measured value, P = predicted value, i = number of values

As opposed to the automatic calibration, manual calibration allows the user to assign a suitable value to a parameter based on the experience relating to the watershed. In this study, the manual calibration technique was followed to calibrate the model using measured data at Colt and Palestine. At Colt, measured total flow, surface flow, base flow, sediment, TP, and NO3-N datasets were compared with the simulated reach outputs for FLOW_OUTcms, ((GW_Qmm + LAT_Qmm) / WYLDmm) * FLOW_OUTcms, FLOW_OUTcms - ((GW_Qmm + LAT_Qmm) / WYLDmm) * FLOW_OUTcms, SED_OUTtons, ORGP_OUTkg + MINP_OUTkg, and NO3-N_OUTkg on a monthly basis, respectively. At Palestine, measured total flow, surface flow, and base flow datasets were compared with the simulated reach output for FLOW_OUTcms, ((GW_Qmm + LAT_Qmm) / WYLDmm) * FLOW_OUTcms, FLOW_OUTcms - ((GW_Qmm + LAT_Qmm) / WYLDmm) * FLOW_OUTcms on a monthly basis, respectively. Flow was calibrated first at Colt; followed by sediment, TP, and NO3-N (Santhi et al., 2001; White and Chaubey, 2005). Calibration was performed simultaneously at Colt and Palestine. Moreover, the output statistics (R^2, NSE, PBIAS, and RSR) at Colt and Palestine were optimized simultaneously as per the procedure suggested by Migliaccio and Chaubey (2007).

3.6 SELECTION OF SUITABLE MARGINAL LAND FOR LAND USE CONVERSION AS WELL AS APPROPRIATE LAND COVER/PLANT GROWTH PARAMETERS AND MANAGEMENT PRACTICES FOR THE BIOFUEL CROPS

In section 3.2, modified land use and land cover layer resulted in 18 reclassified land uses. Out of these 18 land uses, nine overlapped marginal land in the LRW. These overlapping land uses (soybean/SOYM, rice/RICM, corn/CORM, cotton/COTM, generic-agriculture/AGRM, forest/FRSM, pasture/PASM, urban/URBM, and water/WATM) comprised 52 percent of the watershed area. However, based on the practicality of land use conversion, FRSM, PASM, URBM and WATM were discarded from the land use change analyses as it was unlikely that the biofuel crops be grown on forest, pasture, urban land, and water. As a result, the available land uses for biofuel crop simulation were soybean/SOYM, rice/RICM, corn/CORM, cotton/COTM, and generic-agriculture/AGRM. These selected land uses constituted about 40 percent of the watershed area and were regarded as representing marginal lands suitable for simulating biofuel crops. Thus, on absolute area basis, marginal lands obtained with the conventional approach were found to be 209 square kilometers more than that obtained with the novel approach. In both the approaches, the obtained marginal land was simulated with the second generation biofuel crops.

Appropriate land cover/plant growth parameters and management practices for switchgrass and miscanthus were defined in the SWAT model. Most of the land cover/plant growth parameters for switchgrass were already available in the SWAT land cover/plant growth database. Two of its parameters were modified to simulate its growth characteristics in Arkansas (Dr. West, personal communication, 21 July 2011). The modified parameters were maximum potential leaf area index (BLAI), and maximum canopy height (CHTMX). BLAI was modified from 6 to 10 (dimensionless), and CHTMX was modified from 2.5 to 3 (meters). Miscanthus being a relatively new biofuel crop, lacked parameters in the SWAT model. Land cover/plant growth parameters for miscanthus, as defined by Ng et al. (2010) were used in this study. Appendix (D) includes land cover/plant growth parameters used for simulating switchgrass and miscanthus in the model.

Management practices for switchgrass and miscanthus were incorporated as per local recommendations (Dr. West, personal communication, 19 April 2012). The management practices were largely simulated uniformly for both switchgrass and miscanthus (Table 3.6). As can be seen in Table (3.6), the management practices for switchgrass/miscanthus differed only for the first two years followed by no change from third year onwards. These management practices were converted into SWAT equivalent management operations (Table 3.6) and input in the model via the management operations table available in ArcSWAT.

Table 3.5: Summary of measured data in the L'Anguille River watershed (LRW).

Monitoring Station	Drainage Area in the LRW (sq. km)	Data Providing Agency	Time Period	Calibrated/Validated Variables
Colt	552	USGS* (http://www.usgs.gov/)	Calibration – 1990 to 2005 Validation – 2006 to 2008	Total flow Surface flow Base flow Sediment Total Phosphorus Nitrate-nitrogen
Palestine	728	USGS (http://www.usgs.gov/)	Calibration – 1998 to 2005 Validation – 2006 to 2008	Total flow Surface flow Base flow
Vannadale	751	ECO** (http://www.ecoconservation.org/)	Validation – 2006 to 2008	Total flow Sediment Total Phosphorus Nitrate-nitrogen

*United States Geological Survey

**Ecological Conservation Organization

Table 3.6: Crop management practices for switchgrass and miscanthus.

Date	Practice	Amount/acre	SWAT Practice	SWAT kg/ha
First Year				
Apr 20	Phosphorus, Potassium Application	36 lb phosphate (P2O5), 60 lb K12	Fertilizer Application (00-40-60)	112 (19.5 Elemental P, 55.7 Elemental K)
Apr 20	Disking		Tillage (Disk Plow Ge23ft)	
Apr 21	Roller		Tillage (Roller Packer Attachment)	
May 20	Burn down with glyphosate	1 lb a.i.	Pesticide Application (Glyphosate Amine)	1.12
May 21	Plant switchgrass		Plant/Begin Growing Season (Switchgrass)	
Jun 20	Weed control	0.25 a.i.	Pesticide Application (2,4-D Amine)	0.28
Second Year				
Apr 1	Nitrogen Application	70 lb Urea	Fertilizer Application (Urea)	78.46
Jun 20	Weed control	0.25 lb a.i.	Pesticide Application (2,4-D Amine)	0.28
Nov 1	Harvest		Harvest Only (100% Harvesting Efficiency)	
From Third Year Onwards				
Apr 1	Nitrogen Application	70 lb Urea	Fertilizer Application (Urea)	78.46
Nov 1	Harvest		Harvest Only (100% Harvesting Efficiency)	

3.7 COMPARISON BETWEEN THE CONVENTIONAL AND NOVEL APPROACH

Conventional approach represents typical SWAT modeling approach in which switchgrass and miscanthus were simulated on marginal HRUs disregarding the fact that switchgrass and miscanthus could also get simulated on other HRUs within subwatersheds because of the spatial discontinuity among same HRUs. Novel approach represents the new approach in which switchgrass and miscanthus were simulated only on those marginal HRUs which were targeted. In both the conventional and novel approaches, switchgrass and miscanthus were simulated separately. In other words, switchgrass was simulated first on all the marginal land and the pollutant losses exiting the marginal HRUs were analyzed. This was followed by the simulation of miscanthus on all the marginal land and again analyzing the pollutant losses exiting the marginal HRUs. Area-weighted annual pollutant losses (sediment, TP, and TN) exiting the marginal HRUs to their respective subwatershed's reach were obtained for both the conventional and novel approach. Area-weighted annual pollutant losses were averaged over the 19 year study period (excluding warm-up years for the model). These area-weighted average annual pollutant losses were compared for the conventional and novel approach. The area-weighted average annual sediment loads were cross-checked with the values reported by SWAT Check tool, a standalone Microsoft Windows program intended to identify model issues early in the modeling process (White et al., 2011). In this study, TP loss represents the sum of organic, sediment, and soluble phosphorus exiting the marginal HRUs. TN loss represents the sum of NO3-N and organic nitrogen loss in surface runoff, as well as NO3-N loss in lateral and groundwater flows exiting the marginal HRUs. The equations (3.9 and 3.10) for pollutant losses resulting from both the approaches are as follows:

Conventional Approach:

$$X\_trad = X\_marginal + X\_non\_marginal \tag{3.8}$$

Where X_trad is the conventional pollutant loss from all the marginal and non-marginal HRUs, X_marginal is the pollutant loss from the switchgrass and miscanthus simulated marginal HRUs, and X_non_marginal is the pollutant loss from the non-marginal HRUs.

Novel Approach:

$$\begin{aligned} X\_new &= X\_marginal\_targeted + X\_marginal\_nontargeted \\ &+ X\_non\_marginal \end{aligned} \tag{3.9}$$

Where X_new is the new pollutant loss from the targeted and nontargeted marginal HRUs as well as non-marginal HRUs, X_marginal_targeted is the pollutant loss from the switchgrass and miscanthus simulated targeted marginal HRUs, X_marginal_nontargeted is the pollutant loss from the non-targeted marginal HRUs, and X_non_marginal is the pollutant loss from the non-marginal HRUs.

The pollutant losses from the switchgrass and miscanthus simulated marginal HRUs were compared. In other words, X_marginal for the conventional approach was compared with X_marginal_targeted for the novel approach.

3.8 WATER QUALITY IMPACTS OF SWITCHGRASS AND MISCANTHUS ON TARGETED MARGINAL LAND

In this section, marginal land/HRUs represent the targeted marginal land/HRUs. Area-weighted annual sediment, TP, and TN losses were obtained for the actual land uses (current cropping condition) on marginal HRUs. These annual sediment, TP, and TN losses exiting marginal HRUs to their respective subwatershed's reach were referred as baseline losses. Annual baseline losses were averaged over the 19 year study period (excluding warm-up years for the model). These area-weighted average annual baseline losses were compared with the losses resulting from the marginal HRUs simulated with switchgrass and miscanthus, respectively. The procedures for comparing the losses resulting from the novel approach with the baseline are shown in the form of a flow diagram (Figure 3.7). Moreover, the probable causes for the differences between the reductions obtained by simulated switchgrass and miscanthus were also analyzed. Furthermore, annual trends for the pollutant losses were also analyzed over the 19 years study period.

3.9 YIELD ANALYSIS FOR THE SWAT SIMULATED SWITCHGRASS AND MISCANTHUS

An additional analysis was performed for the simulated yield. This analysis was done to compare the simulated yields for switchgrass and miscanthus with literature values, and hence evaluate the level of confidence in model simulations. Area-weighted simulated yields were obtained for switchgrass and miscanthus on an annual scale. These annual yields were then averaged to get the area-weighted average annual yield for switchgrass and miscanthus. These yield values for switchgrass and miscanthus were compared with the field values reported in literatures. Ashworth (2010) had reported nitrogen uptakes for switchgrass production in Fayetteville, Arkansas. Therefore, area-weighted annual values were obtained for the simulated nitrogen uptake for switchgrass. Finally, the average annual nitrogen uptake by switchgrass was compared with that reported by Ashworth (2010).

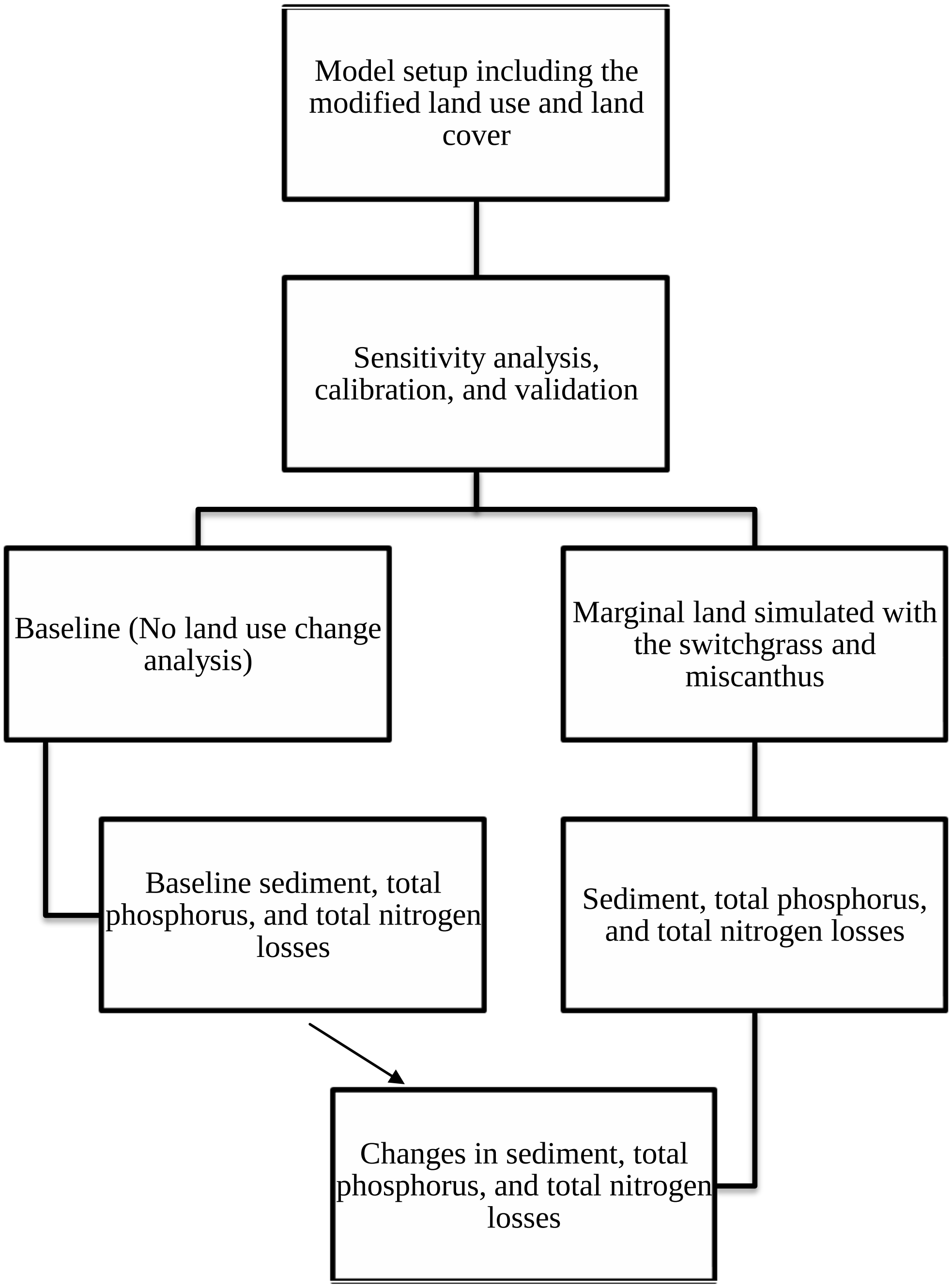


Figure 3.7: Procedure for analyzing changes in pollutant losses from the baseline upon simulating switchgrass and miscanthus on marginal land.

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CHAPTER IV

RESULTS AND DISCUSSION

Sections 4.1, 4.2, and 4.3 are for objective 1**: Development of a novel simulation approach to incorporate marginal land in the SWAT model followed by calibration and validation of the model for the L'Anguille River watershed.** Methodology to develop a novel simulation approach was already explained in the materials and methods chapter. The modeling parts of objective 1 are discussed below. Results for the various analyses were discussed including identification of sensitive parameters, adjustment of parameters for the model calibration, and evaluation of calibration, validation and post-validation results. Once the model was calibrated and validated, results for both the conventional and novel approaches were discussed. Section 4.4 is for objective 2: **Comparison between the conventional and novel approach for water quality impacts of biofuel crop simulation on marginal land.** After analyzing differences between the conventional and novel approach, water quality impacts of biofuel crop simulations were evaluated with the novel approach. Section 4.5 is for objective 3: **Analysis of the water quality impacts of biofuel crop simulation on marginal land (defined by the novel approach) at the HRU scale.** Section 4.6 is for the yield analysis for switchgrass and miscanthus followed by the analysis of simulated nitrogen uptake for switchgrass. Finally, Section 4.7 lists all the references that have been cited in this chapter.

4.1 SENSITIVITY ANALYSIS

This section reports the sensitive parameters identified for flow, sediment, total phosphorus (TP), and nitrate-nitrogen (NO3-N) for the Colt station.

COLT

Hydrology: Sensitive parameters obtained for hydrology were the curve number for the moisture condition II (CN2), soil evaporation compensation factor (ESCO), available water capacity in the soil (SOL_AWC), depth of water necessary for the occurrence of the groundwater flow (GWQMN), and maximum potential leaf area index (BLAI). CN2 was ranked as the most sensitive parameter for flow that mainly affects the overland flow process. Saraswat et al. (2008) identified hydrological soil groups C and D as the dominant soil groups in the L’Anguille River watershed (LRW). The soil groups C and D have been reported to have high runoff potentials (USDA-NRCS, 2009). Therefore, it was no surprise that the overland process mainly affected the flow in the LRW. The modified soil conservation service (SCS) curve number equation relates flow and CN2. Santhi et al. (2001) reported that calibrating CN2 will be always useful as it is not well-defined physically. A higher sensitivity for the ESCO was because the LRW, located in the southern U.S., receives higher solar radiation. CN2 and ESCO were also identified as sensitive for the LRW by Maringanti (2008). As per the sensitivity analysis for flow, SOL_AWC, GWQMN, and BLAI were other parameters identified as sensitive besides CN2 and ESCO.

Sediment: Sensitive parameters obtained for sediments were the universal soil loss equation practice factor (USLE_P), cofficient provided by the user in simulating the maximum amount of sediment allowed to transport from a reach segment (SPCON), universal soil equation cropping factor (USLE_C), exponent cofficient provided by the user in simulating the maximum amount of sediment allowed to transport from a reach segment (SPEXP), and channel cover factor (CH_COV2). USLE_P represents the ratio of soil loss from a specific support practice (contour tillage, strip cropping, etc.) to the loss from an up and down slope culture (Arnold et al., 2011). USLE_P was ranked as the most sensitive parameter for the sediment yield, indicating that a change in the land use practice factor would affect the sediment loadings. The modified universal soil loss equation (MUSLE) relates sediment yield and USLE_P. Apart from USLE_P, USLE_C also affected the sediment loadings due to the change in crop and management factors indicating that a change in the land use and land cover in LRW would impact the sediment loadings. Channel processes also played a role in affecting sediment loadings as depicted by the sensitive parameters: SPCON, SPEXP, and CH_COV2. The LRW was considered as a sediment impacted watershed, and as a result identification of sedimentation sources from L'Anguille River banks was recommended by the Nine-Element Watershed Restoration Plan (Audubon, 2005). Therefore, it was expected that the sediment impacted L'Anguille River would be influenced by both the overland and channel processes.

Total Phosphorus: Sensitive parameters obtained for TP were the phosphorous soil partitioning cofficient (PHOSKD), phosphorous percolation cofficient (PPERCO), nitrate percolation coefficient (NPERCO), deep acquifer percolation fraction (RCHRG_DP), and initial concentration of nitrate in the shallow aquifer (SHALLST_N). Phosphorus soil partitioning coefficient (PHOSKD) was identified as the most sensitive parameter for the TP. PHOSKD represents the soluble phosphorus concentration in the surface 10mm of soil divided by the soluble phosphorus concentration in surface runoff (Arnold et al., 2011). PHOSKD was again related to the overland process similar to CN2 and USLE_P. Therefore, it was observed that the overland process affects most of the flow, sediment, and TP. Moreover, there was a predictable correlation between sediment and TP because of the ability of phosphorus to bind over and transport with sediments. PHOSKD value mainly changes with the diffusion process i.e. migration of ions in the soil solution as a response to the concentration gradient (Arnold et al., 2011). Apart from PHOSKD, parameters representing the underground process: PPERCO, NPERCO, RCHRG_DP, and SHALLST_N also influenced the overall phosphorus loadings.

Nitrate-nitrogen: Sensitive parameters obtained for NO3-N were deep acquifer percolation fraction (RCHRG_DP), nitrate percolation coefficient (NPERCO), phosphorous soil partitioning cofficient (PHOSKD), phosphorous percolation cofficient (PPERCO), and initial concentrate of nitrate in shallow aquifer (SHALLST_N). The deep aquifer percolation fraction (RCHRG_DP) was ranked as the most sensitive parameter for NO3-N. RCHRG_DP represents the fraction of percolation from the root zone which recharges the deep aquifer (Arnold et al., 2011). As the movement of NO3-N is mainly an underground process, it was no surprise that RCHRG_DP was ranked as the most sensitive parameter for NO3-N. Apart from RCHRG_DP, other parameters affecting the NO3-N were NPERCO, PHOSKD, PPERCO, and SHALLST_N. Some of the sensitive parameters for NO3-N were the same as that for TP due to the interaction between parameters.

Parameters were adjusted during the multi-site (Colt and Palestine), multi-variable (total flow, surface flow, base flow, sediment, TP, and NO3-N), and multi-objective (coefficient of determination, Nash-Sutcliffe efficiency, percent bias, and root mean square-standard deviation ratio) calibration, within the ranges recommended by the SWAT manual (Table 4.1). As sensitivity analysis assumes linearity and does not consider correlations between parameters (White and Chaubey, 2005), adjusted parameters were not all the same as sensitive parameters. Some parameters were selected to make a better fit for the measured and simulated data (Santhi et al., 2001). The selected parameters were ALPHA_BF (baseflow alpha factor), GW_REVAP (groundwater revap coefficient), CH_N2 (Manning's 'n' for the main channel), PRF (peak rate adjustment factor for the main channel sediment routing), SURLAG (surface runoff lag cofficient), SOL_Z (depth of soil from the surface to the bottom of the layer), CH_K2 (main channel's effective hydraulic conductivity), SDNCO (denitrification threshold water content), and CDN (denitrification exponential rate cofficient).

4.2 CALIBRATION AND VALIDATION

This section reports the calibration and validation results for total flow, surface flow, base flow, sediment, total phosphorus, and nitrate-nitrogen at the Colt station, and total flow, surface flow, and base flow at the Palestine station.

COLT

Statistical results for the calibration and validation at the Colt site are shown in Table (4.2) and temporal results are shown in Figures (4.1 - 4.2). The coefficient of determination (R^2) and Nash-Sutcliffe efficiency (NSE) ranged from 0.4 to 0.9 and 0.5 to 0.9 respectively. As a result, most of the statistics for total flow, surface flow, base flow, sediment, TP and NO3-N were satisfactory at Colt and showed good correlation between measured and simulated values as per the model evaluation guidelines provided by Moriasi et al. (2007). The percent bias (PBIAS) statistics indicated some underprediction for total flow during the calibration period (positive biases) and overprediction during the validation period (negative biases), which could also be seen in Figure (4.1). According to Figure (4.1), there were high underprediction for total flow during February 1998, 1999, and 2001, and January 2002, and high overprediction during March 2008. Studies have reported spatial variability as a major cause for the under and overprediction for flow (Santhi et al., 2001; Srinivasan et al., 1998). Against an average rainfall of 1152 mm, rainfall in the watershed varied from 1109 mm to 1271 mm during the period of under/overprediction.

SWAT underpredicted sediments for the calibration period; however, validation results reflect that the model performance was very good. As sediment and flow were interrelated, errors in flow predictions were propagated to sediments. As a result, sediment underprediction during February 1998 was likely to be propagated from flow underprediction which could be seen in Figure (4.2). TP statistics were good for the calibration and validation period, but SWAT underpredicted TP during calibration and overpredicted during validation. This under and overprediction of TP was related to flow as most of the phosphorous transportation is through surface runoff (Haggard et al., 2003). Calibration and validation for NO3-N had some overpredicted peaks while the remaining period was dominated by underprediction. The coefficient of determination for NO3-N was 0.4 which was just below the satisfactory level. This occurred because in general NO3-N is difficult to calibrate, resulting in poor simulations (Chu et al., 2004). Overall, most of the statistics were satisfactory or better as per Moriasi et al., (2007).

PALESTINE

Statistical results for the calibration and validation at the Palestine site are shown in Table (4.3) and temporal results are shown in Figure (4.3). The coefficient of determination (R^2) and

Nash-Sutcliffe efficiency (NSE) ranged from 0.4 to 0.9 and 0.3 to 0.8 respectively. Most of the total flow, surface flow, and base flow statistics were satisfactory at Palestine and showed good correlation between measured and simulated values as per the model evaluation guidelines provided by Moriasi et al. (2007). Total flow was underpredicted during calibration (positive biases) and overpredicted (negative biases) during validation. SWAT mainly underpredicted total flow in March 2001, January 2002 and May 2002, and overpredicted in January 2008 (Figure 4.3). This under and overprediction is attributed to SWAT model's inability to simulate storm event as it is designated for long term simulation. Surface flow was somewhat underpredicted during the calibration and overpredicted during the validation period. Nonetheless, the model was considered satisfactory on a holistic basis due to the robustness of multi-site, multi-variable, and multi-objective calibration and validation approach.

4.3 VALIDATION: VANNADALE

Most of the statistical results showed that the model responses at Vannadale were satisfactory (Table 4.4). As can be seen in Figure (4.4), there was a huge localized storm in January 2007. In order to match the peak of this storm, the model overpredicted total flow for other time periods. The coefficient of determination for nitrate-nitrogen and the Nash-Sutcliffe efficiency for total flow and sediment were below the satisfactory level as per the Moriasi et al. (2007). However, these statistics were considered satisfactory based on the statistics reported by other studies (Cao et al., 2006; Onusluel and Rosbjerg, 2010; Qi and Grunwald, 2005; Santhi et al., 2001; Srinivasan et al., 1998; White and Chaubey, 2005).

Table 4.1: Parameters adjusted during the multi-site, multi-variable, and multi-objective calibration.

Variable	Description	Unit	Input file	Sub watershed (S)/Watershed (W)	Recommended Range in SWAT
Hydrology					
CN2	Curve number for the moisture condition II	None	mgt	S	-
ESCO	Soil evaporation compensation factor	None	hru	W	0.01 – 1.0
SOL_AWC	Available water capacity in the soil	mm/mm	sol	S	-
ALPHA_BF	Baseflow alpha factor	days	gw	S	0.1 – 1.0
GWQMN	Depth of water which is necessary for the occurrence of the groundwater flow	mm	gw	S	-
GW_REVAP	Groundwater revap coefficient	None	gw	S	0.02 – 0.20
Sediment					
CH_N2	Manning’s ‘n’ for the main channel	None	sub	S	0.016 – 0.150
USLE_P	Support practice factor of the Universal Soil Loss Equation equation	None	mgt	S	-
SPCON	Cofficient provided by the user in simulating the maximing amount of sediment that is allowed to transport from a reach segment	None	bsn	W	0.0001 – 0.01
SPEXP	Exponent cofficient required to be provided by the user in simulating the maximum amount of sediment that is allowed to transport from a reach segment	None	bsn	W	1.0 – 2.0
PRF	Peak rate adjustment factor for the main channel sediment routing	None	bsn	W	-
USLE_C	Minimum value of USLE C	None	Crop	S	-

	factor for water erosion applicable to the land cover/plant				
Total Phosphorus					
SURLAG	Surface runoff lag cofficient	None	bsn	W	-
SOL_Z	Depth of soil from the surface to the bottom of the layer	mm	sol	S	-
CH_K2	Main channel’s effective hydraulic conductivity	mm/hr	rte	S	0.025 - 127
PHOSKD	Phosphorous soil partitioning cofficient	m^3/Mg	bsn	W	-
PPERCO	Phosphorous percolation cofficient	m^3/Mg	bsn	W	10 – 17.5
Nitrate-nitrogen					
RCHRG_DP	Deep acquifer percolation fraction	None	gw	S	0.0 – 1.0
NPERCO	Nitrate percolation coefficient	None	bsn	W	0.01 – 1.0
SDNCO	Denitrification threshold water content	None	bsn	W	-
CDN	Denitrification exponential rate cofficient	None	bsn	W	0.0 – 3.0

Table 4.2: Statistical results for the calibration and validation at Colt.

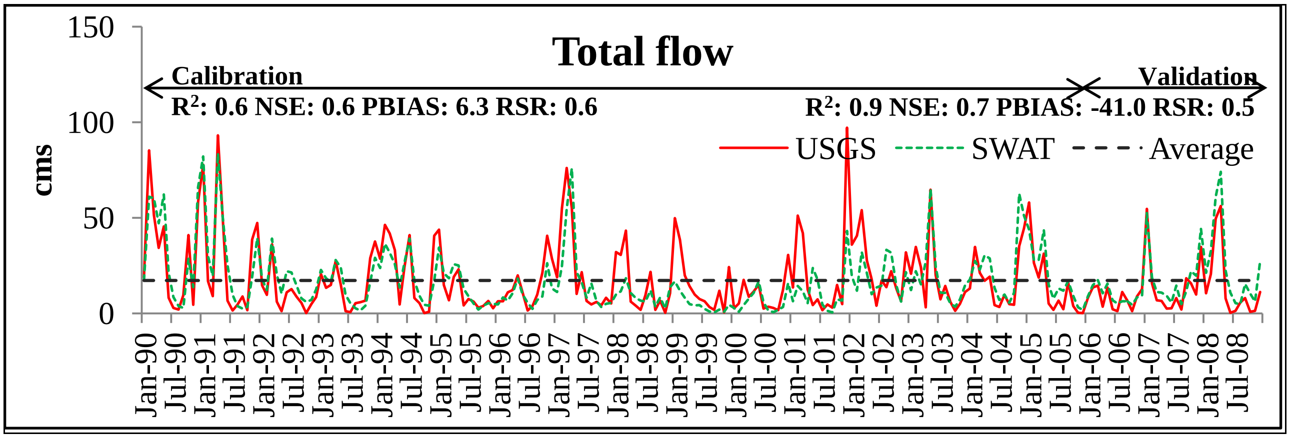
Gauge	Output	Calibration				Validation			
		R^2 *	NSE **	PBIAS ***	RSR ****	R^2	NSE	PBIAS	RSR
Colt	Total flow	0.6	0.6	6.3	0.6	0.9	0.7	-41.0	0.5
	Surface flow	0.7	0.6	-1.6	0.6	0.7	0.6	-47.1	0.7
	Base flow			19.6				-30.6	
	Sediment	0.5	0.5	56.5	0.9	0.9	0.8	27.2	0.6
	Total phosphorous	0.5	0.7	45.3	0.8	0.9	0.9	-4.9	0.5
	Nitrate-nitrogen	0.4	0.5	25.1	1.0	0.6	0.6	1.9	0.8

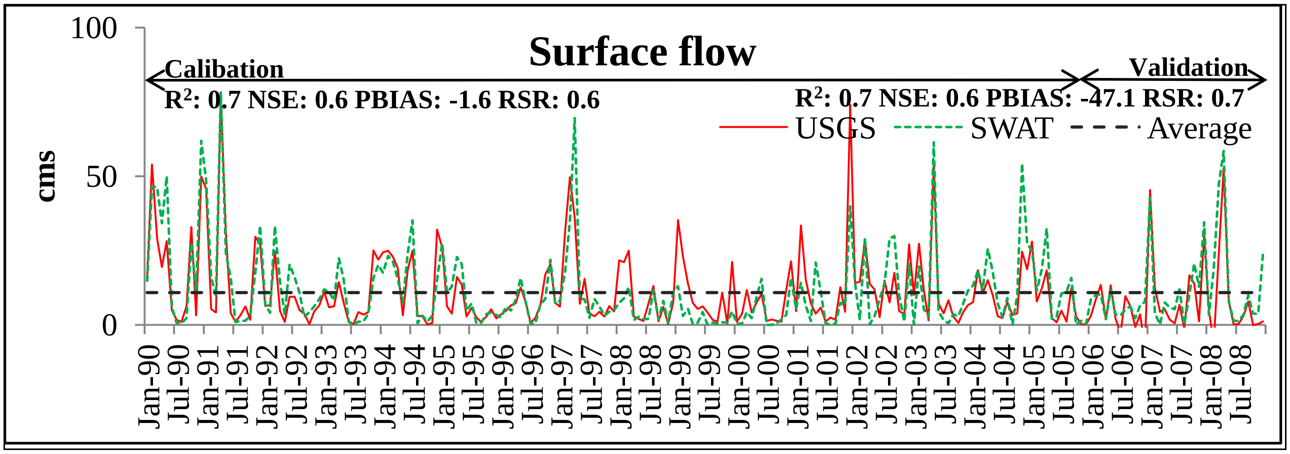
*Coefficient of Determination

**Nash-Sutcliffe Efficiency

***Percent-Bias

****Root mean square error-standard deviation ratio





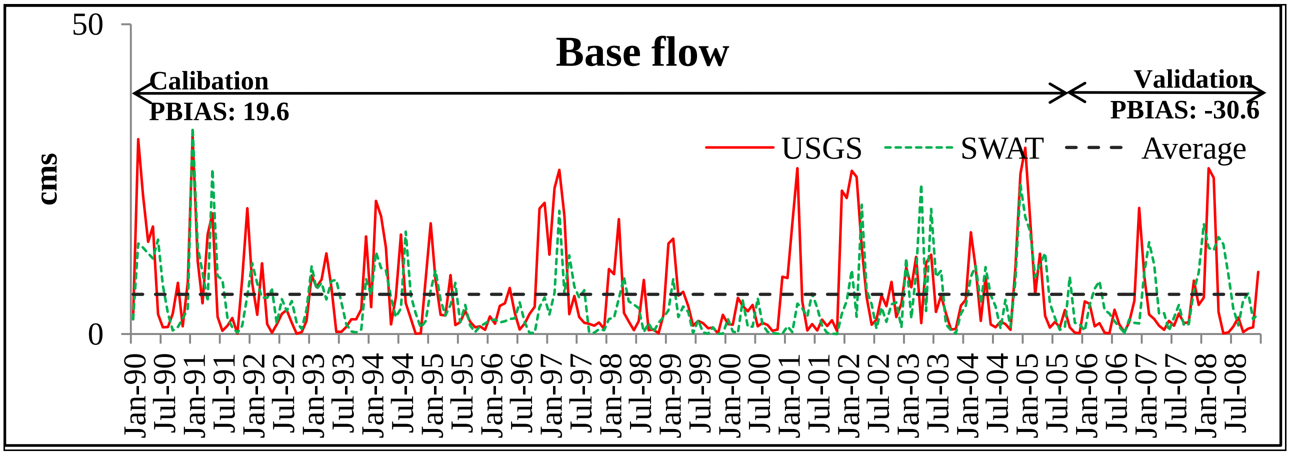
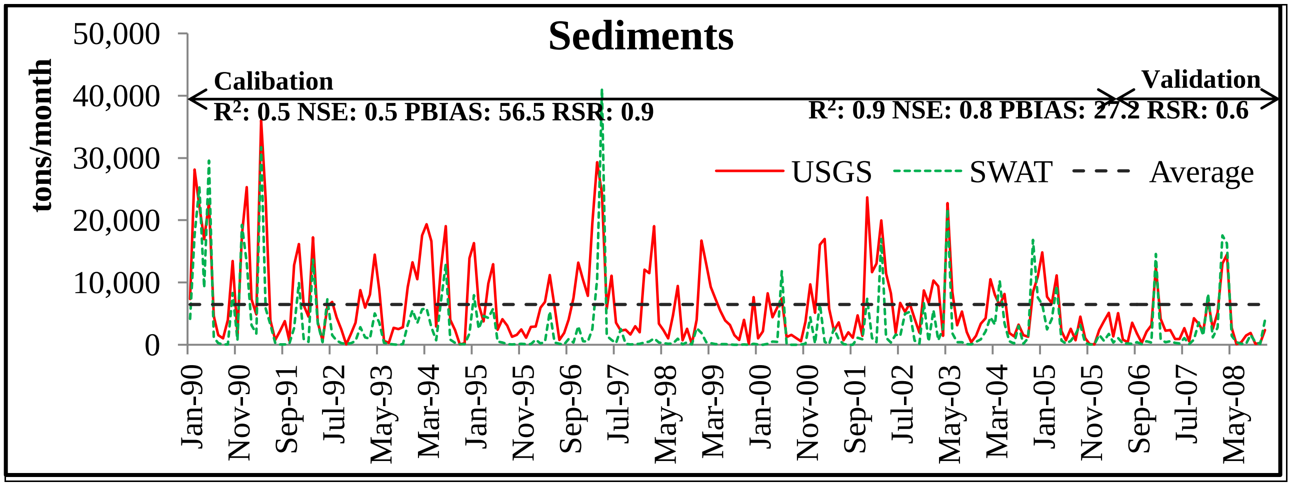
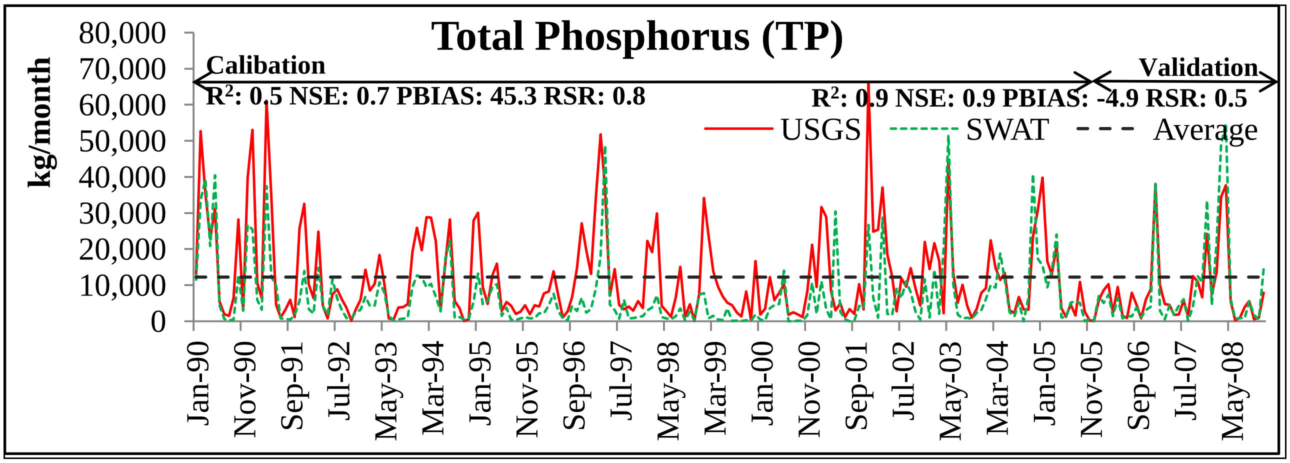


Figure 4.1: Time series plots for total, surface, and base flow calibration and validation at Colt.





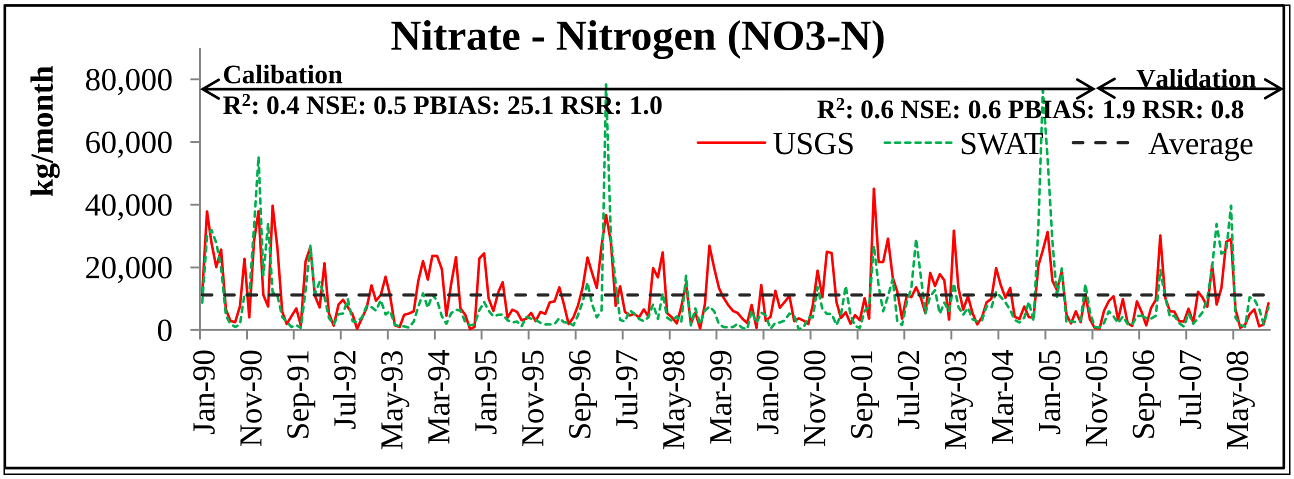


Figure 4.2: Time series plots for sediment, total phosphorus, and total nitrogen calibration and validation at Colt.

Table 4.3: Statistical results for the calibration and validation at Palestine.

Gauge	Output	Calibration				Validation			
		R^2 *	NSE **	PBIAS ***	RSR ****	R^2	NSE	PBIAS	RSR
Palestine	Total flow	0.5	0.5	23.5	0.7	0.9	0.8	-34.8	0.4
	Surface flow	0.4	0.3	26.2	0.8	0.7	0.3	-38.8	0.8
	Base flow			18.5				-26.7	

*Coefficient of Determination

**Nash-Sutcliffe Efficiency

***Percent-Bias

****Root mean square error-standard deviation ratio

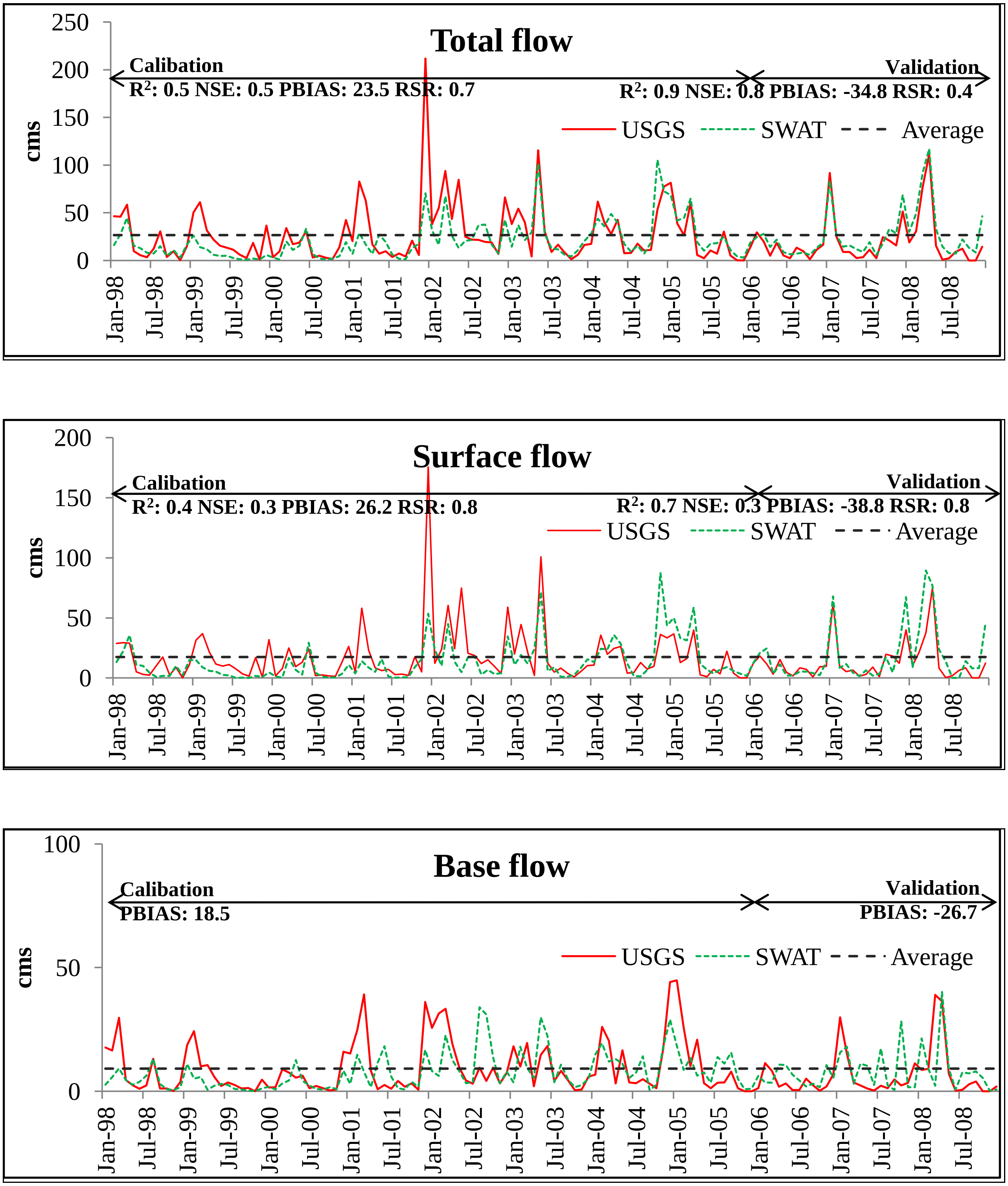


Figure 4.3: Time series plots for total, surface, and base flow calibration and validation at Palestine.

Table 4.4: Statistical results for the validation at Vannadale.

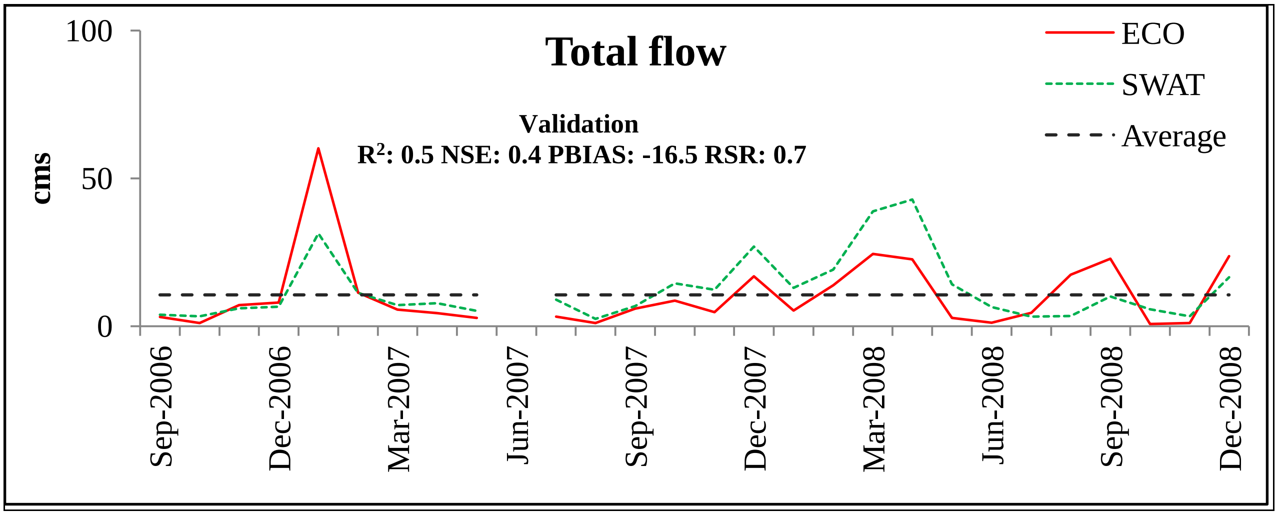
Gauge	Output	Validation			
		R^2*	NSE**	PBIAS***	RSR****
Vannadale	Total flow	0.5	0.4	-16.5	0.7
	Sediment	0.6	0.2	-16.8	1.0
	Total phosphorous	0.7	0.8	56.5	0.8
	Nitrate-nitrogen	0.3	0.5	-11.2	0.9

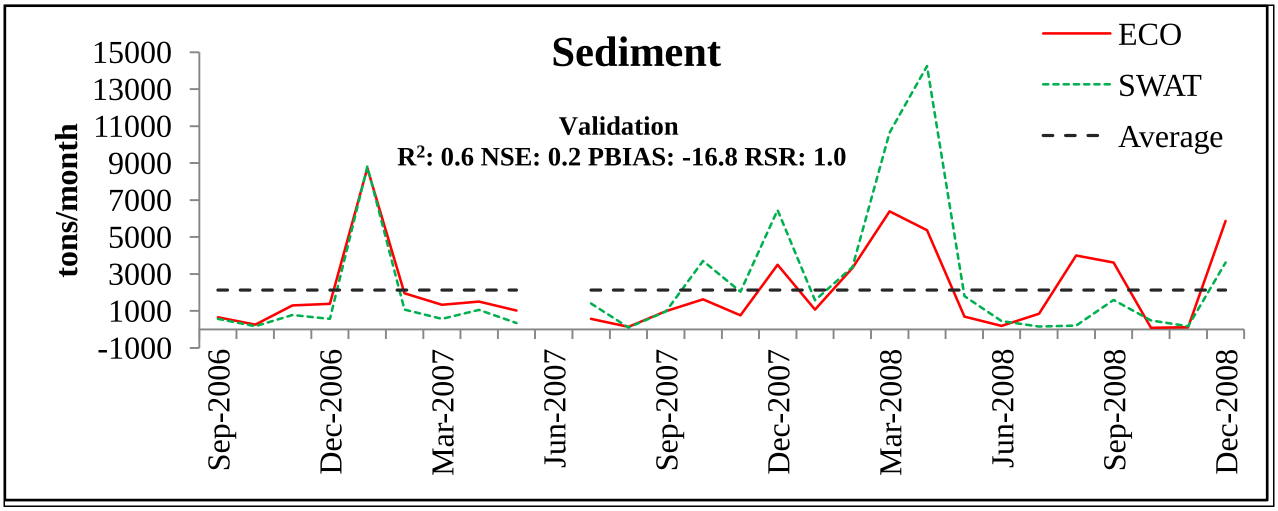
*Coefficient of Determination

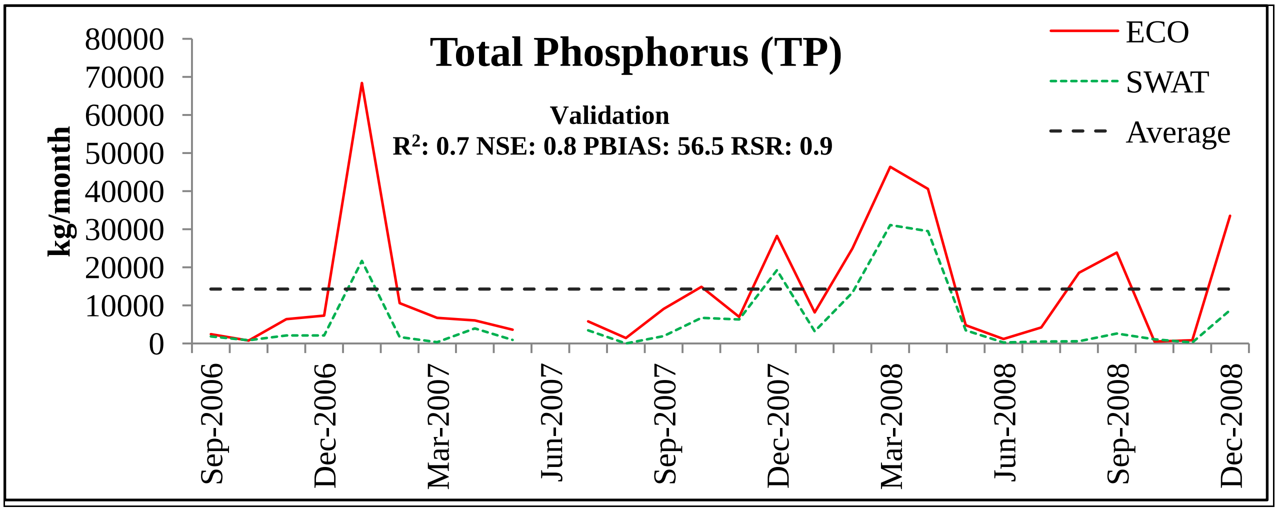
**Nash-Sutcliffe Efficiency

***Percent-Bias

****Root mean square error-standard deviation ratio


Total flow
Validation
R²: 0.5 NSE: 0.4 PBIAS: -16.5 RSR: 0.7
cms
100
50
0
Sep-2006
Dec-2006
Mar-2007
Jun-2007
Sep-2007
Dec-2007
Mar-2008
Jun-2008
Sep-2008
Dec-2008
ECO
SWAT
Average


Sediment
Validation
R²: 0.6 NSE: 0.2 PBIAS: -16.8 RSR: 1.0
tons/month
15000
13000
11000
9000
7000
5000
3000
1000
-1000
Sep-2006
Dec-2006
Mar-2007
Jun-2007
Sep-2007
Dec-2007
Mar-2008
Jun-2008
Sep-2008
Dec-2008
ECO
SWAT
Average


Total Phosphorus (TP)
Validation
R²: 0.7 NSE: 0.8 PBIAS: 56.5 RSR: 0.9
kg/month
80000
70000
60000
50000
40000
30000
20000
10000
0
Sep-2006
Dec-2006
Mar-2007
Jun-2007
Sep-2007
Dec-2007
Mar-2008
Jun-2008
Sep-2008
Dec-2008
ECO
SWAT
Average

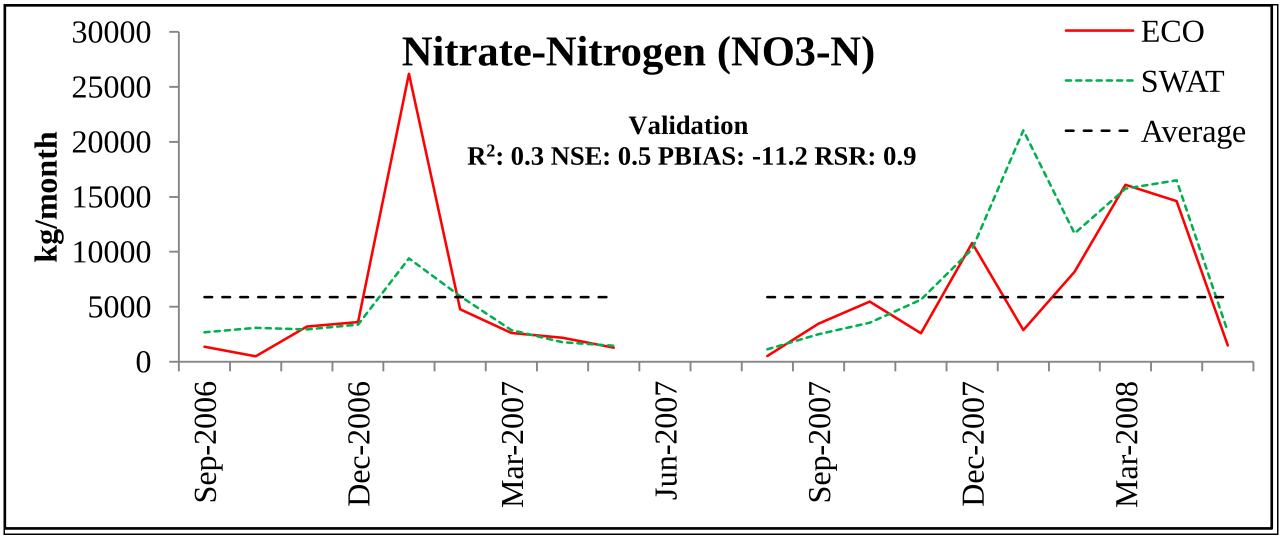


Figure 4.4: Time series plots for total flow, sediments, total phosphorus, and total nitrogen validation at Vannadale.

4.4 COMPARISON BETWEEN THE CONVENTIONAL AND NOVEL (TARGETED) APPROACH

Area-weighted average annual sediment, TP, and total nitrogen (TN) losses resulting from the simulated switchgrass were analyzed for the conventional and novel approach (Figures 4.5 and 4.6). Similarly, area-weighted average annual sediment, TP, and TN losses resulting from the simulated miscanthus were analyzed for the conventional and novel approach (Figures 4.7 and 4.8).

Area-weighted average annual sediment, TP, and TN losses resulting from the simulated switchgrass and miscanthus were less for the novel approach (targeted marginal land) as compared to the conventional approach (Figures 4.5-4.8). Compared to novel approach, the conventional approach resulted in overprediction of sediments by 20 and 61%, TP by 17 and 53%, and TN by 25 and 65% for the simulated switchgrass and miscanthus, respectively. This was expected because of the presence of lesser numbers of HRUs (only targeted marginal HRUs) under the novel approach. In other words, the conventional approach resulted in simulation of switchgrass and miscanthus on the additional HRUs which were not targeted. As a result, the pollutant losses were higher for the conventional approach. Therefore, simulation of switchgrass and miscanthus on the targeted HRUs reduced the sediment, TP, and TN exiting from these HRUs. Thus, it was concluded that there were differences in sediment, TP, and TN with the simulation of switchgrass and miscanthus via conventional and novel approach.

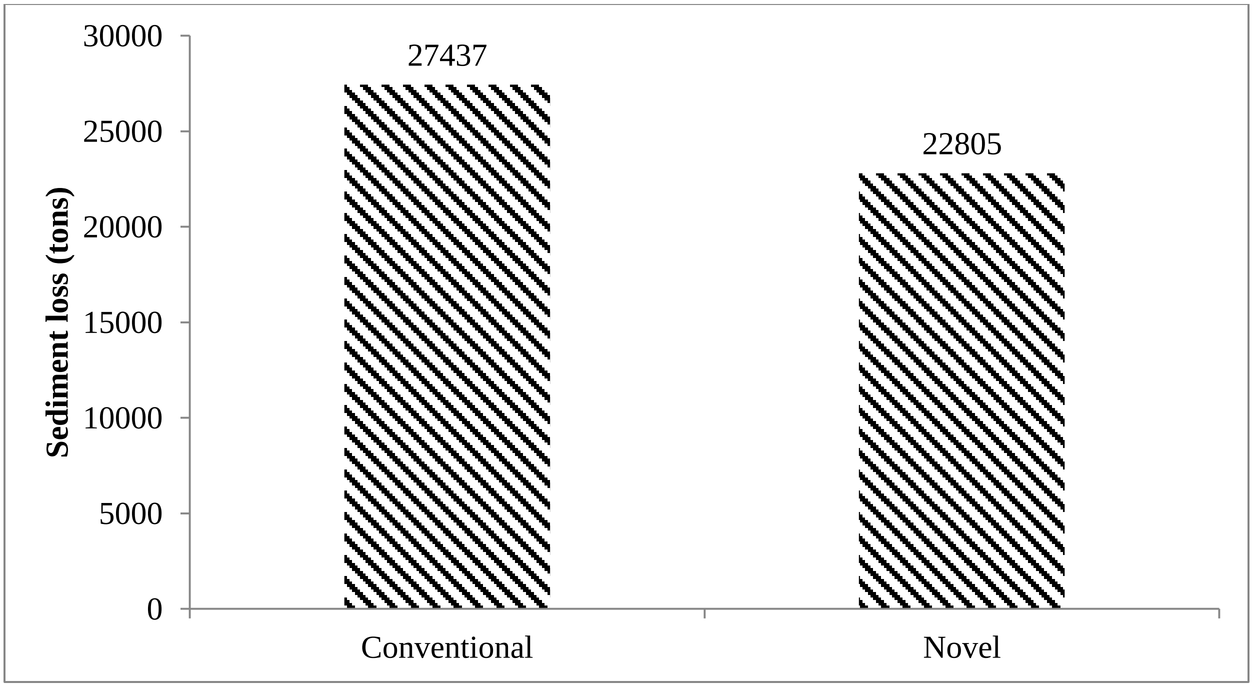


Figure 4.5: Comparison between the conventional and novel approach for the area-weighted average annual sediment losses resulting from the simulated switchgrass.

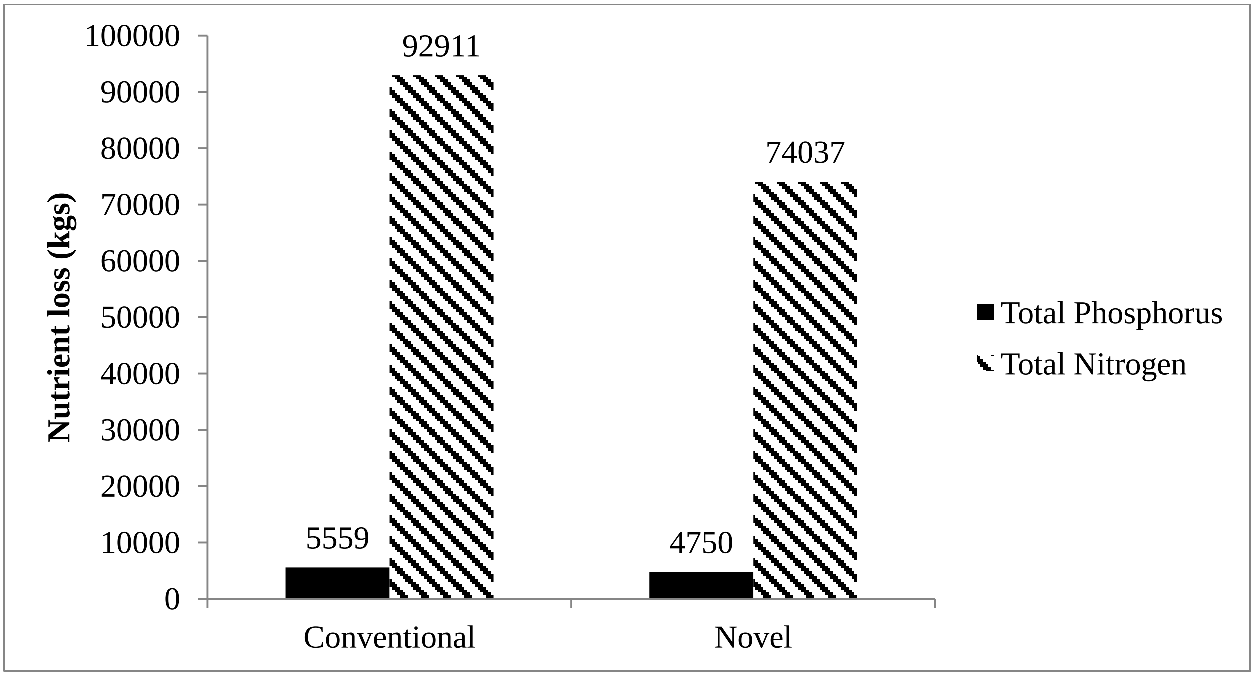


Figure 4.6: Comparison between the conventional and novel approach for the area-weighted average annual nutrient losses resulting from the simulated switchgrass.

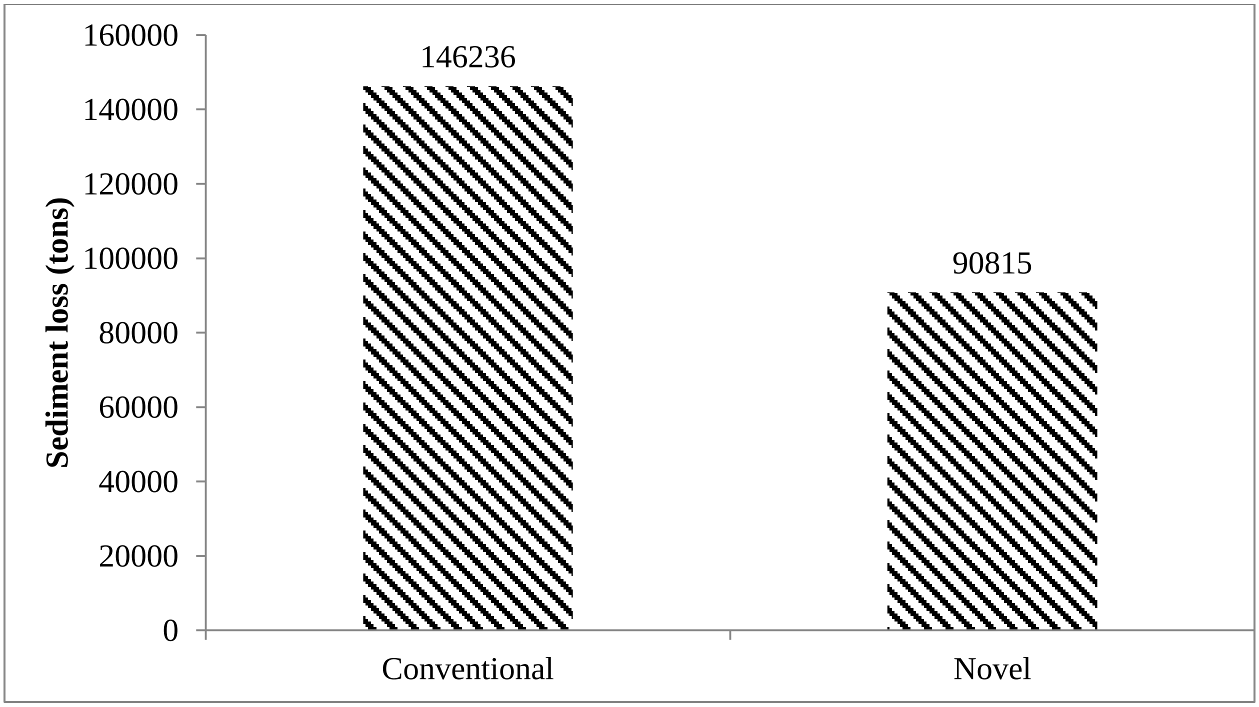


Figure 4.7: Comparison between the conventional and novel approach for the area-weighted average annual sediment losses resulting from the simulated miscanthus.

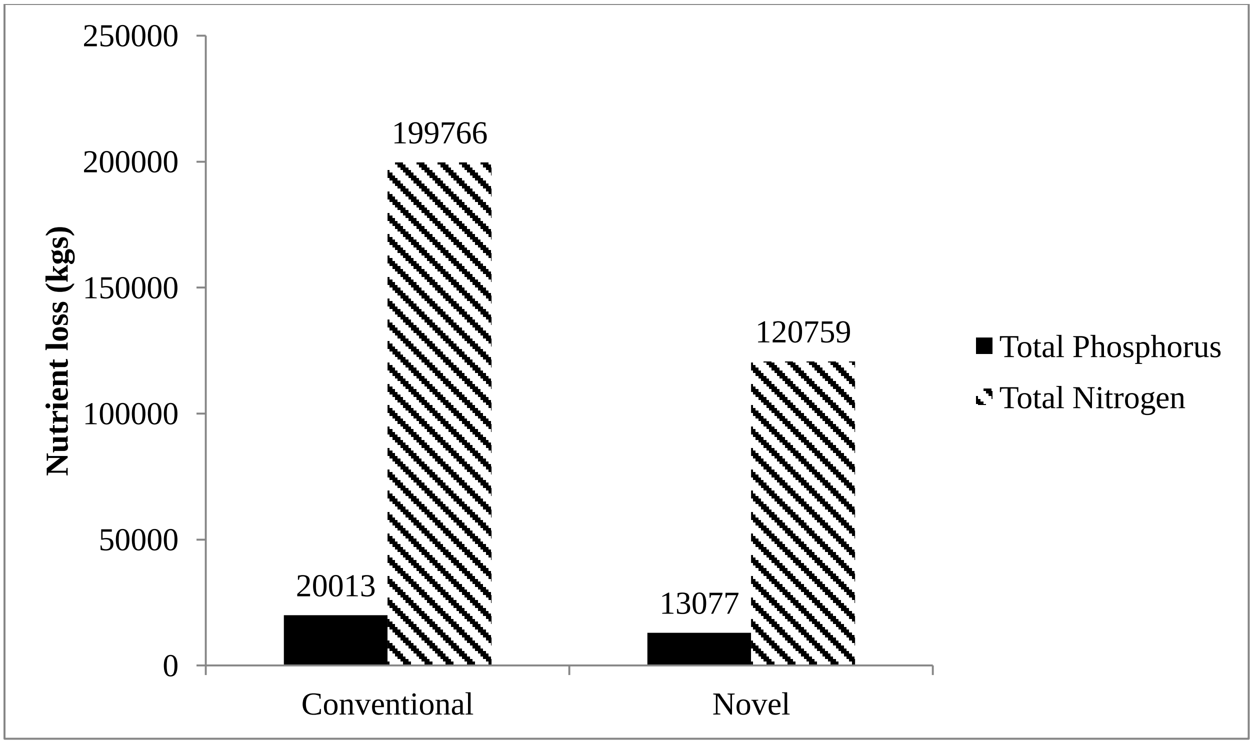


Figure 4.8: Comparison between the conventional and novel approach for the area-weighted average annual nutrient losses resulting from the simulated miscanthus.

4.5 WATER QUALITY IMPACTS OF SWITCHGRASS AND MISCANTHUS ON MARGINAL LAND (DEFINED BY THE NOVEL APPROACH)

Simulation of switchgrass on marginal land resulted in 94% decrease in sediment, 96% decrease in TP, and 80% decrease in TN compared to the baseline losses (baseline represents the current cropping condition) (Figure 4.9). Similarly, simulation of miscanthus on marginal land resulted in 78% decrease in sediment, 90% decrease in TP, and 67% decrease in TN compared to the baseline losses (Figure 4.9). One of the reasons for decrease in sediment loss was the lack of simulating tillage operation after the first year of establishment of switchgrass and miscanthus, respectively. Studies have reported that sediment losses will decrease in the absence of tillage practices (Giri et al., 2012; Yang et al., 2011). Additionally, switchgrass and miscanthus are closely grown, deeply rooted crops that hinder the transport of sediments. Phosphate (36 pounds P2O5) nutrient was applied to switchgrass and miscanthus only in their first year of establishment. As a result, the land use change to switchgrass and miscanthus resulted in TP reduction compared to the baseline losses. In fact, the binding nature of phosphorus on the surface of sediments creates a predictable correlation between TP and sediments. As switchgrass and miscanthus require lower inputs of nitrogenous fertilizer compared to the baseline crops, therefore there was a reduction in TN with the simulation of switchgrass and miscanthus. Sarkar et al. (2011) reported a simulated long-term TN reduction of 87% for the one-cut mature switchgrass which was quite similar to the 80% reduction obtained in the present study. In summary, simulation of switchgrass and miscanthus on marginal land reduced the sediment, TP, and NO3-N losses exiting the marginal HRUs. Based on these results, it can be said that production of both switchgrass and miscanthus on marginal lands have the potential to improve water quality (sediment, TP, and TN) compared to baseline row crops produced on such lands.

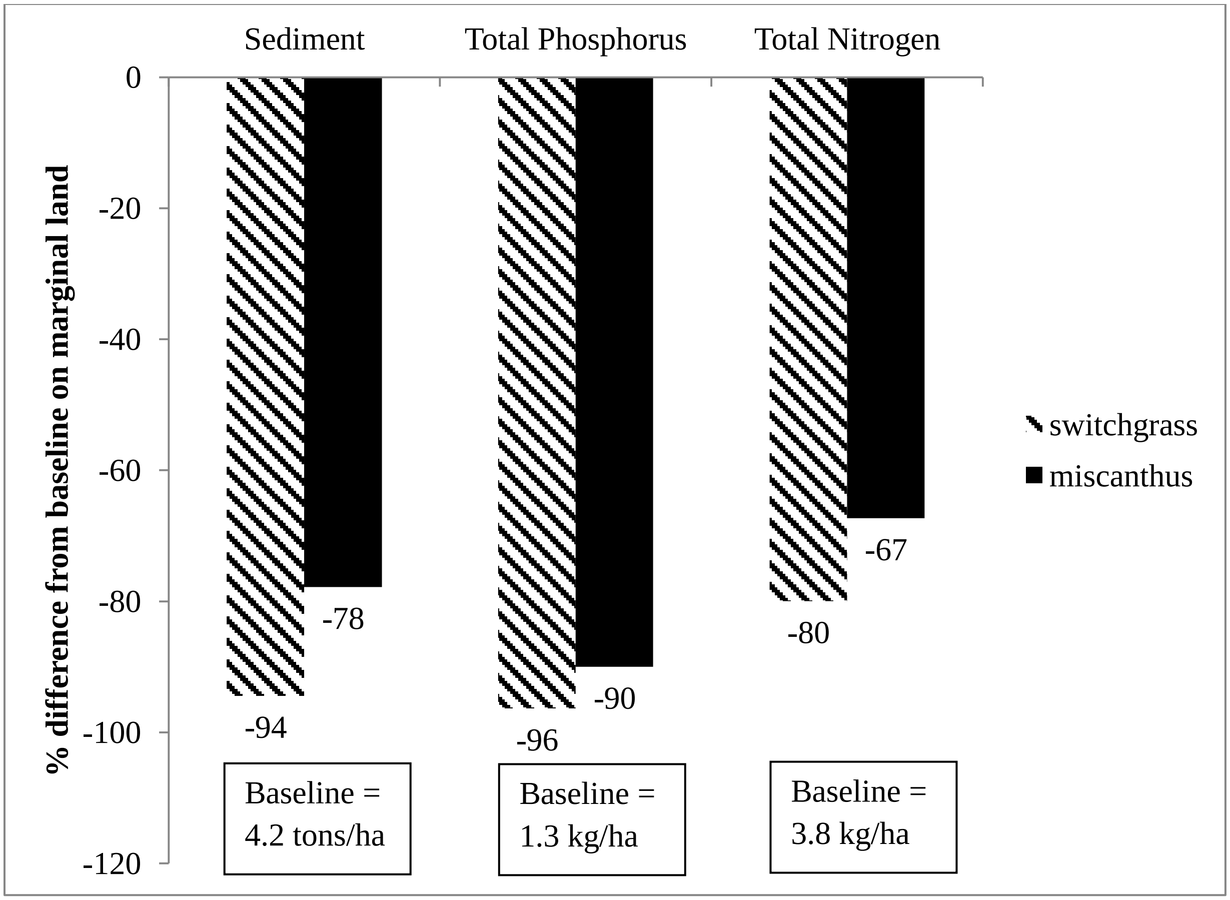


Figure 4.9: Area-weighted average annual changes in sediment and nutrient losses resulting from the simulation of switchgrass and miscanthus on marginal land compared to the baseline scenario.

In general, management practices and land cover/plant growth parameters are the two factors affecting the pollutant losses in the land use change simulation. In the present study, same management practices were defined in SWAT for simulating switchgrass and miscanthus. However, reductions in pollutant losses resulting from the simulated switchgrass and miscanthus were different. It was hypothesized that these differences were because of the difference in land cover/plant growth parameters for switchgrass and miscanthus. Land cover/plant growth parameters for switchgrass and miscanthus are shown in Appendix (D). The hypothesis was verified by replacing all the land cover/plant growth parameters for switchgrass with the defined parameters for miscanthus. The obtained pollutant losses were exactly the same for both the simulated switchgrass and miscanthus. Moreover, percentage reductions in sediment, total phosphorus, and total nitrogen were also analyzed by replacing the land cover/plant growth parameters for switchgrass with the defined parameters for miscanthus one at a time (Table 4.5). HVSTI (Harvest Index: fraction of aboveground biomass removed in harvest) was identified as the major parameter responsible for differences in the pollutant losses when marginal land was simulated with switchgrass and miscanthus. HVSTI was defined as 0.9 for switchgrass and 1.0 for miscanthus in this study. When HVSTI for switchgrass was changed from 0.9 to 1.0, reductions in pollutant losses from the baseline decreased. This was because of the fact that 100% harvest of the aboveground biomass of switchgrass will result in more pollutant losses after the harvest due to no ground cover as compared to the 90% harvest scenario, thereby resulting in less reductions for sediment, total phosphorus, and total nitrogen from the baseline.

As precipitation is the major driving factor for most of the watershed processes, temporal relation between the precipitation and simulated sediment losses for the switchgrass was explored. A direct relation was obtained between the area-weighted annual sediment losses and precipitation over the years 1990 to 2008 (Figure 4.10). Higher precipitation years resulted in higher sediment losses. TP losses followed the similar trend as sediment due to the binding nature of phosphorus on the surface of sediments (Figure 4.11). TN losses did not follow the trend with the precipitation or TP as closely as sediment did (Figure 4.12). This was mainly because of the fact that transport of nitrogen is both an overland and an underground process whereas the transport of sediment and TP are mainly overland processes.

4.6 YIELD ANALYSIS FOR THE SIMULATED SWITCHGRASS AND MISCANTHUS

The simulated yield for switchgrass and miscanthus was 7 and 9 Mg/ha respectively. The simulated yield was compared with the yields expected for the Arkansas conditions. Popp and Hogan (2007) reported that the expected yield of switchgrass in Arkansas can vary from 3-5 tons/ac (7-12 Mg/ha approx.). In Fayetteville, Arkansas, switchgrass yields ranged within 8-12 Mg/ha during field trials (West et al., 2011). Although the SWAT-simulated yield for switchgrass was on the lower side of the expected yield, the simulated yield was considered reasonable (Dr. West, personal communication, 26 June 2012). Moreover, Baskaran et al. (2010) reported that SWAT-predicted yields can be lower than the actual expected yield. Because of the unavailability of data for miscanthus yield in Arkansas, the simulated yield for miscanthus was not validated. However miscanthus yield was considered acceptable, keeping in mind that the yield simulated for miscanthus was greater than that simulated for switchgrass (Heaton et al., 2004; Burner et al., 2009).

The relation between area-weighted nitrogen uptake and the biomass yield was also explored for the switchgrass scenario on an annual scale. In general, it was found that there was a direct relation between the nitrogen uptake and the biomass yield (Figure 4.13). In other words, nitrogen uptakes increase with higher biomass yields. The area-weighted average annual simulated nitrogen uptake was 24 kg/ha (approx.) for switchgrass. Ashworth (2010) conducted field trials in Fayetteville, Arkansas and harvested switchgrass at various time periods (almost every month since its plantation) during the year 2009. She reported that the switchgrass yield varies from 0.18 to 13.2 Mg/ha, and the nitrogen removal in biomass varies from 0 to 80 kg/ha. The nitrogen uptake value for the simulated switchgrass was lower than the peak value reported by Ashworth (2010). The possible reason for this might be the low simulated switchgrass yield as compared to the peak yield reported by Ashworth (2010). Low simulated yield will result in low nitrogen uptake by switchgrass. A scatterplot was plotted between the area-weighted annual nitrogen uptakes and biomass yields for switchgrass, and a regression equation was generated between them (Figure 4.14). From the scatterplot, it was clear that higher simulated yield would result in higher nitrogen uptakes. Moreover, it was also acknowledged that the nitrogen uptakes might differ according to the location of the study area. Kering et al. (2012) conducted a field study in the southern Oklahoma and reported that switchgrass had a biomass yield of 17.8 Mg/ha and a nitrogen removal rate of 40 to 75 kg/ha. Lemus et al. (2009) conducted a field study at eight locations in five states in the upper southern USA. They reported that the average nitrogen removals in switchgrass ranges from 38.3 to 126.8 kg/ha among these eight locations. Therefore, the nitrogen uptake rate for switchgrass may vary from location to location. As a result, it is highly recommended that the yield and its associated variables (especially nitrogen uptakes) should be cross-checked with the field values (if available) in order to increase the confidence in the model simulations.

Table 4.5: Percentage reductions in sediment, total phosphorus, and total nitrogen from baseline when land cover/plant growth parameters for switchgrass were replaced with that for miscanthus one at a time.

Parameter*	**Sediment**	**Total Phosphorus**	**Total Nitrogen**
HVSTI	-64	-86	-57
BIOE	-93	-96	-79
BLAI	-94	-96	-80
CHTMX	-94	-96	-80
RDMX	-94	-96	-80
FRGRW2	-95	-97	-81
DLAI	-95	-97	-81
T_OPT	-94	-96	-80
T_BASE	-96	-97	-82
CNYLD	-94	-96	-80
CPYLD	-94	-96	-80
BN1	-94	-96	-80
BN2	-96	-97	-81
BN3	-93	-96	-79
BP1	-93	-96	-78
BP2	-94	-96	-80
BP3	-94	-96	-80
WSYF	-94	-96	-80
WAVP	-94	-96	-80
EXT_COEF	-96	-97	-83

*Details about the parameters can be obtained from the SWAT Input/Output documentation available at: http://swatmodel.tamu.edu/media/19754/swat-io-2009.pdf

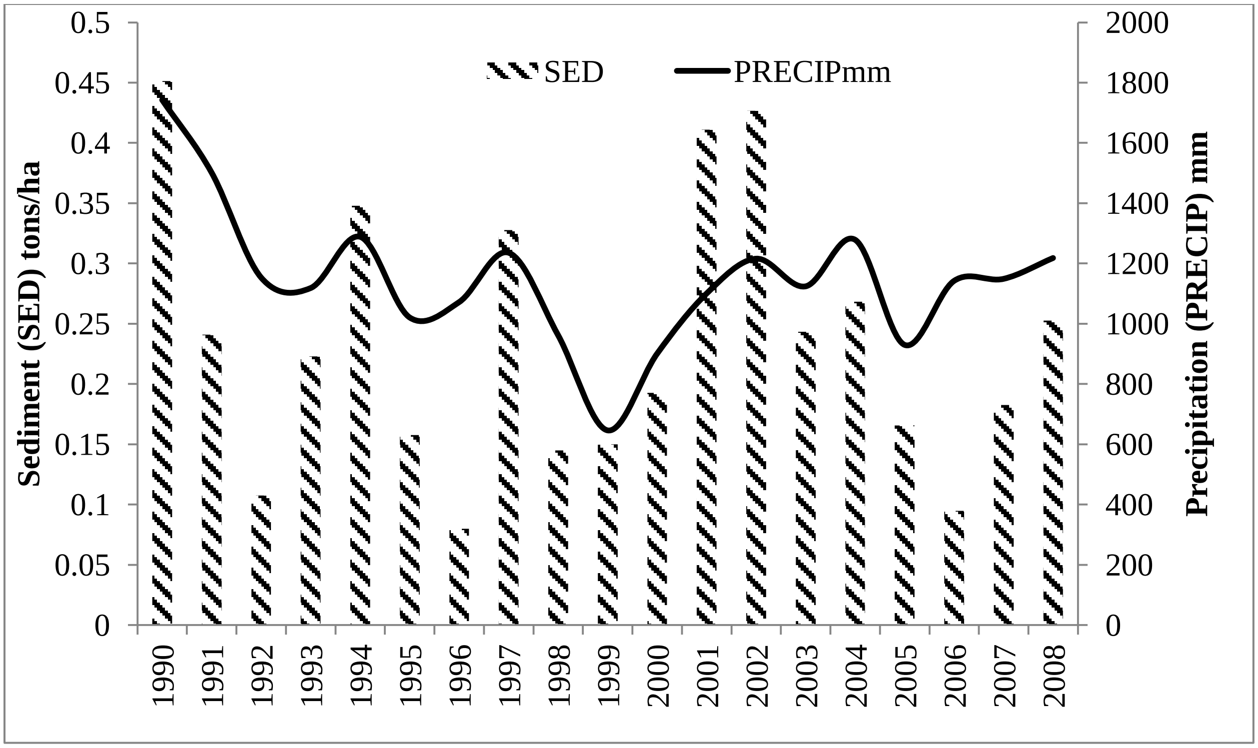


Figure 4.10: Area-weighted annual sediment losses and its relation with precipitation for the simulated switchgrass.

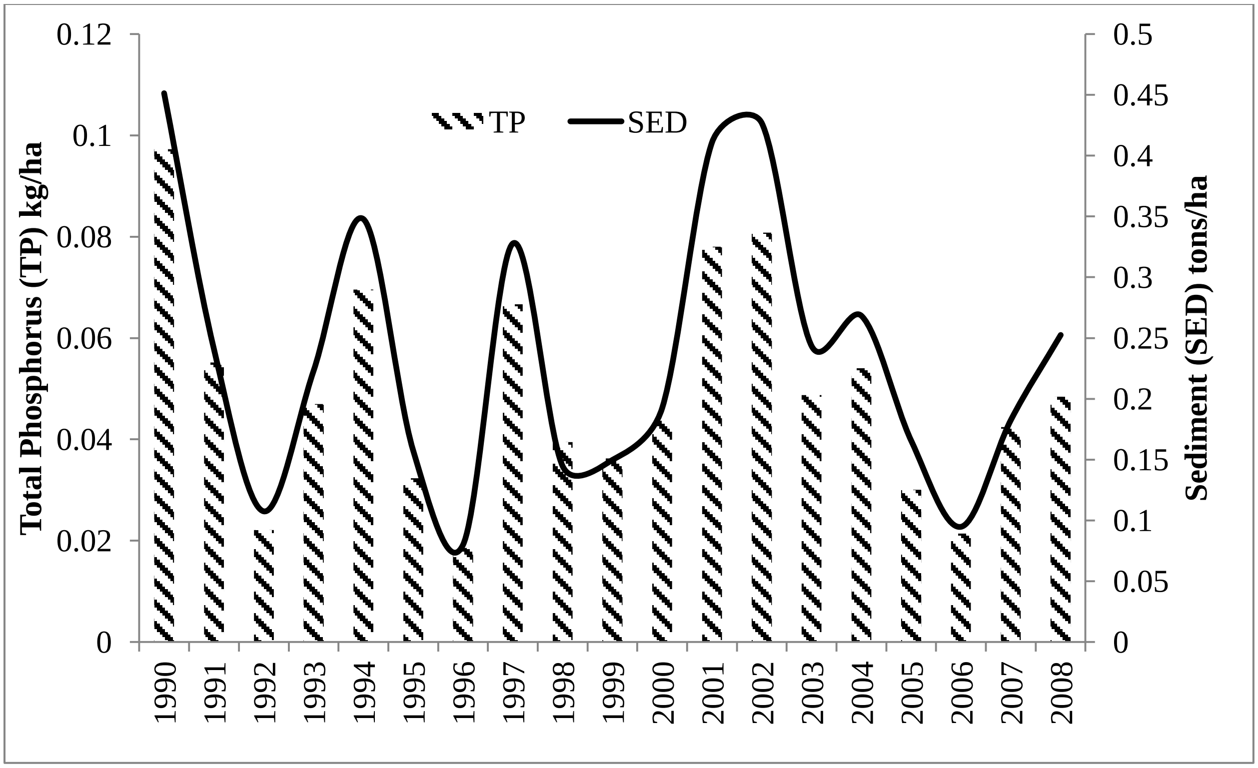


Figure 4.11: Area-weighted annual total phosphorus losses and its relation with sediment losses for the simulated switchgrass.

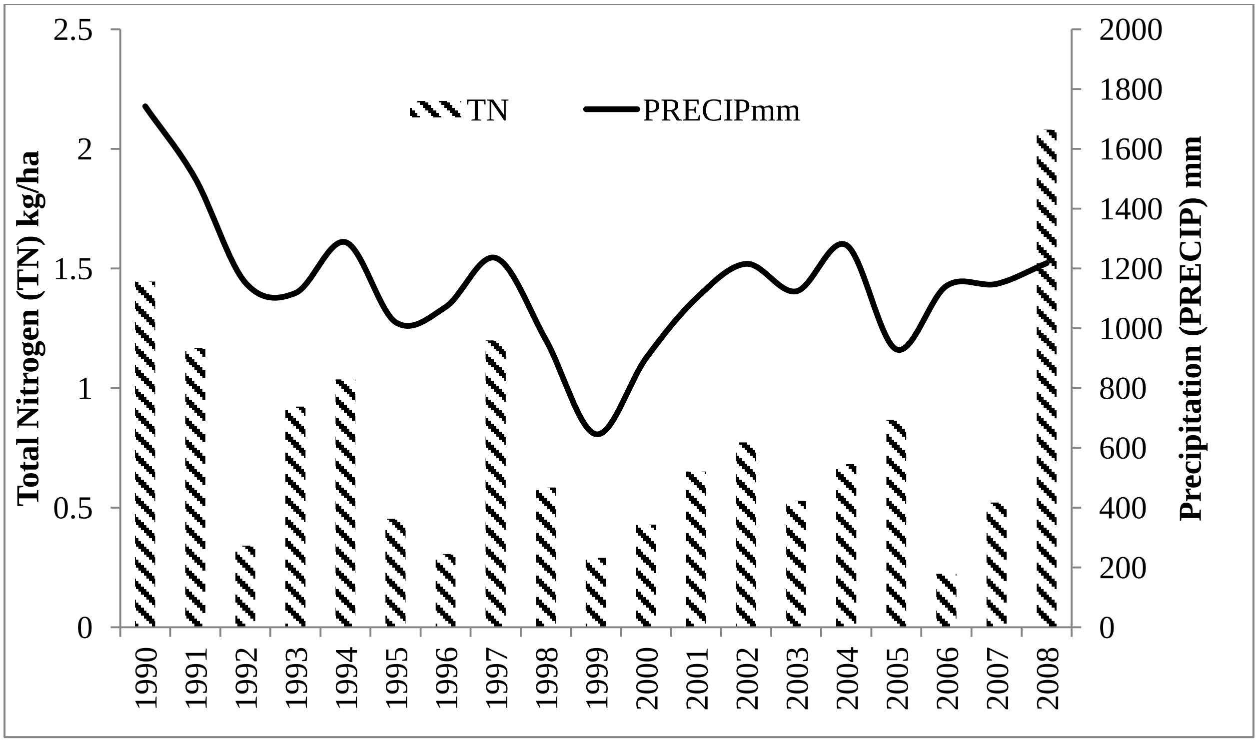


Figure 4.12: Area-weighted annual total nitrogen losses and its relation with precipitation for the simulated switchgrass.

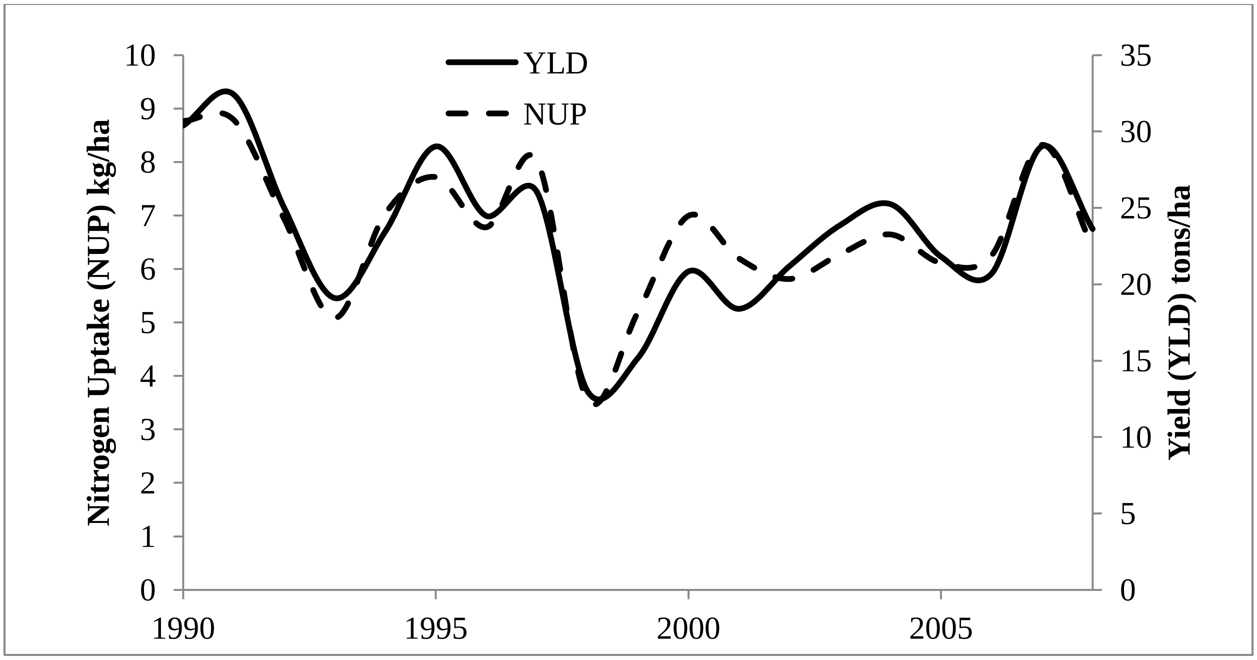


Figure 4.13: Area-weighted annual temporal relation between nitrogen uptake and biomass yield for the simulated switchgrass.

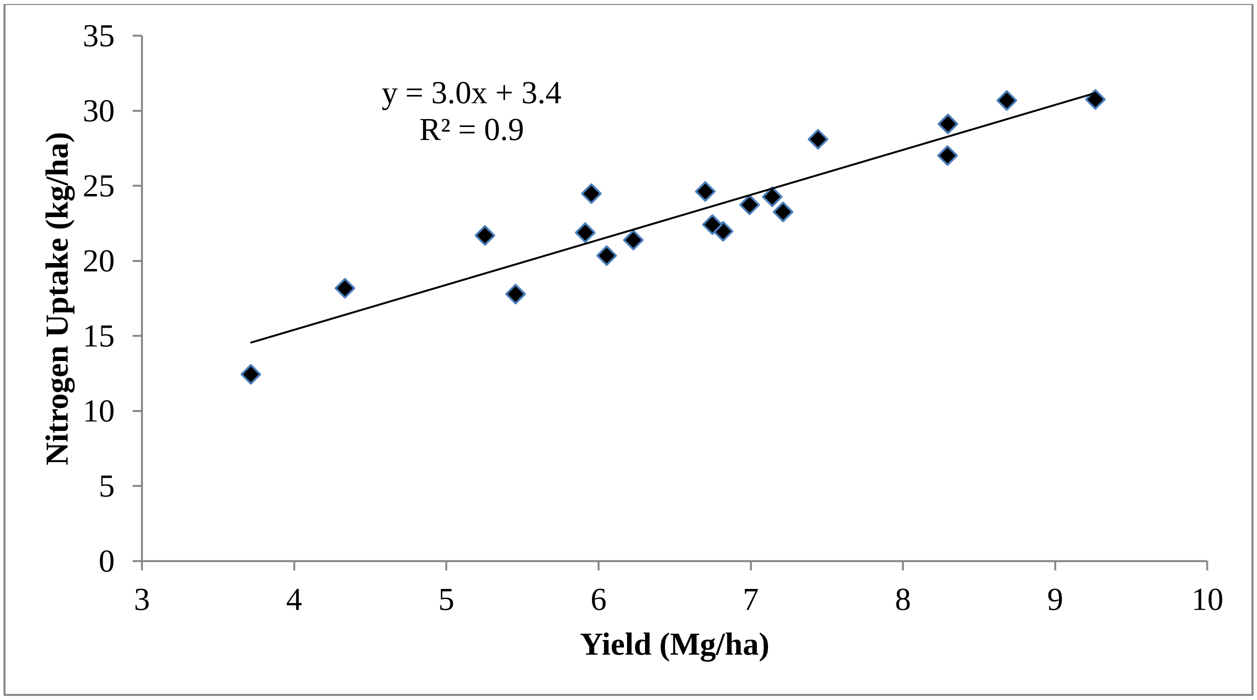


Figure 4.14: Scatterplot for the area-weighted annual nitrogen uptake and the biomass yield for the simulated switchgrass.

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CHAPTER V

CONCLUSIONS

Objective 1: Development of a novel simulation approach to incorporate marginal land in the SWAT model followed by calibration and validation of the model for the L'Anguille River watershed.

A novel simulation approach was developed to implement targeted land use change in the soil and water assessment tool (SWAT) model for simulating biofuel crops on marginal land. A modified land use and land cover data layer was prepared and input in the SWAT model for conducting targeted land use change in the L'Anguille River watershed (LRW). The SWAT model's simulations were performed at daily time step for the period covering 1986 to 2008. Statistical and graphical results for the calibration and validation period, analyzed on a monthly time step for the multi-site, multi-variable, and multi-objective model for output variables (total flow, surface flow, base flow, sediment, and total phosphorus) showed that there was a good correspondence between the simulated and measured data. However, there were a few months during calibration period at which the model underpredicted the total flow, surface flow, base flow, sediment, and total phosphorus and overpredicted during validation. Results for the nitrate-nitrogen simulation were found below satisfactory level as per the evaluation criteria used in this study. The overall performance of LRW SWAT model was considered acceptable for total flow, surface flow, base flow, sediment, and total phosphorus.

Objective 2: Comparison between the conventional and novel approach for water quality impacts of biofuel crop simulation on marginal land.

The conventional approach resulted in higher sediment, total phosphorus, and total nitrogen losses for both the switchgrass and miscanthus as compared to the novel approach. On further investigation, it came to light that there was an additional 209 square kilometers of marginal land that was simulated under the conventional approach due to the model's limitation to exclude non-targeted hydrological response units (HRUs). Pollutant losses from the additional marginal land explained the differences in the sediment, total phosphorus, and total nitrogen losses for the conventional and novel appraoch.

Objective 3: Analysis of the water quality impacts of biofuel crop simulation on the targeted marginal land (defined by the novel approach) at the HRU scale.

Compared to the baseline losses, simulation of switchgrass and miscanthus on marginal land resulted in 94% and 78% decrease in sediment, 96% and 90% decrease in total phosphorus, and 80% and 67% decrease in total nitrogen, respectively. Therefore, the null hypothesis (biofuel crop simulation on marginal land is not predicting reduced pollutant losses from marginal HRUs to their respective subwatersheds's reach) was rejected in this study. The differences in the magnitude of reductions were traced to the land cover/plant growth parameters for switchgrass and miscanthus.

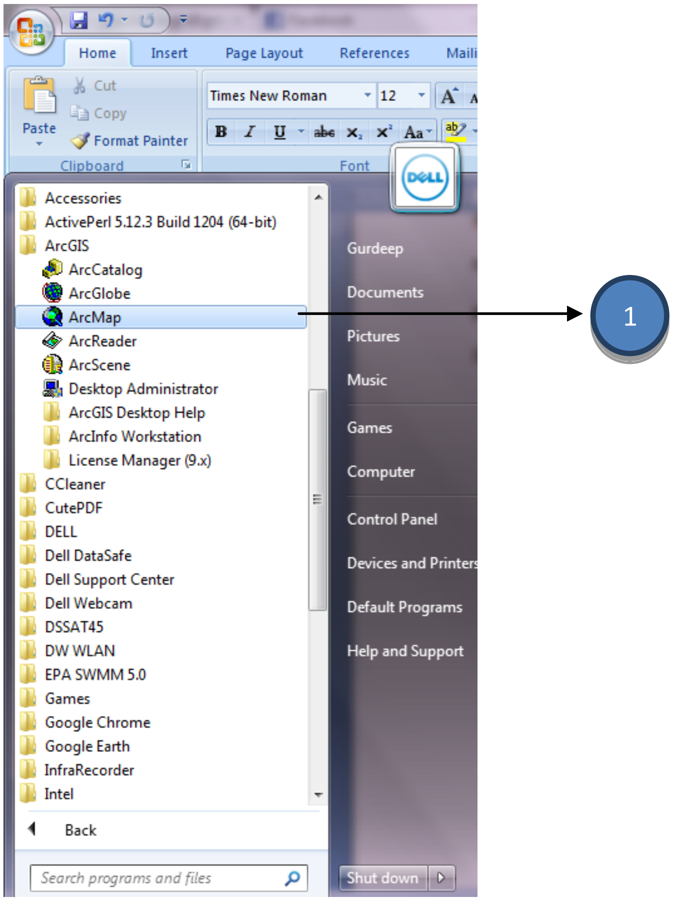
Overall, a novel approach was developed to incorporate marginal land in the SWAT model. The results indicated that the targeted land use change approach would result in lower sediment, total phosphorus, and total nitrogen losses compared to the conventional modeling approach. Moreover, the results for the targeted land use change approach also suggest that substantial reduction in pollutant losses could be achieved by replacing field crops with biofuel crops on marginal lands in the LRW.

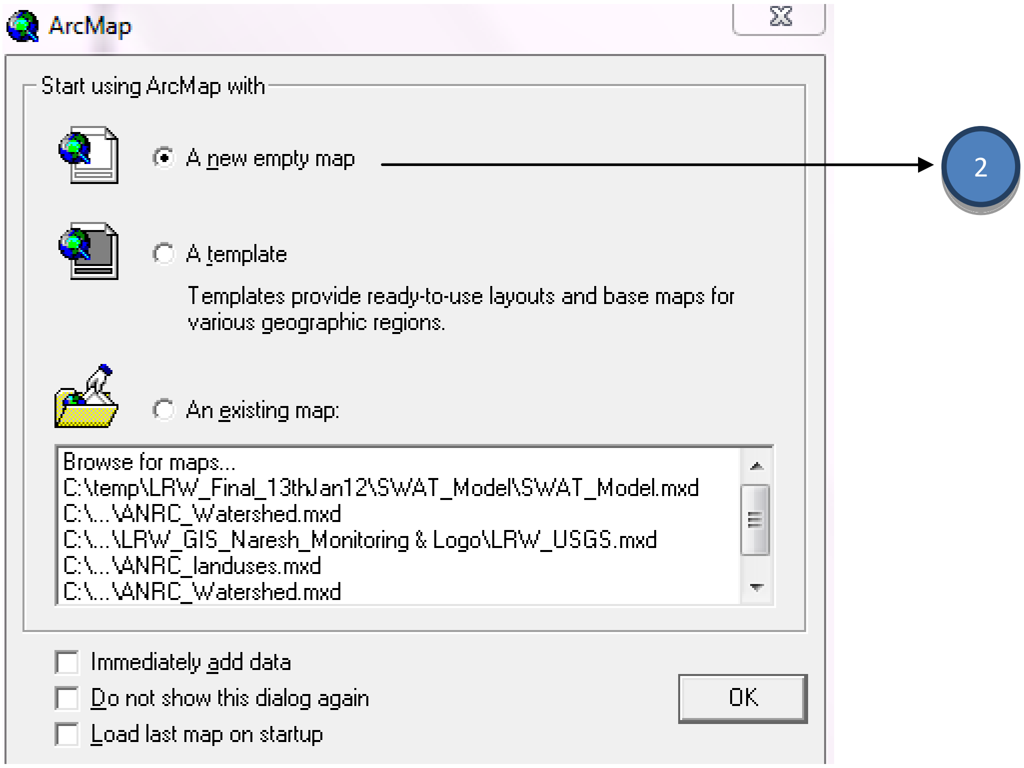
APPENDIX A: STEP-BY-STEP PROCEDURE FOR PREPARING THE MODIFIED LAND USE AND LAND COVER LAYER

STARTING ARCMAP

Steps:

1. Click **Start** > **All Programs** > **ArcGIS** > **ArcMap**.
2. Select **A new empty map** by highlighting the radio button next to it.
3. Click **OK.**





ArcMap

Start using ArcMap with

● A new empty map

○ A template

Templates provide ready-to-use layouts and base maps for various geographic regions.

○ An existing map:

Browse for maps...
C:\temp\LRW_Final_13thJan12\SWAT_Model\SWAT_Model.mxd
C:\...\ANRC_Watershed.mxd
C:\...\LRW_GIS_Naresh_Monitoring & Logo\LRW_USGS.mxd
C:\...\ANRC_landuses.mxd
C:\...\ANRC_Watershed.mxd

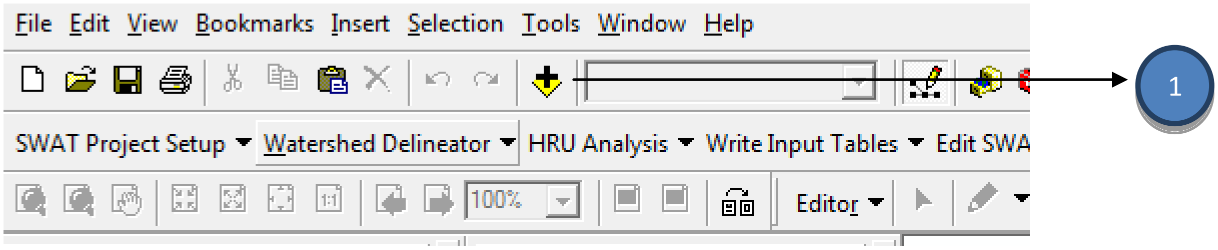
☐ Immediately add data
☐ Do not show this dialog again
☐ Load last map on startup

OK

ADDING DATA

Steps:

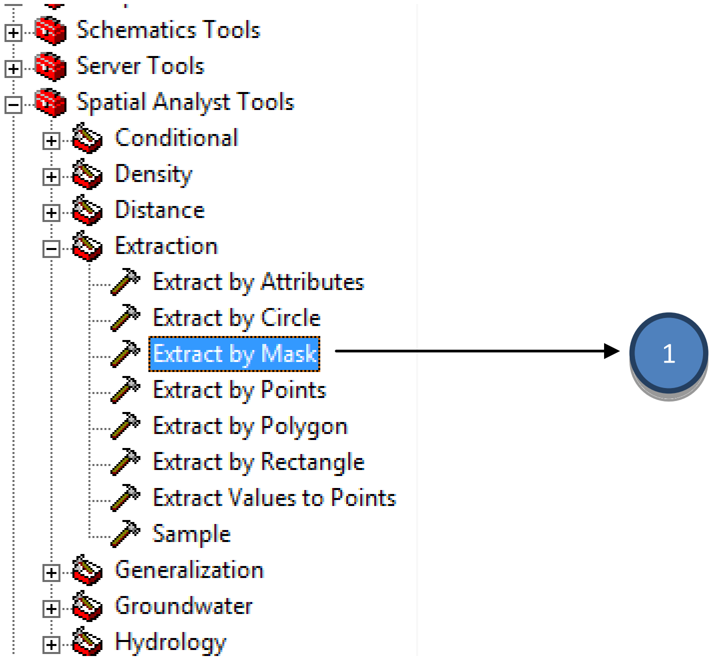
1. Click the **Add Data** button.
2. Navigate to the location on hard drive where input data for the land use and land cover (LULC) layer of the LRW was stored in order to add to ArcMap.
3. Click **Add.**
4. Navigate to the location on hard drive where input data for the marginal land (ML) layer of the LRW was stored in order to add to ArcMap.
5. Click **Add.**



EXTRACTING DATA

Steps:

1. Click **Extract by Mask** under **Spatial Analyst Tools**.
2. Browse to the location of LULC layer and add as **Input raster**.
3. Browse to the location of ML layer and add as **Input raster or feature mask data**.
4. Browse to the location of project data and name the **Output raster** as ML_Extract.
5. Click **OK.**



Input raster

LULC

Input raster or feature mask data

ML

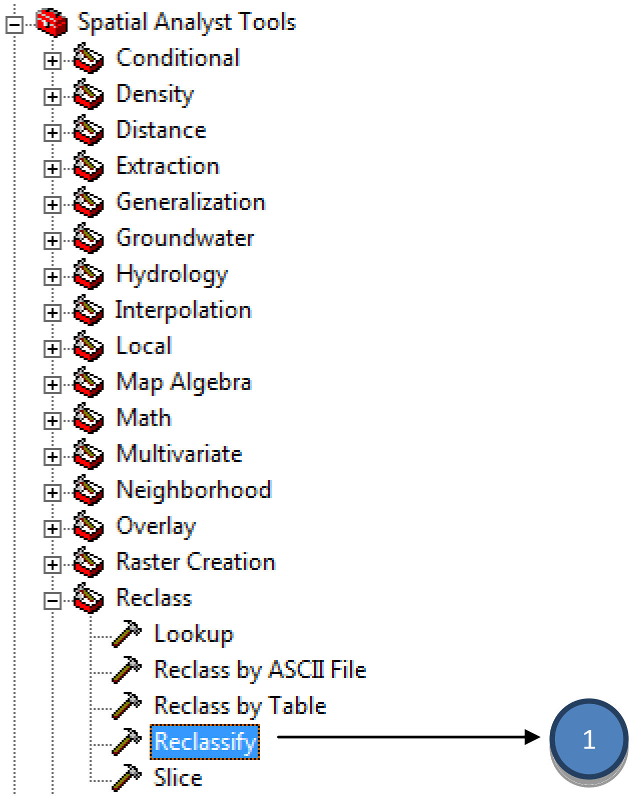
Output raster

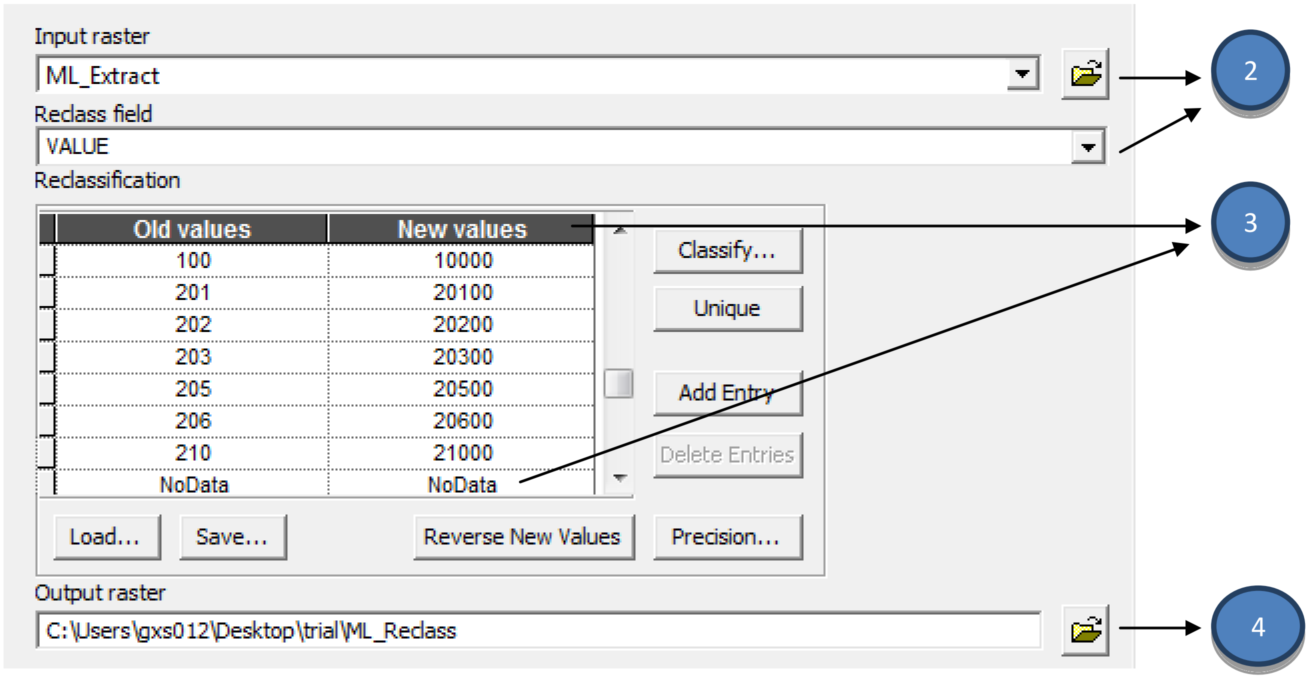
C:\Users\gxs012\Desktop\trial\ML_Extract

RECLASSIFYING DATA

Steps:

1. Click **Reclassify** under **Spatial Analyst Tools**.
2. Browse to the location of ML_Extract and add as **Input raster** with value as a **Reclass field**.
3. Obtain **New Values** by multiplying **Old Values** with 100 (value 10 to 1000, 40 to 4000, etc.). Do not change the ‘NoData’ value.
4. Browse to the location of project data and name the **Output raster** as ML_Reclass.
5. Click **OK.**
6. Click **Reclassify** again under **Spatial Analyst Tools**.
7. Browse to the location of ML_Extract and add as **Input raster** with value as a **Reclass field**.
8. Obtain **New Values** by multiplying **Old Values** with 100 (value 10 to 1000, 40 to 4000, etc.). Replace ‘NoData’ with a value of 0.
9. Browse to the location of project data and name the **Output raster** as ML_Reclass_0.
10. Click **OK**.





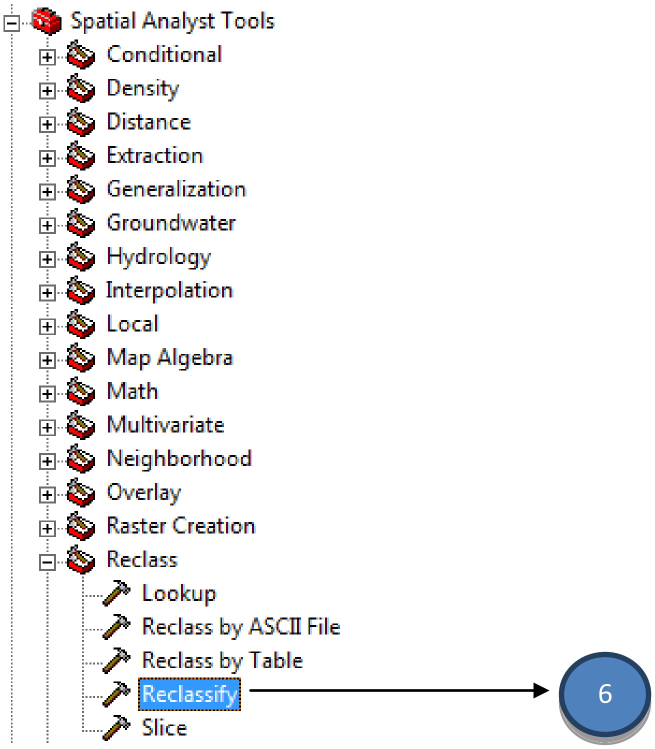
Input raster: ML_Extract

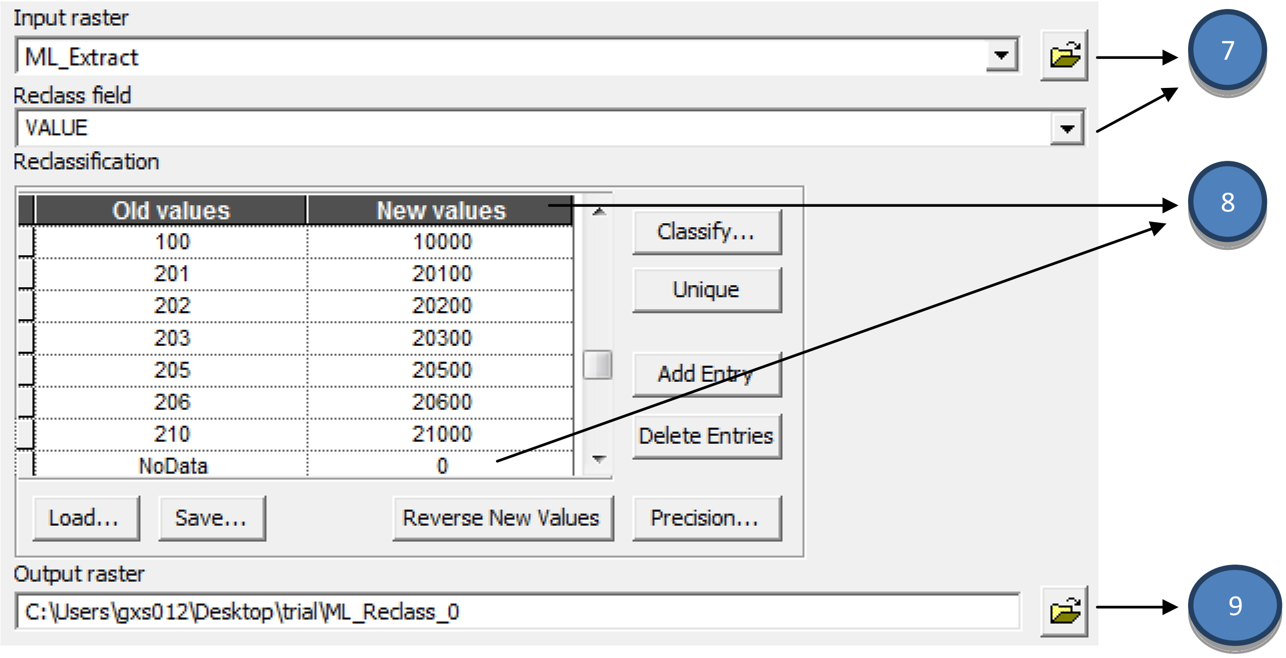
Reclass field: VALUE

Reclassification

Old values	New values
100	10000
201	20100
202	20200
203	20300
205	20500
206	20600
210	21000
NoData	NoData

Output raster: C:\Users\gxs012\Desktop\trial\ML_Reclass





Input raster: ML_Extract

Reclass field: VALUE

Reclassification

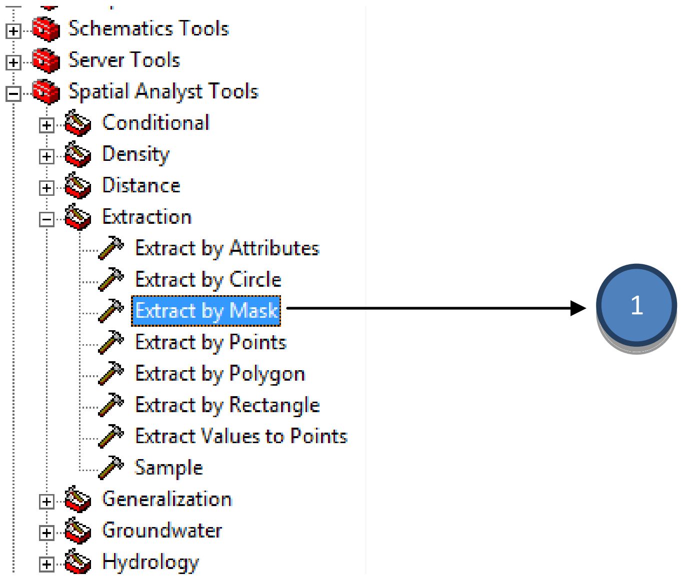
Old values	New values
100	10000
201	20100
202	20200
203	20300
205	20500
206	20600
210	21000
NoData	0

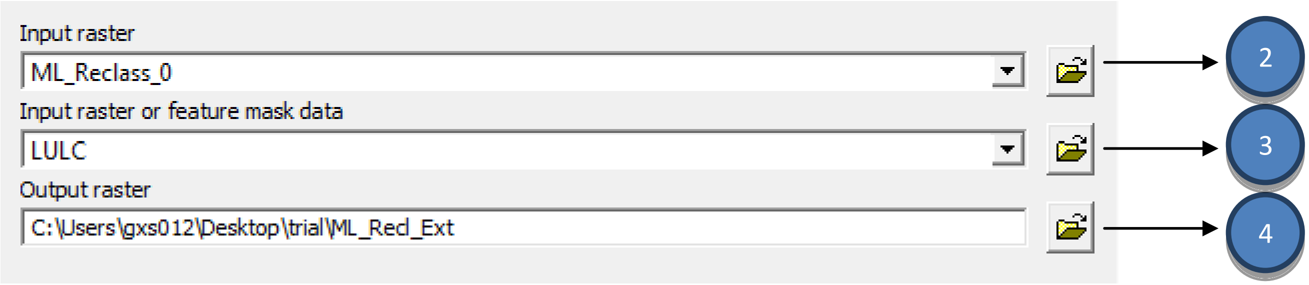
Output raster: C:\Users\gxs012\Desktop\trial\ML_Reclass_0

EXTRACTING DATA

Steps:

1. Click **Extract by Mask** under **Spatial Analyst Tools**.
2. Browse to the location of ML_Reclass_0 and add as **Input raster**.
3. Browse to the location of LULC and add as **Input raster or feature mask data**.
4. Browse to the location of project data and name the **Output raster** as ML_Recl_Ext.
5. Click **OK**.



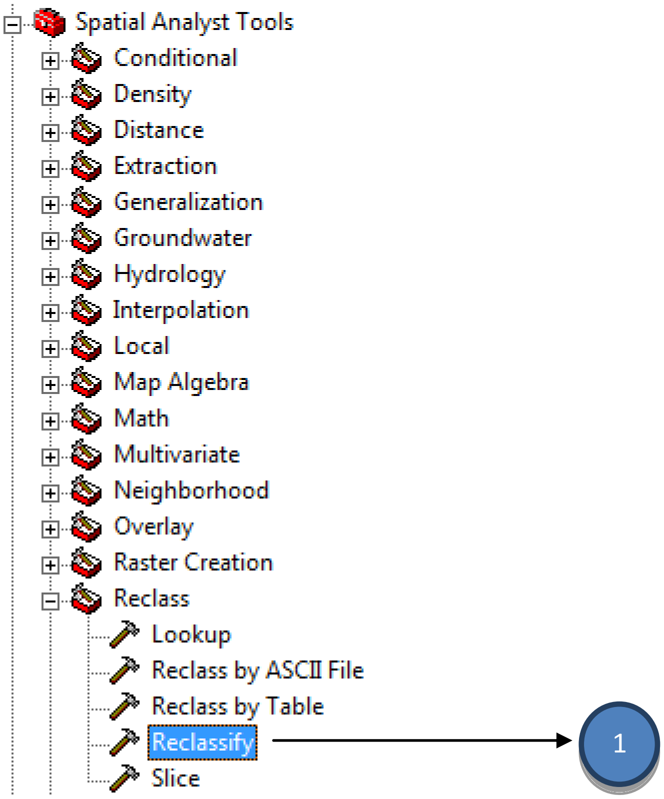


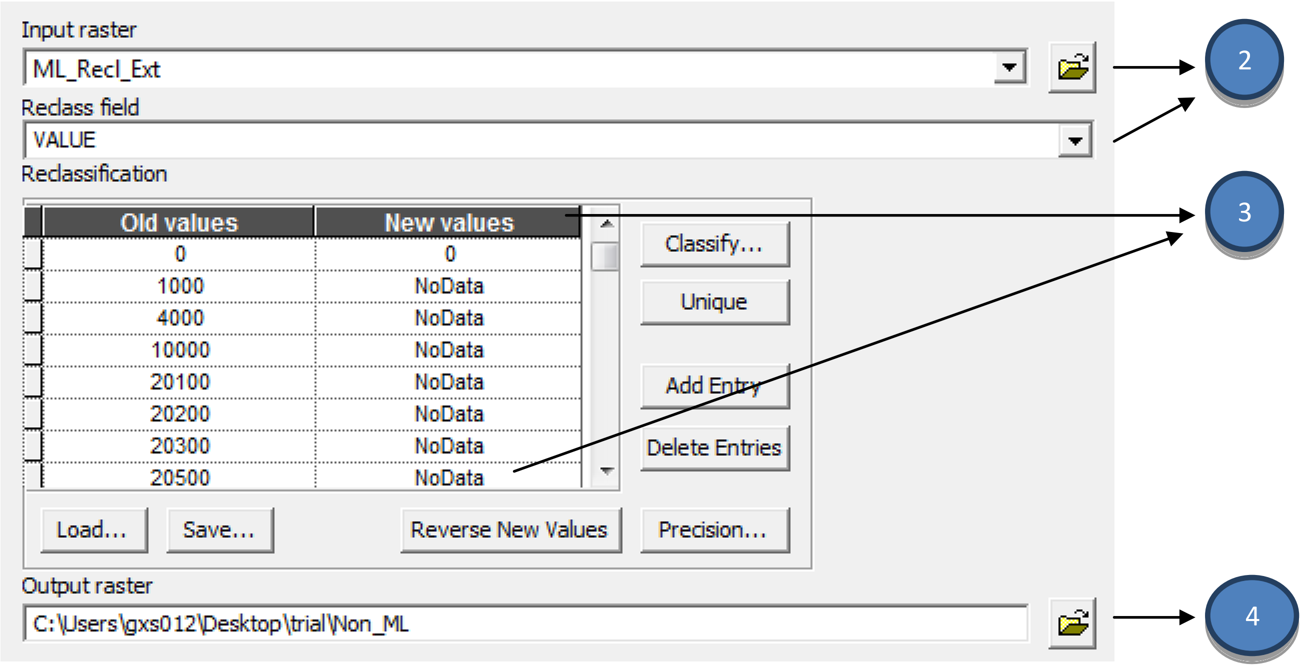
Input raster
ML_Reclass_0
Input raster or feature mask data
LULC
Output raster
C:\Users\gxs012\Desktop\trial\ML_Recl_Ext

RECLASSIFYING DATA

Steps:

1. Click **Reclassify** under **Spatial Analyst Tools**.
2. Browse to the location of ML_Recl_Ext and add as **Input raster** with value as a **Reclass field**.
3. Obtain **New Values** by replacing **Old Values** with Nodata (value 10 to NoData, 40 to NoData, etc.). Do not change the '0' value.
4. Browse to the location of project data and name the **Output raster** as Non_ML.
5. Click **OK**.




Input raster
ML_Recl_Ext

Reclass field
VALUE

Reclassification

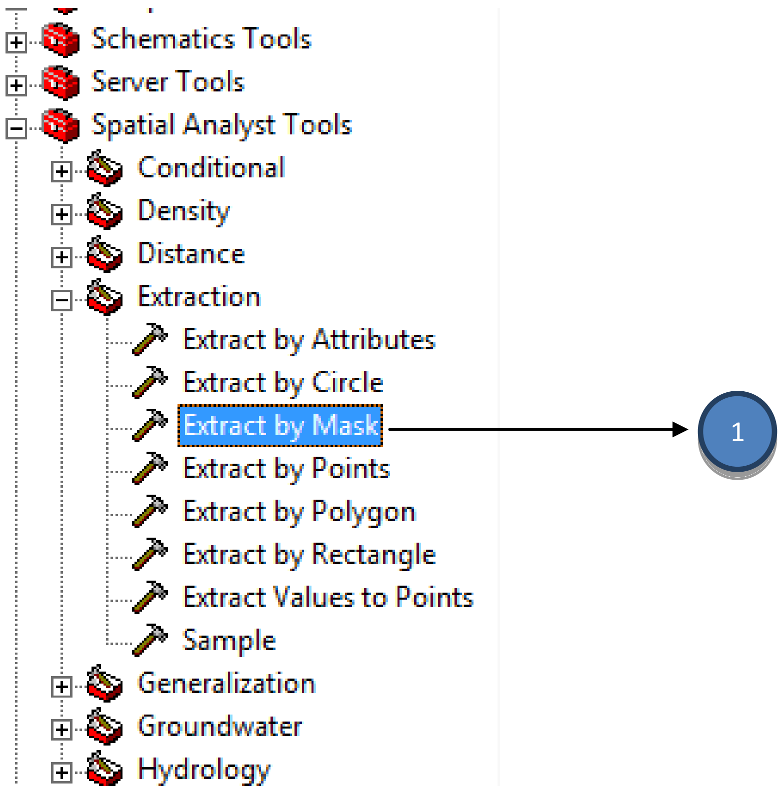
Old values	New values
0	0
1000	NoData
4000	NoData
10000	NoData
20100	NoData
20200	NoData
20300	NoData
20500	NoData

Output raster
C:\Users\gxs012\Desktop\trial\Non_ML

EXTRACTING DATA

Steps:

1. Click **Extract by Mask** under **Spatial Analyst Tools**.
2. Browse to the location of LULC and add as **Input raster**.
3. Browse to the location of Non_ML and add as **Input raster or feature mask data**.
4. Browse to the location of project data and name the **Output raster** as Non_ML_Ext.
5. Click **OK**.




Input raster
LULC

Input raster or feature mask data
Non_ML

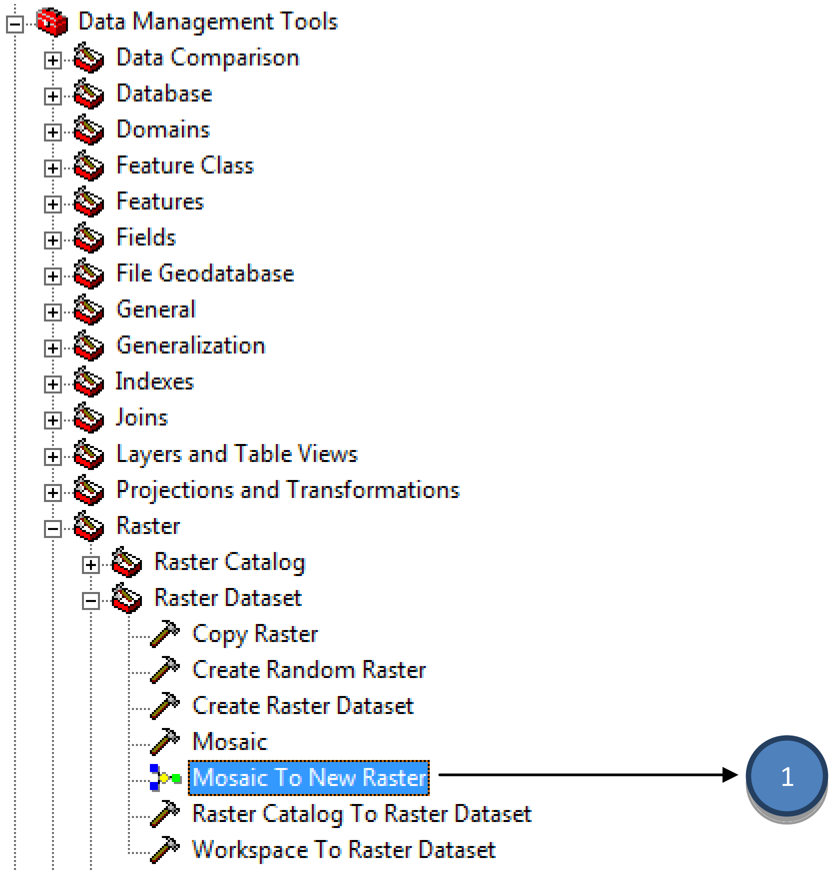
Output raster
C:\Users\gxs012\Desktop\trial\Non_ML_Ext

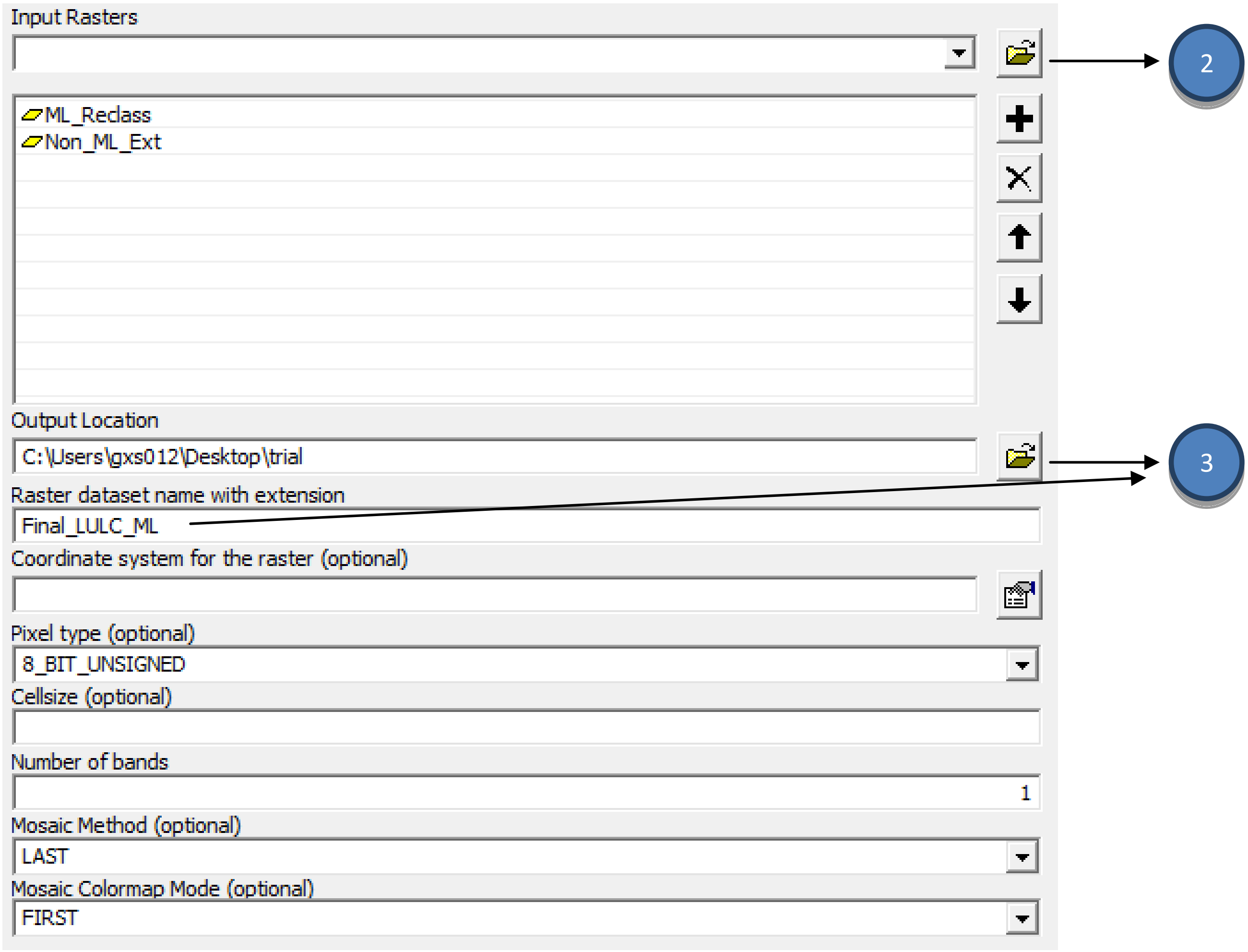
DEVELOPMENT OF FINAL MODIFIED LAND USE AND LAND COVER LAYER

Steps:

1. Click **Mosaic to New Raster** under **Data Management Tools**.
2. Browse to the locations of ML_Reclass and Non_ML_Ext and add as **Input Rasters**.
3. Browse to the location of project data and name the **Raster dataset** as Final_LULC_ML.

4. Click **OK**.


Data Management Tools
Data Comparison
Database
Domains
Feature Class
Features
Fields
File Geodatabase
General
Generalization
Indexes
Joins
Layers and Table Views
Projections and Transformations
Raster
Raster Catalog
Raster Dataset
Copy Raster
Create Random Raster
Create Raster Dataset
Mosaic
Mosaic To New Raster
Raster Catalog To Raster Dataset
Workspace To Raster Dataset
1



Input Rasters

ML_Reclass
Non_ML_Ext

Output Location

C:\Users\gxs012\Desktop\trial

Raster dataset name with extension

Final_LULC_ML

Coordinate system for the raster (optional)

Pixel type (optional)

8_BIT_UNSIGNED

Cellsize (optional)

Number of bands

1

Mosaic Method (optional)

LAST

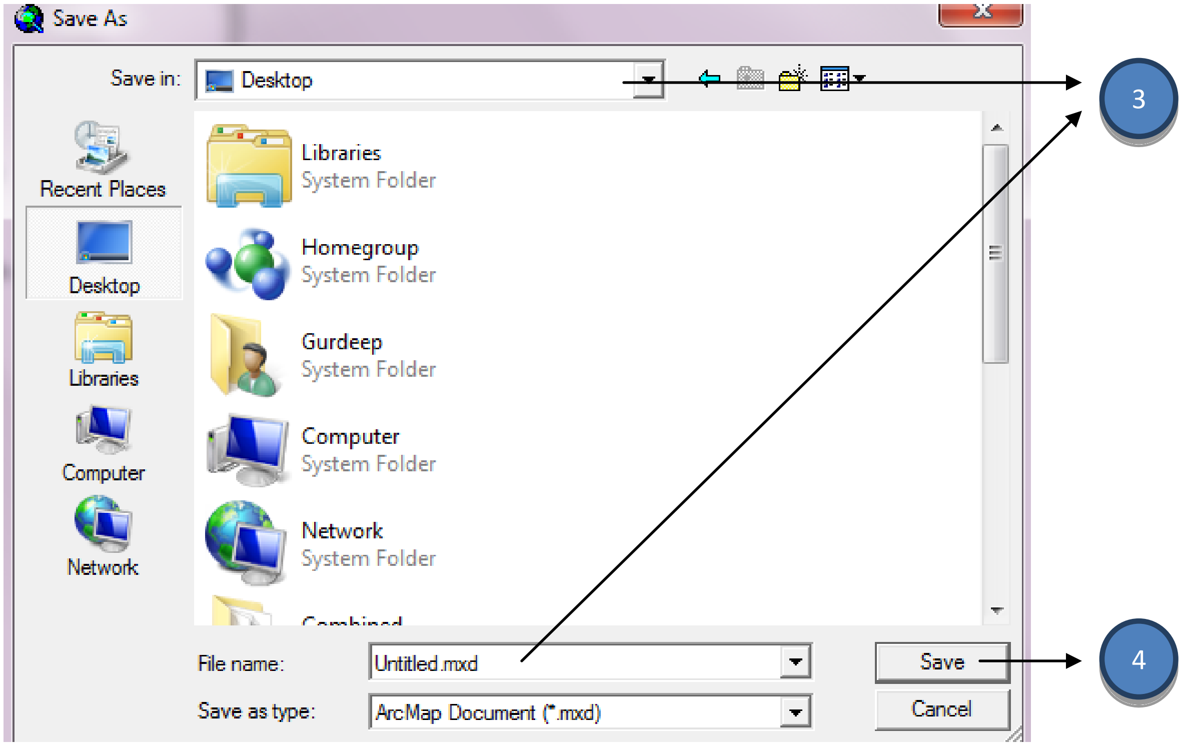
Mosaic Colormap Mode (optional)

FIRST

SAVING THE ARCMAP DOCUMENT

Steps:

1. Click the **File** menu
2. Click **Save As** from the dropdown list.
3. Select the **Save in** location and specify appropriate **File name** for the ArcMap document.
4. Click Save.



Save in: Desktop

File name: Untitled.mxd

Save as type: ArcMap Document (*.mxd)

APPENDIX B: LAND COVER/PLANT GROWTH PARAMETERS FOR SOYBEAN.

Parameter*	**Values**
BIO_E [(kg/ha)/MJ/m2)]	25
HVSTI [(kg/ha)/(kg/ha)]	0.31
BLAI (m2/m2)	3
FRGRW1 (fraction)	0.15
LAIMX1 (fraction)	0.05
CHTMX (m)	0.8
RDMX (m)	1.7
FRGRW2 (fraction)	0.5
LAIMX2 (fraction)	0.95
DLAI (heat units/heat units)	0.6
T_OPT (C)	25
T_BASE (C)	10
CNYLD (kg N/kg seed)	0.065
CPYLD (kg P/ kg seed)	0.0091
BN1 (kg N/kg biomass)	0.0524
BN2 (kg N/kg biomass)	0.0265
BN3 (kg N/kg biomass)	0.0258
BP1 (kg P/kg biomass)	0.0074
BP2 (kg P/kg biomass)	0.0037
BP3 (kg P/kg biomass)	0.0035
WSYF [(kg/ha)/(kg/ha)]	0.01
USLE_C	0.2
GSI (m/s)	0.007
VPDFR (kPa)	4
FRGMAX (fraction)	0.75
WAVP (rate)	8
CO2HI (uL/L)	660
BIOEHI (ratio)	34
RSDCO_PL (fraction)	0.05
ALAI_MIN (m2/m2)	0
BIO_LEAF (fraction)	0
MAT_YRS (years)	0
BMX_TREES (tons/ha)	0
EXT_COEF	0.45
BM_DIEOFF	0.1

*Details about the parameters can be obtained from the SWAT Input/Output documentation available at: http://swatmodel.tamu.edu/media/19754/swat-io-2009.pdf

APPENDIX C: MANAGEMENT OPERATIONS FOR THE LAND USES IN THE L'ANGUILLE RIVER WATERSHED.

RICE

Month	Day	Operation	SWAT Practice	Fertilizer (kg/ha)	Pesticide (kg/ha)	Irrigation (mm)
April	15	Plant/begin growing season	Rice			
April	29	Pesticide	Clomazone		0.6	
May	7	Pesticide	Propanil		3.36	
May	15	Fertilizer	Elemental Phosphorus	44.83		
May	15	Fertilizer	Urea	336.25		
May	30	Pesticide	Lambda-Cyhalothrin		0.016	
June	1	Irrigation				1.511
June	1	Release/Impound	Initiate water impound			
June	10	Irrigation				1.511
June	13	Fertilizer	Urea	112.08		
June	20	Irrigation				1.511
June	30	Irrigation				1.511
July	10	Irrigation				1.511
July	20	Irrigation				1.511
July	30	Irrigation				1.511
August	10	Irrigation				1.511
August	20	Irrigation				1.511
August	30	Irrigation				1.511
September	1	Release/Impound	Initiate water release			
September	11	Harvest and kill operation				

COTTON

Month	Day	Operation	SWAT Practice	Fertilizer (kg/ha)	Pesticide (kg/ha)	Irrigation (mm)
April	8	Tillage	Disk Plow Ge23ft			
April	8	Fertilizer	Elemental Phosphorus	9.775		
April	8	Fertilizer	Elemental Nitrogen	7.85		
April	9	Tillage	Field Cultivator Ge 15ft			
April	10	Pesticide	Trifluralin		1.98	
April	10	Tillage	Hipper 1 Row			
May	19	Tillage	Hipper 1 Row			
May	20	Tillage	Landall, Do-all			
May	20	Plant/begin growing season	Upland Cotton			
June	16	Fertilizer	Elemental Nitrogen	52.69		
July	11	Fertilizer	Elemental Nitrogen	59.41		
July	17	Irrigation				24.13
August	17	Irrigation				20.32
August	20	Irrigation				27.94
August	30	Irrigation				22.86
November	9	Harvest and kill operation				

CORN

Month	**Day**	**Operation**	**SWAT Practice**	**Fertilizer (kg/ha)**	**Pesticide (kg/ha)**	**Irrigation (mm)**
March	1	Tillage	Hipper 1 Row			
April	1	Tillage	Hipper 1 Row			
April	2	Tillage	Bed Roller 4 Row			
April	10	Fertilizer	Elemental Phosphorus	27.37		
April	11	Tillage	Hipper 1 Row			
April	21	Pesticide	Metolachlor		1.61	
April	21	Plant/begin growing season	Corn			
May	5	Pesticide	Atrazine		1.79	
May	5	Fertilizer	Elemental Nitrogen	174.85		
May	25	Irrigation				20.32
June	10	Irrigation				20.32
June	25	Irrigation				20.32
July	10	Irrigation				20.32
July	25	Irrigation				20.32
August	10	Irrigation				20.32
August	17	Harvest and kill				

SOYBEAN AND WHEAT ROTATION

Month	**Day**	**Operation**	**SWAT Practice**	**Fertilizer (kg/ha)**	**Pesticide (kg/ha)**	**Irrigation (mm)**
February	26	Fertilizer	Urea	210.16		
March	20	Fertilizer	Urea	146.2		
June	5	Harvest and kill				
June	6	Tillage	Disk Plow Ge23ft			
June	7	Tillage	Land Planer-leveler			
June	8	Tillage	Field Cultivator Ge15ft			
June	10	Plant/begin growing season	Soybean			
June	25	Pesticide	Glyphosate Amine		0.63	
July	11	Pesticide	Glyphosate Amine		0.63	
July	16	Irrigation				31.49
August	12	Irrigation				35.05
August	22	Irrigation				51.3
September	8	Irrigation				34.36
October	19	Harvest and Kill				
November	7	Tillage	Disk Plow Ge23ft			
November	9	Fertilizer	Elemental Nitrogen	52.68		
November	10	Plant/begin growing season	Winter Wheat			

APPENDIX D: LAND COVER/PLANT GROWTH PARAMETERS FOR SWITCHGRASS AND MISCANTHUS.

Parameter*	Switchgrass	Miscanthus
BIO_E [(kg/ha)/MJ/m2)]	47	39
HVSTI [(kg/ha)/(kg/ha)]	0.9	1
BLAI (m2/m2)	10	11.5
FRGRW1 (fraction)	0.1	0.1
LAIMX1 (fraction)	0.2	0.2
CHTMX (m)	3	4
RDMX (m)	2.2	4
FRGRW2 (fraction)	0.2	0.5
LAIMX2 (fraction)	0.95	0.95
DLAI (heat units/heat units)	0.7	0.85
T_OPT (C)	25	30
T_BASE (C)	12	10
CNYLD (kg N/kg seed)	0.016	0.005
CPYLD (kg P/ kg seed)	0.0022	0.00063
BN1 (kg N/kg biomass)	0.035	0.0304
BN2 (kg N/kg biomass)	0.015	0.0074
BN3 (kg N/kg biomass)	0.0038	0.0057
BP1 (kg P/kg biomass)	0.0014	0.00337
BP2 (kg P/kg biomass)	0.001	0.00104
BP3 (kg P/kg biomass)	0.0007	0.00082
WSYF [(kg/ha)/(kg/ha)]	0.9	1
USLE_C	0.003	0.003
GSI (m/s)	0.005	0.005
VPDFR (kPa)	4	4
FRGMAX (fraction)	0.75	0.75
WAVP (rate)	8.5	7.2
CO2HI (uL/L)	660	660
BIOEHI (ratio)	54	54
RSDCO_PL (fraction)	0.05	0.05
ALAI_MIN (m2/m2)	0	0
BIO_LEAF (fraction)	0	0
MAT_YRS (years)	0	0
BMX_TREES (tons/ha)	0	0
EXT_COEF	0.33	0.65
BM_DIEOFF	0.1	0.1

*Details about the parameters can be obtained from the SWAT Input/Output documentation available at: http://swatmodel.tamu.edu/media/19754/swat-io-2009.pdf