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National Geo-Database for Biofuel Simulations and Regional Analysis of Biorefinery Siting Based on Cellulosic Feedstock Grown on Marginal Lands

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April 2012



Pacific Northwest
NATIONAL LABORATORY

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Executive Summary

The goal of this project undertaken by GLBRC (Great Lakes Bioenergy Research Center) Area 4 (Sustainability) modelers is to develop a national capability to model feedstock supply, ethanol production, and biogeochemical impacts of cellulosic biofuels. The results of this project contribute to sustainability goals of the GLBRC; i.e. to contribute to developing a sustainable bioenergy economy: one that is profitable to farmers and refiners, acceptable to society, and environmentally sound. A sustainable bioenergy economy will also contribute, in a fundamental way, to meeting national objectives on energy security and climate mitigation.

The specific objectives of this study are to: (1) develop a spatially explicit national geodatabase for conducting biofuel simulation studies and (2) locate possible sites for the establishment of cellulosic ethanol biorefineries.

To address the first objective, we developed SENGBEM (Spatially Explicit National Geodatabase for Biofuel and Environmental Modeling), a 60-m resolution geodatabase of the conterminous USA containing data on: (1) climate, (2) soils, (3) topography, (4) hydrography, (5) land cover / land use (LCLU), and (6) ancillary data (e.g., road networks, federal and state lands, national and state parks, etc.). A unique feature of SENGBEM is its 2008-2010 crop rotation data, a crucially important component for simulating productivity and biogeochemical cycles as well as land-use changes associated with biofuel cropping.

ARRA support for this project and to the PNNL Joint Global Change Research Institute enabled us to create an advanced computing infrastructure to execute millions of simulations, conduct post-processing calculations, store input and output data, and visualize results. These computing resources included two components installed at the Research Data Center of the University of Maryland. The first resource was “deltac”: an 8-core Linux server, dedicated to county-level and state-level simulations and PostgreSQL database hosting. The second resource was the DOE-JGCRI “Evergreen” cluster, capable of executing millions of simulations in relatively short periods. ARRA funding also supported a PhD student from UMD who worked on creating the geodatabases and executing some of the simulations in this study.

Using a physically based classification of marginal lands, we simulated production of cellulosic feedstocks from perennial mixtures grown on these lands in the US Midwest. Marginal lands in the western states of the US Midwest appear to have significant potential to supply feedstocks to a cellulosic biofuel industry. Similar results were obtained with simulations of N-fertilized perennial mixtures. A detailed spatial analysis allowed for the identification of possible locations for the establishment of 34 cellulosic ethanol biorefineries with an annual production capacity of 5.6 billion gallons.

In summary, we have reported on the development of a spatially explicit national geodatabase to conduct biofuel simulation studies and provided simulation results on the potential of perennial cropping systems to serve as feedstocks for the production of cellulosic ethanol. To accomplish this, we have employed sophisticated spatial analysis methods in combination with the process-based biogeochemical model EPIC. The results of this study will be submitted to the USDOE Bioenergy Knowledge Discovery Framework as a way to contribute to the development of a sustainable bioenergy industry. This work provided the opportunity to test the hypothesis that marginal lands can serve as sources of cellulosic feedstocks and thus contribute to avoid potential conflicts between bioenergy and food production systems. This work, we believe, opens the

door for further analysis on the characteristics of cellulosic feedstocks as major contributors to the development of a sustainable bioenergy economy.

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Acronyms and Abbreviations

ANPP	Aboveground Net Primary Productivity
CDL	USDA Crop Data Layer
DEM	Digital Elevation Model
EERE	USDOE Energy Efficiency and Renewable Energy
EISA	2007 Energy Independence and Security Act of the United States of America
EPIC	Environmental Policy Integrated Climate model
GIS	Geographic Information System
GLBRC	Great Lakes Bioenergy Research Center
HCU	Hydrologic Catalogue Unit
HDOS	Hierarchical Data Organization System
HSMU	Homogenous Spatial Modeling Unit
LCA	Life Cycle Analysis
LCC	Land Capability Class
LCGHGE	Lifecycle Greenhouse Gas Emission
NASS	USDA National Agricultural Statistical Census
NHD	National Hydrography Dataset
NOAA	National Oceanographic and Atmospheric Administration
NRC	National Research Council of the United States of America
OBP	USDOE EERE Office of Biomass Program
RIMA	Regionally Intensive Modeling Area
RFS	Renewable Fuel Standard, a component of the 2005 Energy Policy Act of the United States of America
SEIMF	Spatially Explicit Integrated Modeling Framework
SENGBEM	Spatially Explicit National Geodatabase for Biofuels and Environmental Modeling
SRTM	Shuttle Radar Topography Mission
SSURGO	USDA Soil Survey Geographic Database
TPI	Topographic Position Index
USDA	United States Department of Agriculture
USDOE	United States Department of Energy

Acronyms and Abbreviations

Mg	Equivalent to 1 metric ton or 1,000 kg
Gg	Equivalent to 1,000 Mg

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1.0 Introduction

1.1 Background and Rationale

Biofuels have been emerging as viable alternatives to fossil fuels. Two major factors have determined their rise in prominence in the United States: energy security and climate change (NRC, 2011). Energy security concerns about high oil prices and a continued dependence of the U.S. on foreign oil, led the U.S. Congress to establish the Renewable Fuel Standard (RFS) as part of the 2005 Energy Policy Act. The RFS established the first renewable fuel volume in the U.S. in the form of a requirement to blend 7.5 billion gallons of renewable fuel with gasoline by 2012. The 2007 Energy Independence and Security Act expanded the RFS mandate by requiring an increase in the fuel blending from 9 billion gallons in 2008 to 36 billion gallons by 2022. Of the 36 billion gallons by 2022, about 58% has to originate from advanced biofuels; i.e. a renewable fuel that has a lifecycle greenhouse gas emission (LCGHGE) that is at least 50% lower than that of the baseline LCGHGE in 2005 (EISA, 2007). Cellulosic ethanol, an advanced biofuel, is expected to cover 44% of the 2022 target.

The second factor relates to climate change and the societal need to reduce anthropogenic greenhouse-gas (GHG) emissions to the atmosphere. Biofuels are promising because they can contribute to replace energy use from fossil fuels and reduce GHG emissions to the atmosphere (Kim and Dale, 2004). Satisfying bioenergy production targets in the U.S. will create a demand for land to grow biomass crops and some have expressed concern about the ultimate impact of these transformations on food prices and the environment (Crutzen et al., 2008; Fargione et al., 2008; Searchinger et al., 2008).

Ensuring the sustainable production of biofuels is a key mission of the Great Lakes Bioenergy Research Center (GLBRC) created in 2007 by the U.S. DOE Office of Science and led by the University of Wisconsin and Michigan State University (Slater et al., 2010). The GLBRC is organized around four major discovery areas: (1) improved plant production, (2) improved processing, (3) improved catalytical processes, and (4) sustainable biofuels production practices. Six major research activities describe the sustainability area: novel production practices, plant-microbial interactions, biogeochemical practices, biodiversity, economic analysis, and integrated modeling (biophysical, biogeochemical, economic, and LCA).

Most of the integrated modeling research at the GLBRC has been conducted at biorefinery scale, a multi-county area where a theoretical cellulosic ethanol biorefinery could draw enough plant biomass to produce 100 million gallons of ethanol per year. These areas are known within the GLBRC research community as RIMAs (Regionally Intensive Modeling Areas). Zhang et al. (2010) reported on SEIMF (Spatially Explicit Modeling Framework), a spatially explicit approach designed to model biomass productivity and environmental impacts of diverse biofuel crops. Egbendewe-Mondzozo et al. (2011) expanded on the work by Zhang et al. (2010) by developing a spatially explicit bioeconomic model of biomass supply from alternative cellulosic crops and crop residues as well as explored policy scenarios for handling various environmental outcomes. Current modeling work focuses on integrating the SEIMF approach with biogeochemical and biodiversity experiments together with LCA modeling. Emerging results from field experiments are utilized to test as well as improve modeling capabilities of current and novel biofuel-production practices.

In fall 2008, the USDOE EERE Office of Biomass Program (OBP) provided support to the GLBRC to enhance field research and modeling activities of sustainable biofuels production practices. Here we report on efforts to develop a national-scale methodology to simulate biofuel crops and on regional modeling results of biomass productivity and potential ethanol production resulting from the collection and processing of this biomass.

1.2 General and Specific Objectives

The objective of this work is to develop predictive land-use change modeling capabilities to address how biomass can be produced on a sustainable basis. The results of experimental field research will be combined with theoretical modeling capabilities to create the ability to examine land-use changes in a broad context with relation to many sustainability criteria such as water use, CO₂ emissions, and related factors.

Specific objectives of this report are to describe: 1) a spatially explicit national geodatabase to conduct biofuel simulation studies and 2) results of a regional analysis of biorefinery siting based on cellulosic feedstock grown on marginal lands.

2.0 Materials and Methods

2.1 Overall Approach

The overall approach used in this project was to extend the integrated modeling research experience gained with the SEIMF approach (Zhang et al., 2010) at RIMA (multi-county) scale and extend it for the modeling of larger (multi-state) regions. As described by Zhang et al. (2010), the SEIMF contains three modules: 1) a GIS-based geodatabase, 2) a terrestrial ecosystem model, and 3) a multi-objective optimization algorithm (Figure 1). The geodatabase is used to process input data, define homogenous spatial modeling units (HSMUs) from moderate to high spatial-resolution data, and extract input data needed to execute the terrestrial ecosystem model EPIC (Williams et al., 1989; Kiniry et al., 1995), the second module of the SEIMF. The last module of SEIMF is a multiobjective optimization algorithm designed for the evaluation of the production and environmental tradeoffs of diverse biofuel production practices.

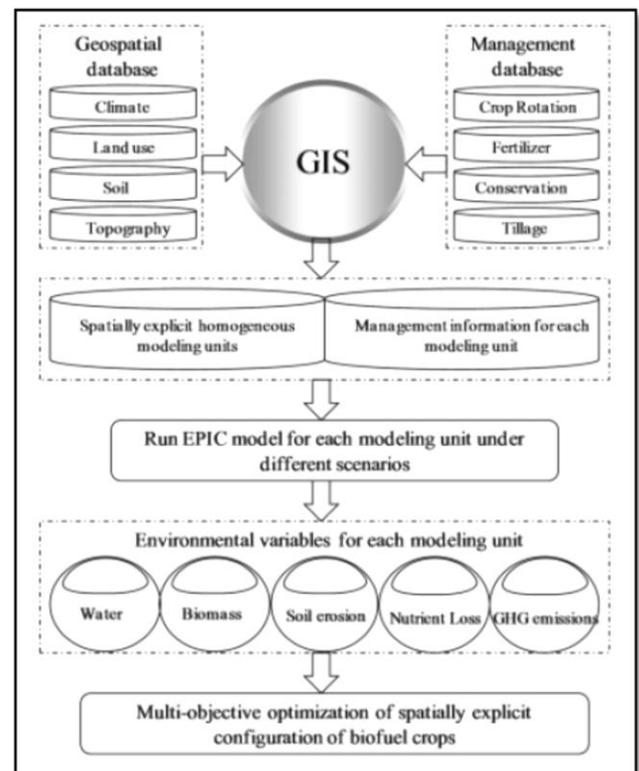


Figure 1. Structure of the Spatially Explicit Modeling Framework (Zhang et al., 2010).

2.2 Preparation of a Spatially Explicit National Geodatabase for Biofuel and Environmental Modeling (SENGBEM)

The main purpose for developing a high-resolution spatial and temporal geodatabase was to be able to model, at field scale, the performance of diverse biofuel crops under various management scenarios. In particular, there was the need to examine the potential of marginal lands for the placement of perennial biofuel crops. The procedure described by Zhang et al. (2010) demonstrated the possibility of identifying and modeling the productivity and environmental impacts of biofuel crops grown on marginal lands.

The SENGBEM geodatabase contains five main types of data: 1) climate, 2) soils, 3) topography, 4) hydrography, and 5) land cover / land use (LCLU). In addition, SENGBEM contains other types of ancillary data such as road networks, federal and state lands, national and state parks, etc. Following is a description of the data and datasets used in constructing SENGBEM.

Climate Data. The climate database contains historical daily values of weather variables needed to drive EPIC and other biophysical models. The weather variables are air temperature (maximum and minimum, °C), precipitation (mm), solar radiation (MJ m^{-2}), wind speed (m s^{-1}), and relative humidity (as a fraction). Climate data can be extracted from multiple sources, including Daily Surface Weather and Climatological Summary (DayMet) (<http://www.daymet.org/>), the North American Regional Reanalysis (NARR) (<http://www.esrl.noaa.gov/psd/data/gridded/data.narr.html>), and the North American Land Data Assimilation System (NLDAS) (<http://www.emc.ncep.noaa.gov/mmb/nldas/>). The datasets differ in terms of spatial resolution and length of period of record.

The DayMet dataset provides the highest spatial resolution (1 km) and accounts for the influence of orography on weather. DayMet was developed at the University of Montana, Numerical Terradynamic Simulation Group (NTSG) to provide the biophysical modeling community the daily meteorological and climatological data necessary to run simulation models. The NARR and NLDAS datasets are both from NOAA and the main difference between them is the spatial resolution: 32 km for NARR and 12 km for NLDAS. The main advantage of the NOAA datasets over DayMet is that they are available from 1979 to the present, with approximately a 6-month lag. While DayMet data are also available from about the same start period (1980), the delay for more recent data is much longer.

Topography and Hydrography Data. Topographic data are essential to delineate watersheds and determine slope characteristics (elevation, gradient, length, and aspect) needed for hydrological and erosion modeling. Topographic data were derived from the Shuttle Radar Topography Mission (SRTM), which produced the highest resolution digital elevation model (DEM) of the Earth at a resolution of 30 m (Farr et al., 2007). In addition, the National Hydrography Dataset (NHD-plus) (Simley and Carswell, 2009) was used to extract hydrologic catalogue unit (HCU) boundary information for modeling soil sediment yield, surface runoff, subsurface flow, and nutrient transport with runoff.

Soils. There are two major soil databases available in the U.S. for environmental modeling: State Soil Geographic (STATSGO) and Soil Survey Geographic (SSURGO) both developed by USDA-NRCS. The STATSGO database was designed mainly for regional, multistate, river basin, state and

multicounty resource planning, management, and monitoring. Instead, the SSURGO database was designed primarily for farm and ranch, landowner/user, township, county, or parish natural resource planning and management. The main difference between the two is the level of detail contained in the map units; STATSGO map units can have up to 21 different component soils while SSURGO map units usually contain one component and can contain up to a maximum of three components. The SSURGO database, now available for almost the entire conterminous U.S., was selected for building SENGBEM. Data from SSURGO (<http://datagateway.nrcs.usda.gov>) were extracted to map soils at scales of ~1:24,000 (~30 m). Data retrieval also included a suite of physical and chemical soil properties needed for biophysical and biogeochemical modeling: albedo, layer depth (m), bulk density (Mg m^{-3}); mineral fractions (sand, silt, clay, coarse fragments), organic C (%), total N (mg kg^{-1}); and pH. The SSURGO database provides an interpretive classification variable [i.e. land capability (LC)] that is represented by land classes based on use limitation (e.g., soil depth, erosion risk, slope, etc.) (Klingebiel and Montgomery, 1961). There are eight LC classes: I–VIII. Class I is (prime) land without any limitations for use. Class VIII is land that cannot be used for anything but wildlife. Classes I–IV can support cropland agriculture, whereas classes V–VIII contain non-arable land. LC can be used for two purposes: (1) identifying marginal land (e.g. low yield cropland) for biofuel production and (2) qualitatively validating the results of biophysical and biogeochemical modeling. Land capability classes are subdivided into land capability subclasses according to the kind of limitation (susceptibility to erosion, excess water, shallowness of the rooting zone, climate hazard). All map unit components, including miscellaneous areas, are assigned a capability class and subclass.

Land Cover and Land Use. Crop rotation information (e.g. corn-soybean, continuous corn) is important for driving cropland ecosystem simulations via a spatially explicit terrestrial ecosystem model. Land cover / land use data to build SENGBEM were derived from the USDA Cropland Data Layer (CDL) remote sensing product available at national scale at a resolution of 56m x 56m since 2008 (<http://datagateway.nrcs.usda.gov>) for the coterminous U.S. The CDL land cover was developed by the USDA to utilize seasonal satellite imagery to monitor how the acreage of major crop types varies from one year to the next. To generate a high-resolution crop rotation map of the U.S, multiple years (2008, 2009, and 2010) of CDL images were overlaid to derive historical crop rotations. A novel time series analysis based algorithm was implemented to aggregate all observed rotations into representative rotations. In all, nearly 170 unique crop rotations representing the entire U.S were generated. The product is highly accurate with >95% accuracy for corn and soybean growing regions in U.S. when compared to census data from NASS (USDA National Agricultural Statistical Services).

Crop rotations were then combined with data on soils, elevation, and hydrography to provide historical input data for the biophysical and biogeochemical modeling. For future biofuel-scenario analyses, current CDL land use classes are summarized into several major categories, including field crops (FC), herbaceous vegetation (HV), and woody vegetation (WV), to reduce the number of modeling units and the computational burden of SEIMF implementation.

2.3 Preparing and Implementing Spatially Explicit Simulations with the EPIC Model

2.3.1 The EPIC Model

The EPIC model can simulate the growth and development of over 100 plant species including all major crops, grasses, legumes, and some trees (Williams, 1995). Crops can be grown as sole crops or as intercrops (up to 10 species), in complex rotations, and under a wide range of management operations including tillage, irrigation, fertilization, and liming. EPIC uses the concept of radiation-use efficiency (Monteith, 1977) by which a fraction of daily photosynthetically active radiation is intercepted by the plant canopy and converted into plant biomass. Daily gains in plant biomass are affected by vapor pressure deficits and atmospheric CO₂ concentration (Stockle et al., 1992 a,b). Plant phenology is controlled via heat-unit calculations where each crop / plant species has base and optimal air temperatures for growth. Potential daily gains in biomass are affected by environmental stresses such as water, temperature, nutrients (primarily N and P), and aeration. All stresses are calculated every day during the simulation, but only the value of the most severe stress is used to reduce potential plant growth and crop yield. Stress factors for soil strength, temperature, and aluminum toxicity are also calculated daily and used to adjust potential root growth (Jones et al., 1991). EPIC is driven by daily weather consisting of solar radiation, air temperature, precipitation, wind speed, and relative humidity, which is either predicted from weather parameters or read from input files. Simulated processes are modified by topographical (e.g. slope gradient and length) characteristics and field / watershed dimensions, soil layer properties (e.g., layer depth, bulk density, C and N contents, pH), and management information (e.g. cropping systems, planting, fertilization, irrigation, harvesting), as inputs to EPIC (Gassman et al., 2005; Williams et al., 1995; Zhang et al., 2010).

For this work, the parameterization of the EPIC model was revised to ensure adequate representation of biofuel cropping systems (Izaurre et al., 2012). Specific crop parameters / variables that underwent evaluation and eventual change included radiation use efficiency, root-to-shoot ratio (Zhang et al., 2011), and planting density. Further, the rate of transformation of standing live to standing dead vegetation was reduced from 1% to 0.1% per day to better model the reduced loss of yield in fall-harvested cellulosic crops.

2.3.2 Spatially Explicit Modeling Framework

The high spatial resolution of operational modeling units (from tens to hundreds of meters, with finer resolutions preferred) provides more homogeneous land units and improves model accuracy. However, agricultural statistics (e.g. crop yields, nutrient applications, tillage types) are only available at regional scale (county or state level). Therefore, a hierarchical data organization system (HDOS) (Figure 2) was designed to facilitate fusing geospatial data from multiple sources at different spatial resolutions, including climate input, land use, soil, and topography, to derive homogeneous spatial modeling units (HSMU) at fine scale, while simultaneously allowing georeferencing of crop management information from different sources to specific HSMUs (Figure 3). The HDOS is designed to be flexible to use data at different levels of detail. Using the conterminous U.S. as an example, the HDOS is illustrated in Figure 2. Given this HDOS, the modeling results can be flexibly aggregated into several levels: county, state, and conterminous

U.S. modeling units. The finest resolution is ~ 60 m, which is determined by the maximum resolution of the CDL and SSURGO data. The HSMU is determined by the unique combination of state, county, LCLU, soil, and hydrologic catalogue unit (Figure 3). Each HSMU has a unique ID and the associated attribute variables that allow preparing climate, land surface, and management parameters for input to the EPIC model.

For each HSMU, EPIC simulates all of the land management scenarios. From the output of these scenarios, a set of variables (Table 2) represents the productivity and environmental impacts of all possible biofuel crop production systems. These results are stored in 3 alternative formats to facilitate multi-platform data access:

Microsoft Excel worksheets, Access databases, and PostgreSQL databases. Internet based data transfer is also available by using PostgreSQL. These modeling results are linked to the HSMU map by using the unique ID field (Figure 3), which allows users to visualize the spatial distribution of the output variables.

2.3.3 Site Validation

Site-scale simulations based on specific data were conducted to calibrate the EPIC model before applying it to the regional-scale simulations. Data from two Long-term Ecological Research (LTER) sites at the Kellogg Biological Station (KBS) in Michigan and at Cedar Creek (CDR) in Minnesota were used to parameterize EPIC and model aboveground net primary productivity (ANPP) of successional vegetation growing on former agricultural fields. Data included in the parameterization and initialization included historical weather, terrain characteristics, and soil properties. The treatment selected for the simulation was natural herbaceous vegetation or early successional (ES). The treatment was initiated in 1989 when agricultural management ceased and natural vegetation was allowed to re-establish. Spring burning was implemented in 1997 and whenever necessary thereafter to inhibit colonization of woody species. Dominant species of successional vegetation included *Solidago canadensis*, *Elytrigia repens*, *Poa pratensis*, *Aster pilosus*, *Phleum pratense*, *Trifolium pratense*, *Apocynum cannabinum*, *Daucus carota*, *Hieracium* spp., and *Rhus typhina* (<http://lter.kbs.msu.edu/>).

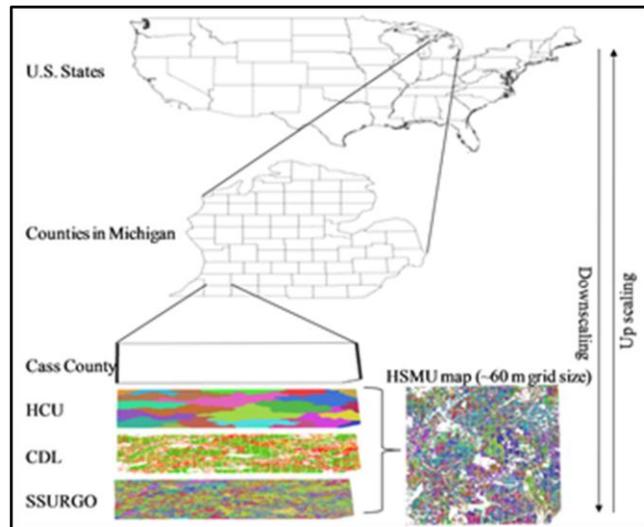


Figure 2. Illustration of the hierarchical and flexible downscaling and upscaling schemes in United States lands (Zhang et al., 2010).

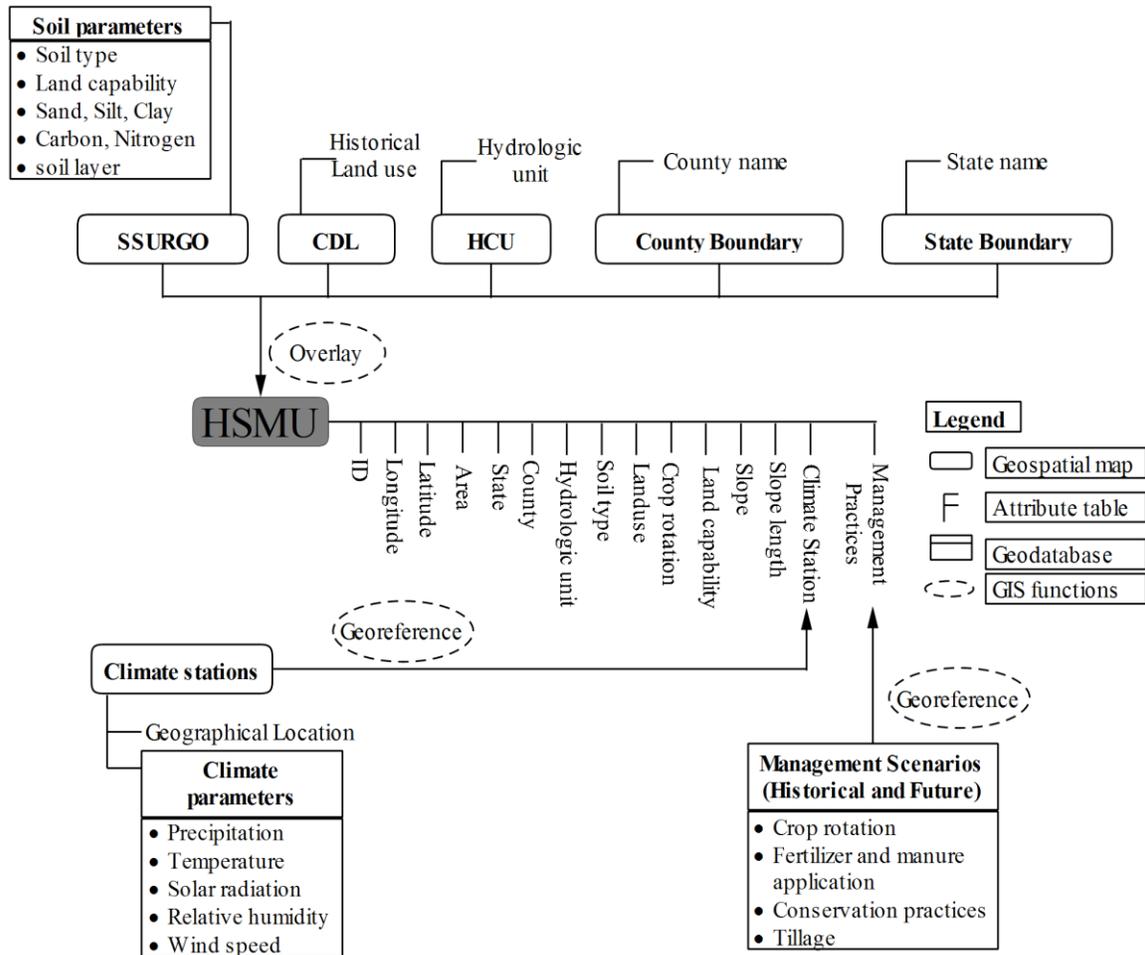


Figure 3. Schematic diagram describing the procedures for defining HSMUs (Homogenous Spatial Modeling Units).

The EPIC calibration with KBS LTER results was achieved by simulating the composition of the ES plant community with three species from the EPIC crop database (*Poa pratensis*, *Phleum pratense*, and *Trifolium pratense*). Spring burning with 80% efficiency was simulated in 1997, 2003, 2004, 2006, and 2008. Aboveground NPP was simulated under three different scenarios; one was left completely unmanaged (no harvest and no N addition), and the other two were simulated with fall harvest with N at 0 and 123 kg ha⁻¹ yr⁻¹. EPIC model runs were based on historical records of daily maximum and minimum air temperature and precipitation from the KBS LTER dataset (<http://lter.kbs.msu.edu/datatables>). Daily solar radiation, relative humidity, wind speed, and missing temperature and precipitation were acquired from Gull Lake NWS weather station (42° 24' N 85° 23' W) also at KBS. Soil layer properties used in the simulations were those of the Kalamazoo soil series (fine-loamy, mixed, mesic Typic Hapludalf).

The EPIC simulations of ANPP for Cedar Creek, MN were conducted with data from the CDR LTER site. A 60-yr chronosequence experiment was simulated according to Zak et al. (1990). The chronosequence consisted of a series of 14 agricultural fields on Alfic and Typic Udipsamments (Soil Survey Staff, accessed March 2012) left unmanaged during periods ranging from one to 60 years. Floristic surveys conducted in 1987 revealed the presence of *Ambrosia artemisiifolia*, *Andropogon gerardii*, *Agropyron repens*, *Agrostris scabra*, *Polygonum*

convolvulus, *Poa pratensis*, and *Schizachyrium scoparium*, among others. C3 species appeared to dominate over C4 species during the first half of the chronosequence period while an equal mix appeared to prevail during the second. The chronosequence was simulated with an equal mix of generic C3 and C4 species from the EPIC crop database and driven by simulated daily weather generated from data of weather station at Rosemount, MN near CDR LTER station. Weather parameters were used to simulate ANPP during a 60-yr period intended to approximate environmental conditions for 1928 – 1987. The only simulated external N addition was 7.7 kg ha⁻¹ yr⁻¹ via wet deposition.

2.4 Regional Simulations

2.4.1 Simulation of Biomass Feedstock across the 10-State US Midwest

The EPIC-based Spatially Explicit integrative modeling framework (SEIMF) (Zhang et al., 2010) was used to simulate yields of perennial herbaceous species grown on marginal lands across the 10-state North Central USA study region. This region extends from North Dakota in the NW corner, south to Nebraska in the SW corner, east to Ohio in the SE corner, and up to Michigan in the NE corner. The Canadian – U.S. border defines the northern border of the study region. A geospatial database containing soil, terrain, weather, land use/land cover and management data was used to obtain relevant parameters for running the EPIC model.

Pertinent details of the geospatial database as described in Section 2.2 of this report follow:

- a) Daily weather files at 32-km resolution to run EPIC were derived from the North America Regional Reanalysis (NARR) (<http://www.esrl.noaa.gov/psd/data/gridded/data.narr.html>);
- b) Elevation data (elevation, slope gradient and length) were extracted from the SRTM DEM product while geospatial analysis was used to derive slope length and gradient of each HSMU.
- c) Land use and land cover. Cropland data layer (CDL) for 2008 and SSURGO map were combined to define LCLU and soil type at a spatial resolution of 60 m for the simulation domain. Federal lands, golf courses, parks, large-lot single-family housing units, and vegetation planted in developed settings for erosion control, recreation, or aesthetic purposes were excluded from the simulation domain.
- d) Soils and marginal lands. Soil layer properties to run EPIC originated from the SSURGO database. Marginal lands were identified as rural lands falling into Land Capability Classes V-VII with slope gradients <20% under non-forested vegetation.

Special consideration was given to the Sandhills of Nebraska (located in North Central Nebraska) whose unique grass-stabilized sand dune topography distinguishes them from the surrounding prairies (Eggemeyer et al., 2006). These dunes can be up to one hundred meters tall and several kilometers long. The inter-dune valleys are the largest sources of hay for the cattle industry in Nebraska (Gosselin et al., 2006). To keep only the inter-dune valleys and exclude the fragile dune ridges and slopes from the analysis, we used the Topographic Position Index (TPI) algorithm in ArcGIS (Tagil and Jenness, 2008).

2.4.2 Methodology for Siting Biorefineries

For each grid of marginal land, we simulated ANPP by the calibrated EPIC model under three levels of N fertilization: 0, 68, and 123 kg N ha⁻¹ yr⁻¹. The ANPP values obtained from EPIC were used to identify the location of potential biorefineries that could process the cellulosic feedstock. Only results belonging to an N fertilization rate of 68 kg N ha⁻¹ yr⁻¹ are used in this analysis. The siting of a potential biorefinery was limited to areas where potential feedstock derived from fields fertilized with 68 kg N ha⁻¹ yr⁻¹ could add at least 768 Gg yr⁻¹ of cellulosic biomass on marginal lands from within an economically feasible transportation distance of 80 km. To accomplish this, a moving window algorithm was implemented over the study region. Subsequently, non-overlapping circles with the highest biomass yields were selected for potential biorefinery locations. We used the following equation to convert biomass yields into liters of ethanol:

$$\text{Yield} \times 0.06 \text{ km} \times 0.06 \text{ km} \times 380.0 \text{ L Mg}^{-1} \times 100 = \text{Yield} \times 136.8 \quad (\text{Eqn 1})$$

Where, Yield (Mg ha⁻¹) is biomass production, 0.06 × 0.06 km is the cell size of the model, 380.0 L Mg⁻¹ is the conversion factor for converting cellulosic biomass to ethanol, and 100 is number of hectares in 1 km².

3.0 Results and Discussion

The results reported here address the two specific objectives described in Section 1.2: 1) a spatially explicit national geodatabase to conduct biofuel simulation studies and 2) a regional analysis of biorefinery siting based on cellulosic feedstock grown on marginal lands. They are also part of a submitted manuscript examining the sustainability of bioenergy production from marginal lands in the US Midwest (Gelfand et al., submitted)

3.1 Features of the National Geodatabase to Simulate Biofuel Production

The National Geodatabase of Contemporary Land Cover and Use in the Conterminous USA is shown in Figure 4. The map is presented in highly aggregated form representing only some predominant crop rotations (e.g. corn-based rotation, winter wheat – fallow) and land covers (e.g. forests, grasslands, urban). This level of aggregation and abstraction is necessary in order to visualize some of the predominant land uses and land covers. However, the map / database retains all the richness

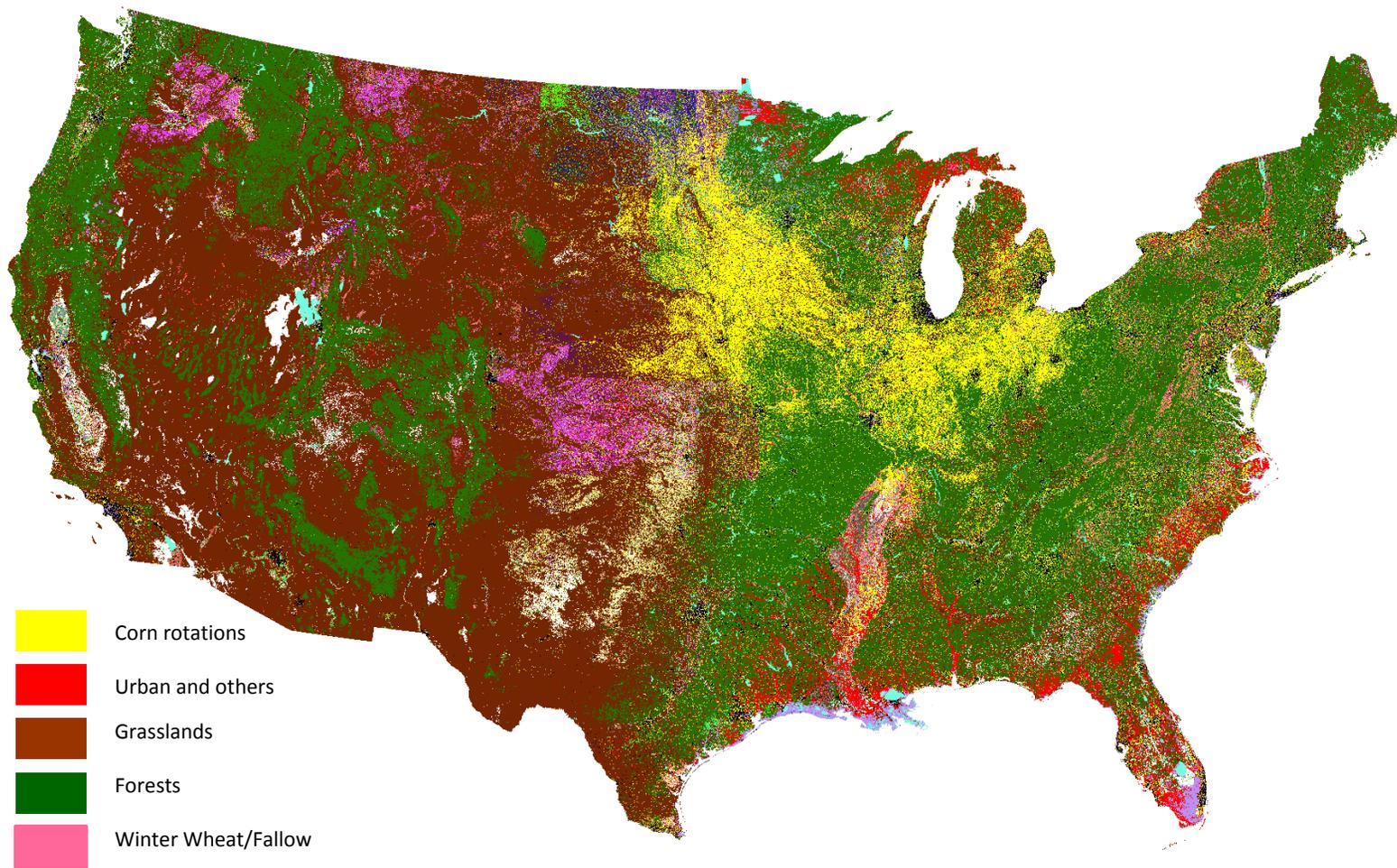


Figure 4. National Geodatabase of Land Cover and Use in the Conterminous USA.

of the high resolution data from which the map was built. In other words, it would be possible to zoom in to a particular 60 m x 60 m field and see the details of its topography, soil properties, and LCLU. Conversely, simulations conducted at the HSMU scale can be scaled-up to watershed, county, state, and even national level without losing any information.

The level of detail included in this database would allow a user to exclude a number of features not needed in the aggregation such as federal and provincial parks, protected areas, recreational areas, urban, suburban, and commercial areas.

The crop rotation (land use) component is a unique feature of the database. Information on the contemporary distribution of field crops on a given field and their change in sequence over time (i.e. crop rotation) is crucial for the understanding of land issues such as soil quality, carbon management, soil emissions of greenhouse gases, etc. As such, we believe the database presented here represents a major advance for increasing the accuracy of environmental modeling and, in particular, for biofuel modeling.

3.2 Simulations Results

3.2.1 Site Simulations

Aboveground NPP simulated EPIC calibration during 2000 and 2008 averaged $60.0 \pm 11.0 \text{ kg ha}^{-1} \text{ yr}^{-1}$ for the scenario without biomass harvest and fertilization, which is similar to the observed average of $59.8 \pm 4.4 \text{ kg ha}^{-1}$ (Table S6). Similarly, simulated ANPP for the scenario with harvest and fertilization was very close to field-based estimation, 96 ± 8 vs. $87.8 \pm 6.4 \text{ kg ha}^{-1} \text{ yr}^{-1}$.

Direct comparisons of biomass productivity results are not possible for the CDR data because the simulations are not time specific. Simulated standing aboveground biomass during the July-August period averaged $51.3 \pm 11.3 \text{ kg ha}^{-1}$ during the first three years. In comparison, Zak et al. (1990), observed 50.9 kg ha^{-1} in the 1-yr old field and 29.6 kg ha^{-1} in the 3-yr old field. Simulated biomass during the last three years of the simulation averaged $76.7 \pm 12.7 \text{ kg ha}^{-1}$, while Zak et al. (1990) observed 78.3 kg ha^{-1} in the 60-yr old field. While EPIC failed to capture the decrease in plant productivity observed during the first years of the chronosequence, it did capture the increase in productivity toward the end of the simulation period. Similar to observations, simulated annual biomass productivity correlated moderately well with N mineralization and soil N. However, correlations obtained with observed data ($R^2 = 0.78$ for potential N mineralization; $R^2 = 0.94$ for soil N) (Zak et al., 1990) were considerably stronger than those obtained with simulated data ($R^2 = 0.34$ for net N mineralization; $R^2 = 0.32$ for soil N).

Overall, EPIC appeared to capture adequately the observed plant productivity patterns from both KBS and CDR LTER sites under different environmental constraints and management scenarios. In addition, Izaurrealde et al. (2006) used EPIC for simulations of the effects of unmanaged grasses on soil carbon accrual on marginal lands in Nebraska, Kansas, and Texas and found good agreement between EPIC predictions and long-term field data, which provides further justification for using the model for large-scale simulations.

3.2.2 Potential Biomass Production from Marginal Lands

The available acreage of marginal lands varied considerably by state (Figure 5). Overall, available acreage of marginal lands varied between <100,000 ha in Ohio (1% of total land) to more than 6.4 million ha in Nebraska (30% of total land). Nebraska was also the only state where marginal land acreage exceeded that of arable lands.

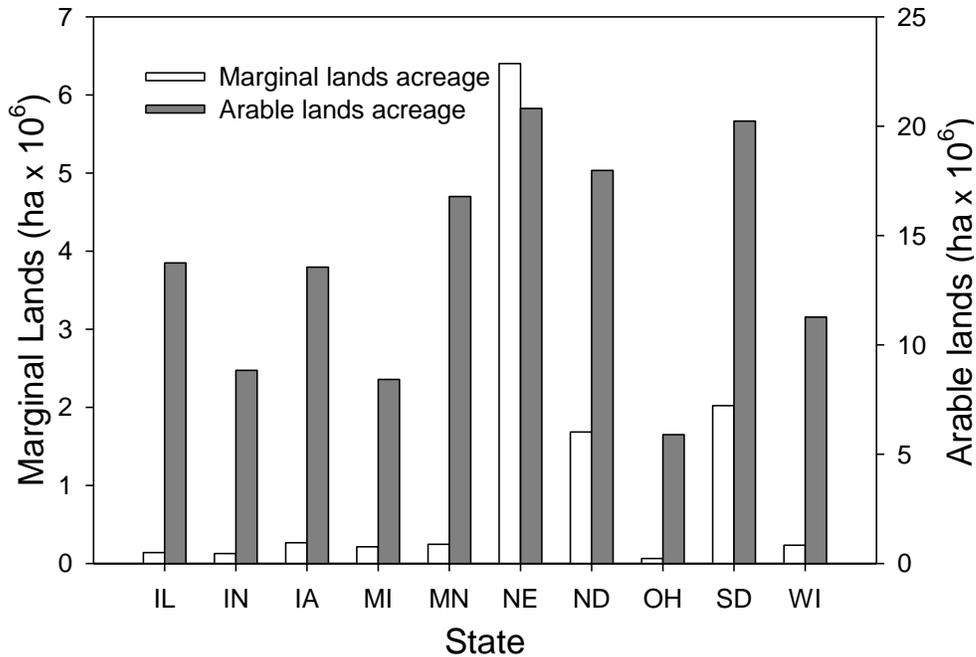


Figure 5. Marginal lands acreage ($\times 10^6$ ha) in 10-state US North Central region

We simulated ANPP by the calibrated EPIC model under three levels of N fertilization: 0, 68, and 123 kg N ha⁻¹ yr⁻¹, and two levels of harvest efficiency: 55% and 90%. Modeled field size for the estimation of potential productivity varied substantially, with a minimum size of 3,600 m² and a maximum >650 $\times 10^6$ m². Overall, we simulated 78,184 fields having unique combinations of soil type, land-use, and LCC. The connectivity between each field and nearby fields was not assessed. Average biomass yields (Mg ha⁻¹ yr⁻¹) for 78,184 parcels of marginal land as modeled by EPIC for three levels of N fertilizer application and two harvest efficiencies are presented in Table 1. Values in parentheses are standard deviations. Ethanol yields are based on a conversion factor of 380.0 L Mg⁻¹ of cellulosic biomass.

Table 1. Average biomass yields (Mg ha⁻¹ yr⁻¹) for 78,184 parcels of marginal land as modeled by EPIC for three levels of N fertilizer application and two harvest efficiencies.

<i>EPIC model</i>		Average Yields	
		Biomass <i>Mg ha⁻¹ yr⁻¹</i>	Ethanol <i>L×10³ ha⁻¹ yr⁻¹</i>
Harvest efficiency (%)	55	4.3 (1.7)	1.6 (0.6)
	90	6.0 (2.6)	2.3 (1.0)
N Fertilization (<i>kg ha⁻¹ yr⁻¹</i>) [†]	0	6.0 (2.6)	2.3 (1.0)
	68	8.2 (2.7)	3.1 (1.0)
	123	8.9 (2.8)	3.3 (1.0)

[†] Simulations under different N fertilization regimes with assumed 90% harvest efficiency.

3.2.3 Comparison with Estimates from Billion Ton Study Update

We also compared our results of biomass production rates with recent Billion-Ton Study Update (Perlack et al. (2011) (Table 2). Our estimation differs significantly and exhibited no relation to the Billion-Ton Study Update ($R^2 = 0.004$). The Spearman rank-order correlation coefficient (r_s) is -0.0061 with a p-value of 0.98. An r_s value below zero implies negative agreement between the two rankings.

Table 2. EPIC simulated and Billion-Ton Study Update estimated biomass yields on marginal lands across the 10-state US Midwest Region.

	Average biomass yield	
	EPIC*	BTS-U
	----- Mg ha ⁻¹ -----	
Illinois	8.16	12.52
Indiana	8.35	13.07
Iowa	7.81	11.73
Michigan	9.98	7.44
Minnesota	10.63	6.04
Nebraska	6.01	8.87
North Dakota	5.55	4.59
Ohio	7.16	14.03
South Dakota	4.75	7.59
Wisconsin	8.96	10.29

* EPIC simulated for unfertilized marginal land.

The difference between our EPIC simulated yields and the results from the Billion-Ton study update can be attributed to three different factors: First, by simulating the production of

mixed species assemblages of existing vegetation, we are able to avoid carbon debt associated with the establishment of new perennial plantings on land not now farmed. Further, we simulate production only on marginal lands rather than to a combination of all marginal and up to 25% of current cropland. Third, rather than using a statistical model based on field data scaled by growing season precipitation and temperature, we employ a process-level crop model operating at a fine grained (0.4 ha) scale to fully capture the soil and climate interactions.

3.2.4 Identifying Location of Biorefineries in the 10-State US Midwest Region

We implemented a moving window algorithm to assess availability of cellulosic biofuel from marginal lands in the 10-State US Midwest region. The placement of biorefineries for cellulosic biomass production from marginal lands in ten North Central states is shown in Figure 6. Each circle represents an 80 km radius area with sufficient biomass resources to produce at least 89.3 ML ethanol yr⁻¹ based on quantitative simulation of yields from non-forested marginal lands at a 60×60 m resolution. Corn acreages (in ha) by county have been derived from the CDL of 2008. The inset map shows a close up of a potential biorefinery location where the yield is not clearly visible on the main map. Figure 5 shows the placement of biorefineries for cellulosic biomass production from marginal lands in ten North Central states with identification numbers corresponding to Figure 6. Overall, nearly 21 GL of cellulosic ethanol can be produced (Table 3), meeting ~30% of the 2022 target for cellulosic biofuel mandated by the 2007 US Energy Independence and Security Act.

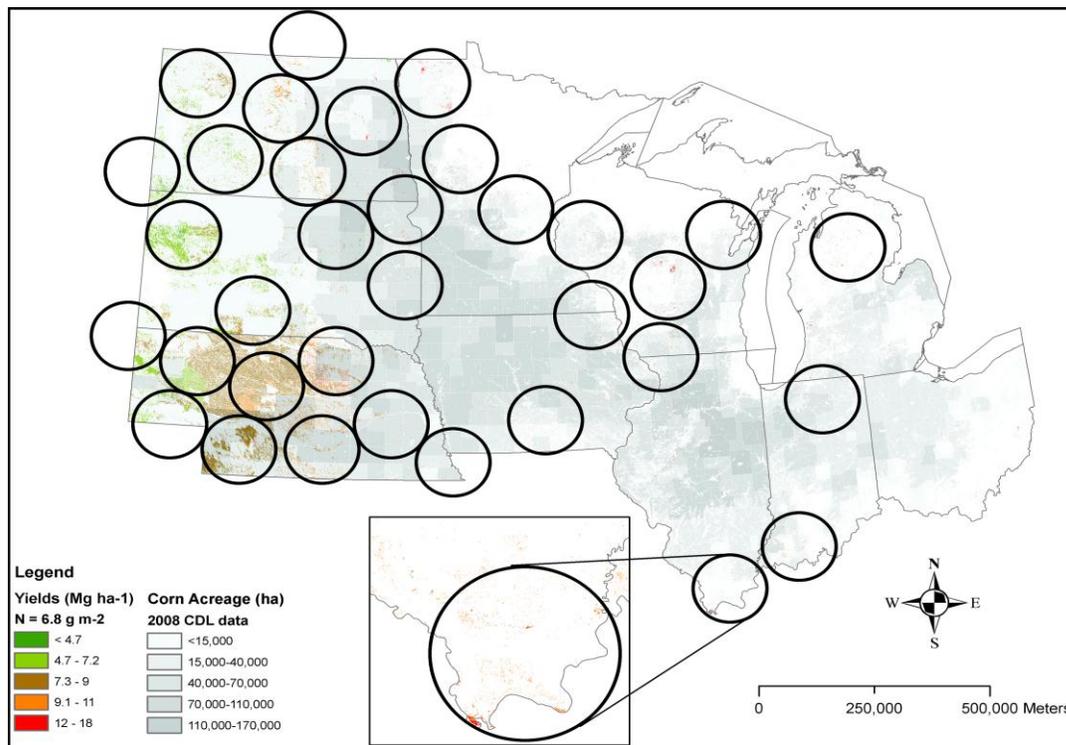


Figure 5. Potential cellulosic ethanol biorefinery locations in the 10-state US Midwest Region.

Table 3. EPIC modeled biomass and cellulosic ethanol production by state assuming 90% harvest efficiency and two N-fertilization levels (0 and 68 kg ha⁻¹).

ID [§]	State [†]	Total biomass production		Total cellulosic ethanol production	
		F*=0	F=68	F=0	F=68
		----- Mg × 10 ⁶ -----		----- GL yr ⁻¹ -----	
1	Illinois‡	1.35	1.88	0.18	0.26
2	Illinois 1	0.67	0.8	0.09	0.11
3	Indiana‡	1.18	1.43	0.16	0.19
4	Indiana 1‡	0.77	0.96	0.11	0.13
5	Iowa	1.67	2.27	0.23	0.31
6	Iowa 1‡	0.87	1.17	0.12	0.16
7	Michigan	1.78	2.29	0.24	0.31
8	Minnesota	2.38	2.55	0.32	0.35
9	Minnesota 1	0.86	1.10	0.12	0.15
10	Minnesota 2	0.90	1.11	0.12	0.15
11	Nebraska	13.72	19.13	1.88	2.62
12	Nebraska 1‡	10.44	14.66	1.43	2.01
13	Nebraska 2‡	9.75	13.83	1.33	1.89
14	Nebraska 3	8.89	11.54	1.22	1.58
15	Nebraska 4	6.43	9.01	0.88	1.23
16	Nebraska 5‡	4.05	5.33	0.55	0.73
17	Nebraska 6	2.55	3.40	0.35	0.46
18	Nebraska 7‡	1.68	2.30	0.23	0.31
19	Nebraska 8	0.61	0.80	0.08	0.11
20	North Dakota	5.48	7.50	0.75	1.03
21	North Dakota 1	4.01	5.19	0.55	0.71
22	North Dakota 2	3.75	5.12	0.51	0.7
23	North Dakota 3	3.59	4.62	0.49	0.63
24	North Dakota 4‡	1.52	1.89	0.21	0.26
25	North Dakota 5	1.28	1.80	0.17	0.25
26	North Dakota 6‡	0.74	0.95	0.10	0.13
27	South Dakota	7.22	10.97	0.99	1.50
28	South Dakota 1‡	4.25	6.07	0.58	0.83
29	South Dakota 2	1.97	2.77	0.27	0.38
30	South Dakota 3‡	1.86	2.42	0.26	0.33
31	South Dakota 4‡	0.93	1.22	0.13	0.17
32	Wisconsin	1.64	2.03	0.22	0.28
33	Wisconsin 1‡	1.20	1.58	0.16	0.22
34	Wisconsin 2‡	0.53	0.65	0.07	0.09
	<i>Total</i>	110.52	150.34	15.1	20.57

* N fertilizer application in kg N ha⁻¹ yr⁻¹.

[†] If more than one potential biorefinery could be placed in a state, we name potential placements with serial numbers.

[‡] Biomass collection for the biorefinery location involves collection across state boundaries.

[§] Biorefinery placements associated with biorefinery ID are presented in Figure 6.

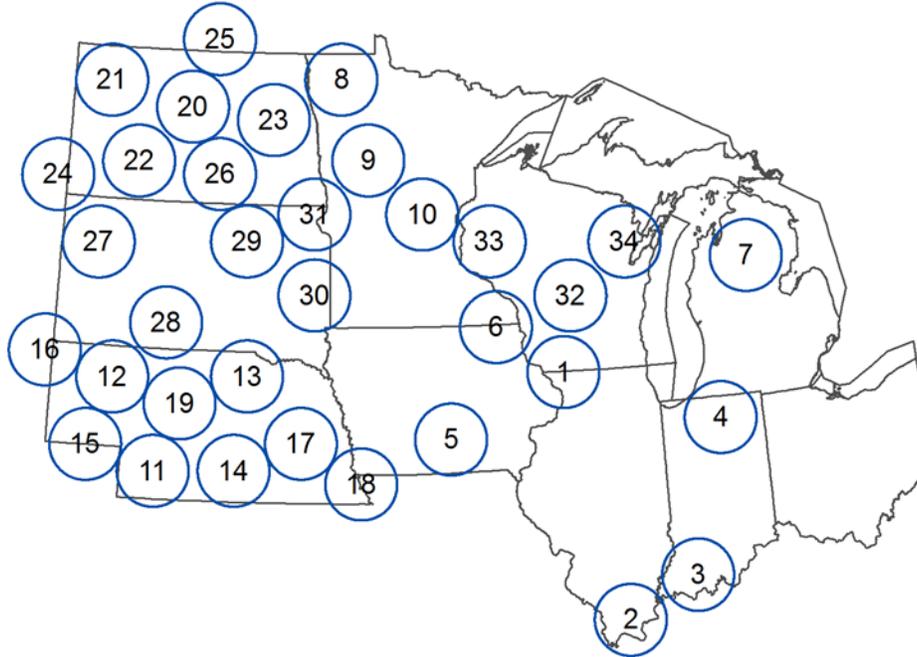


Figure 6. The placement of biorefineries for cellulosic biomass production from marginal lands in ten North Central states with identification numbers corresponding to Table 3.

3.3 Perennial Biomass Crop Production in the Sandhills of Nebraska

The dune ridges and slopes of the Sandhills of Nebraska were removed from analysis by applying the TPI algorithm available in ArcGIS. The TPI is a classification scheme based on the difference in elevation values between a cell in a DEM raster and its neighbors. The extent to which a cell is higher or lower as compared to its neighbors, combined with its slope, can be used to assign it a landform classification like valley, ridge etc.

Removing the dune ridges and slopes reduced the area available for consideration as marginal lands in Nebraska by more than 200,000 ha. This constitutes nearly 3% of the marginal lands identified by our approach. The inter-dune valleys falling under LCC V-VII and with slope gradients < 20% were then used for further analysis using EPIC model with yields shown in Figure 7.

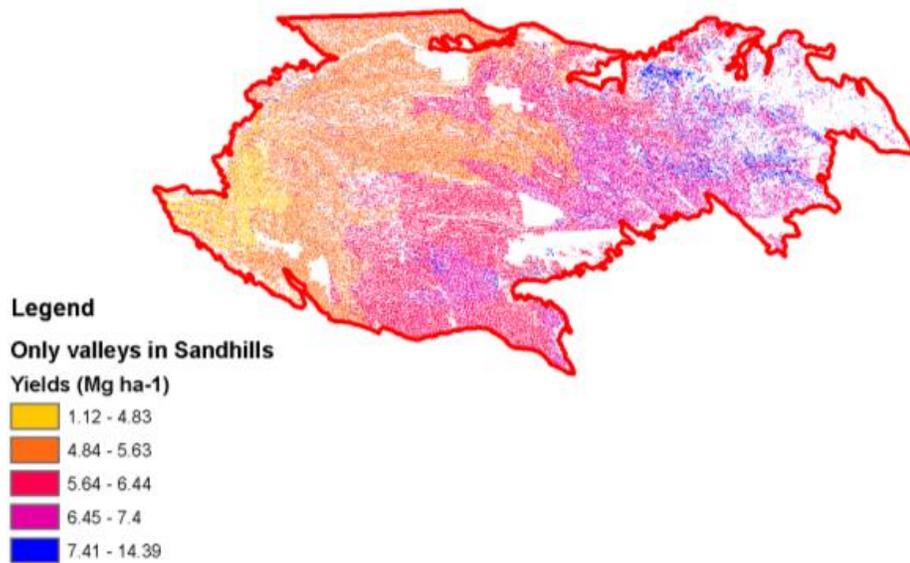


Figure 7. Production capability across the Sandhills for a native prairie mix. The dune ridges and slopes of the Sandhills have been excluded from analysis.

4.0 Conclusions

We have developed a spatially explicit geodatabase containing data for 10 of the US Midwest states for the primary purpose of conducting simulation studies of potential biofuel scenarios. In addition, we have used this geodatabase to perform simulation studies in these states using the EPIC biogeochemical model. The results of this study will be submitted to the USDOE Bioenergy Knowledge Discovery Framework as a way to contribute to the development of a sustainable bioenergy industry.

In order to perform these high-resolution analyses, it was vital to have a computing infrastructure in place that would allow us to simulate 78,184 individual land units for each of the three fertilization and two harvest efficiency scenarios and would allow us to aggregate and visualize the resulting data. The first part of this infrastructure was the server “deltac”: an eight-core Linux server, acquired with ARRA support, used to conduct the initial county-level and state-level simulations and host the PostgreSQL database where data from the national-scale simulations were stored. Had we not received funding for this vital resource, this report would not have been possible in the time allotted. ARRA funding also supported a PhD student from UMD who worked on creating the geodatabases and executing the simulations in this study.

While the available acreage of marginal lands varied considerably by state, we determined that 34 potential biorefineries could be situated among 10 of the US Midwest states, each of which could produce at least 23.6 million gallons ethanol yr⁻¹ (**Error! Reference source not found.**). EPIC simulated annual yields for all marginal lands in the region averaged 6.0±2.6 Mg ha⁻¹ (Table 9). Modest fertilization rates of 68 kg N ha⁻¹ yr⁻¹ increased estimated average yields by 36% to 8.2±2.7 Mg ha⁻¹. Spatially explicit biophysical modeling of cellulosic feedstock production on marginal lands within 80 km of a potential biorefinery suggests an annual potential ethanol production of ~5.6 billion gallons yr⁻¹, or ~30% of the 2022 target for cellulosic biofuel mandated by US legislation.

In summary, we have reported on the development of a spatially explicit national geodatabase to conduct biofuel simulation studies and provided simulation results on the potential of perennial cropping systems to serve as feedstocks for the production of cellulosic ethanol. Our results show that management of marginal lands to permit the growth of mixed species assemblages can provide cellulosic biofuel feedstock without creating the carbon debt associated with land use change to new plantings. This would also lead to additional GHG benefits because of lesser dependence on N inputs and higher amounts of soil C sequestration. This work, we believe, opens the door for further analysis on the characteristics of cellulosic feedstocks as major contributors to the development of a sustainable bioenergy economy. Examples of research questions that could be pursued with the modeling framework presented here include:

- How can the modeling framework be improved? (e.g. adding irrigation, improving winter wheat simulations)
- What is the performance of emerging biofuel feedstocks such as miscanthus, energy cane, and energy sorghum? Where are the best regions to grow them?

- What is the potential of marginal lands across the conterminous USA to provide sustainable levels of biomass feedstocks to the cellulosic ethanol industry?
- What are the full GHG impacts of diverse biofuel production systems?

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