

Research Article

Exploring a United States Maize Cellulose Biofuel Scenario Using an Integrated Energy and Agricultural Markets Solution Approach

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Abstract

Biofuel feedstock production in the United States (US) is an emergent environmental nutrient management issue, whose exploration can benefit from a multi-scale and multimedia systems modeling approach that explicitly addresses diverging stakeholder interests. In the present analysis, energy and agricultural markets models and a hybrid process-based agricultural production model are integrated to explore the potential environmental consequences of increased biofuel production from maize grain and stover feedstocks. Yield and cropland reallocation projections are simulated for 20 agricultural crops at a 12km grid resolution across the continental United States. Our results are presented across multiple, spatially expanding domains, and our results for the Upper Mississippi River Basin (UMRB) are compared to previous studies. Our analysis highlights the critical continuing role of agricultural and crop science to provide physically plausible estimates and physical process drivers of yield increases, and suggests that while the UMRB is the target of the greatest agricultural changes under our scenarios, its response does not necessarily reflect the interests of a broad stakeholder community.

Keywords: EPIC; Cropland reallocation; Yield trend simulation; Nitrogen; MARKAL; CARD

Abbreviations and Acronyms

2002_{BASE}: Baseline scenario for present study; 2022_{BASE}: Future scenario including yield and CO₂ trends; 2022_{CROP}: Future scenario including yield, CO₂ trends and cropland reallocation; A2: Scenario of continuous corn with high yield; ALMANAC: Agricultural and Management Alternative with Numerical Assessment Criteria; APEX: Agricultural Policy/Environment Extender; APSIM: Agricultural Production Systems SIMulator; B1: Scenario of continuous corn with 25% stover removal; CARD: Center for Agricultural and Rural Development; CO₂: Carbon Dioxide; CRP: Conservation Reserve Program; DIN: Dissolved Inorganic Nitrogen; DSSAT: Decision Support System for Agrotechnology Transfer; EISA: Energy Independence and Security Act; EPIC: Environmental Policy Integrated Climate Model; FEST-C: Fertilizer Emission Scenario Tool for CMAQ; LUC: Land Use Change; MARKAL: Market Allocation Model; Markets Solution: the integrated CARD-MARKAL model solution; MRB: Mississippi River Basin; N: Nitrogen; NEWS2-DIN: Nutrient Export from Watersheds version 2 for dissolved inorganic nitrogen; NLCD: National Land Cover Data Layer; MODIS: Moderate Resolution Imaging Spectroradiometer; P: Phosphorus; RFS: Renewable Fuel Standards; SI: Scenario of increased maize yield and no stover harvest; SII-4: Scenario of increased maize yield and 24% stover harvest; SWAT: Soil and Water Assessment Tool; TIMES: Integrated MARKAL Energy Flow Optimization model; UMRB: Upper Mississippi River Basin; US: United States; USDA: United States Department of Agriculture

Introduction

Many potential drivers of environmental impairment involve complex physical and chemical processes, which operate across multiple media, span a wide range of temporal and spatial scales, and touch upon a wide range of stakeholder concerns. Environmental nutrients such as Nitrogen (N) and Phosphorus (P) are particularly sensitive to these complex interactions (Figure 1), and their sustainable maintenance at levels that are healthful for both humans and ecosystems poses significant management challenges for the 21st century [1-3]. An improved understanding of such complex systems requires that stakeholders be included as essential system components and encourages a “one-biosphere” approach. One emergent environmental challenge having implications for nutrient cycling is presented by United States (US) biofuel feedstock production in response to enactment of the Renewable Fuel Standards (RFS) rules, which originated with the Energy Policy Act of 2005, and were expanded and extended by the Energy Independence and Security Act (EISA) of 2007. This issue is well-suited to the one-biosphere approach in light of the number and diversity of stakeholder interests, e.g., energy and agricultural markets, feedstock producers, biotechnology developers and those potentially effected by downstream changes in air, land and water quality. Our understanding of agricultural system drivers and responses can be improved using a one-biosphere paradigm that highlights production system strengths, flexibility and resilience as well as showing opportunities for further expansion of aspects of biofuels production that form important parts of the bioeconomy.

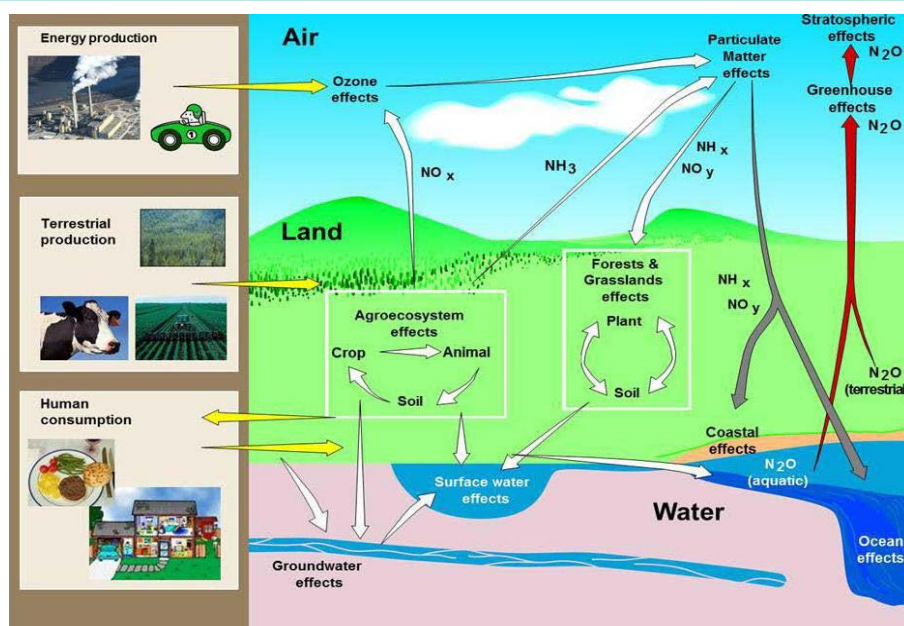


Figure 1: The nitrogen cascade (Source: [60], adapted from [61]).

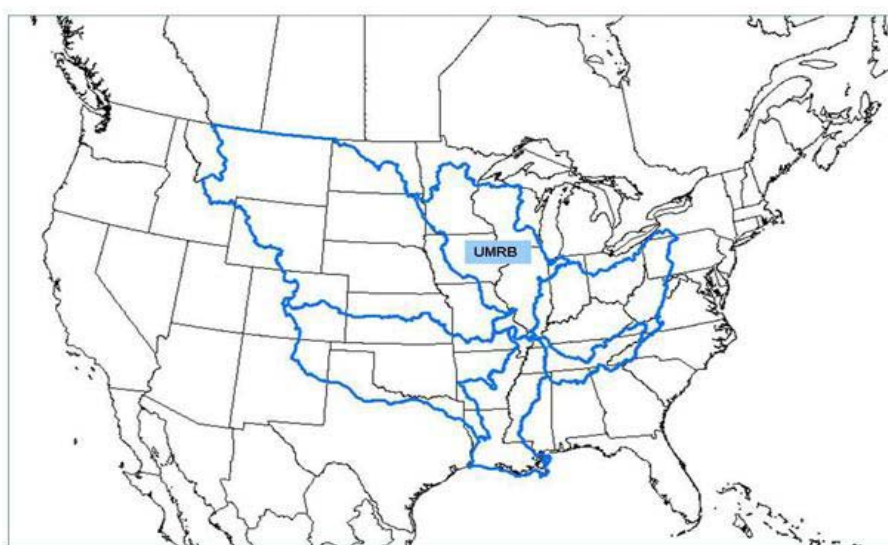


Figure 2: US modelling domain. Hydrologic sub-basins that define in the Mississippi River Basin (MRB) are outlined in blue. Upper Mississippi River Basin (UMRB) sub-basin is labeled.

Previous analyses have employed similar systems approaches, e.g., [4-8]. The present study, however, differs from previous ones by its temporal and spatial scale, use of coupled agricultural and energy market drivers, the number of agricultural crops that are simulated, the method of production simulation employed and the use of these results in analyses relevant to both human health and ecosystems [9,10]. We illustrate our one-biosphere approach by using a scenario for cellulosic biofuel feedstock production that leverages previous innovative economic analyses. The viability of this biofuel feedstock scenario in the US is discussed at length in [11]. Figure 2 illustrates the domain for this simulation, which is the continental US. The most productive agricultural region in the US, the Mississippi River Basin

(MRB) is outlined and an important sub-basin for analysis, the Upper Mississippi River Basin (UMRB) is highlighted. Our simulation timeframe spans from 2002 to 2022. 2002 represents conditions prior to land use and production changes influenced by RFS and EISA policies. The full one-biosphere modeling system defined for this application is provided in (Figure 3). The models listed represent a combination of social science, process-based, hybrid empirical and empirical models that were identified as appropriate in terms of scientific credibility, temporal and physical scale, physical detail and ability to represent or inform the diversity of biofuel Stakeholder interests. In particular, models were selected that have a significant international user base. This is but one possible model configuration,

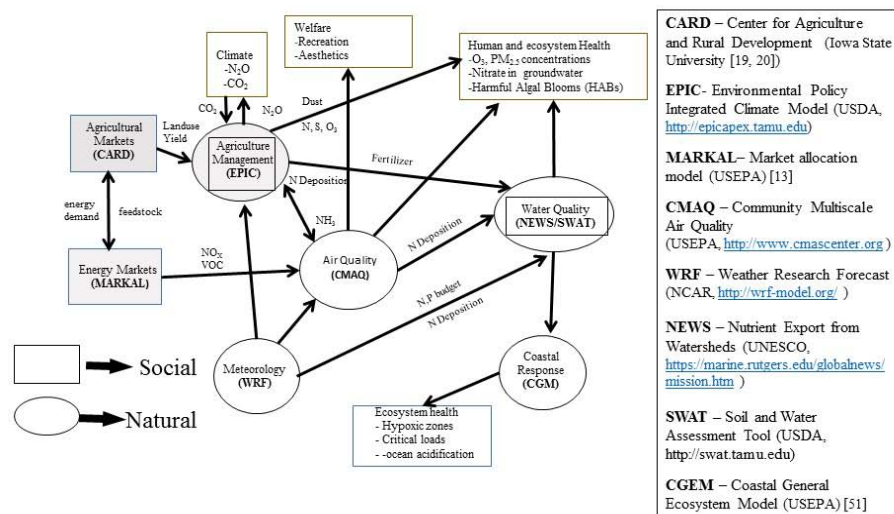


Figure 3: A one-biosphere modeling system to explore nutrient input, fate and transport in the US. Shaded components are the focus of the present analysis.

and other combinations could be selected as long as proper linkages across model components are established. The present discussion focusses on the linkage of models for the agricultural market (CARD), the energy market (MARKAL) and for agricultural production (EPIC) (shaded (Figure 3) components).

Materials and Methods

The CARD and MARKAL models

The present analysis builds on the work of Elobeid *et al.* [12], who develop an integrated energy and agricultural market solution to a hypothetical, policy-driven biofuels demand projection through the year 2022 in which biofuel demand is met through growth in existing maize starch-derived fuels and the introduction of maize stover cellulosic bioenergy fuel production. The MARKet Allocation (MARKAL) model is a linear programming optimization model that solves for the least-cost system-wide solution for meeting end-use energy service demands, given primary energy resources and technologies that convert primary energy into fuels and electricity for end-use sectors [13]. It is a technology-rich bottom-up modeling framework that requires a detailed multi-sector database specific to the country or region being modeled. MARKAL and The Integrated MARKAL/EFOM (Energy Flow Optimization Model) System (TIMES) family of energy system models have both been applied at the global, national, regional and local scales for Sweden, Ireland, the UK, Portugal, Norway, Spain, Greece, all of Europe and China [14-17]. For this application, we use the US nine-region database [18] calibrated to information from the Annual Energy Outlook [19,20], which provides historical data for 2005 and projections to 2035 (all results are annual).

The Center for Agriculture and Rural Development (CARD) US agricultural markets model is part of a broad modeling system of the world agricultural economy comprised of a set of multimarket simulation models [21,22]. The CARD model includes behavioral equations that determine crop planted acreage, domestic feed, food and industrial uses, trade, and ending stocks in marketing years and produces projections for agricultural commodity supply, utilization,

and prices. The model solves for a set of prices that bring annual supply and demand into balance throughout the world market for biofuels, grains and oilseeds.

The integration of MARKAL and CARD systems represents a more realistic approach than assuming maize prices as static, or assuming similar price points for ethanol going out into the future. Maize prices will, in reality, show sensitivity to shifting ethanol demand so that the integrated MARKAL-CARD system represents important science advancement over previous application approaches. For instance, while the Irish TIMES model application includes emissions from direct and indirect Land-Use Changes (LUCs), it does not model the impacts on agricultural markets dynamically. Instead, the authors used a series of best professional judgment assumptions to assign LUC emissions to domestic *versus* imported crops based on a review of the literature [23,24].

Three integrated markets model production scenarios have been developed to explore the response of our one-biosphere system to stakeholder behaviors associated with biofuel production. Baseline 2002 agricultural market conditions are those reported in United States Department of Agriculture (USDA) [25]. Two future scenarios, 2022_{BASE} and 2022_{CROP}, are then developed. We assume that the integrated markets model yield trend is independent of the energy market status and it is applied to both future scenarios. Ethanol can be produced using starch from edible biological feedstocks such as grain, or using cellulose feedstocks made up of inedible biological materials such as wood, grass, and agricultural residues such as maize stover. The 2022_{BASE} projection employs the 2007 Annual Energy Outlook of 0.25 billion gallons of forest cellulose-based ethanol production and 12.29 billion gallons of maize starch based ethanol [19]. The 2022_{CROP} scenario represents a hypothetical situation in which projected ethanol production levels reflect an integrated CARD-MARKAL model solution, hereafter referred to as the “Markets solution” [12]. Biofuel production reaches 8 billion gallons of maize cellulosic-based ethanol production and 18 billion gallons of maize starch-based ethanol and an additional 2 billion gallon cellulosic production from non-cropland feedstocks.

Land use change (cropland reallocation)

One of the key outputs of the Markets solution is agricultural land use change needed to meet projected agricultural commodity demands. These changes reflect economic and population-driven adjustments required to meet not only projected biofuel feedstock demand, but also demand for food and livestock feed spanning 20 (irrigated and rainfed) crops (see Supplementary Information Part I). The Markets solution projects 2022 agricultural land use, but a one-biosphere approach requires the delineation of both agricultural and non-agricultural land. The most widely used source of land use information for the US is the United States Geological Survey (USGS) National Land Cover Data Layer (NLCD) [26]. Our baseline crop production simulations use NLCD 2001 (2011-edition) pasture/hay (class 81) and cultivated crop (class 82) to delineate total cropland areas. Although NLCD data are available only for the US, Moderate Resolution Imaging Spectroradiometer (MODIS) data are available world-wide and could be used for projections outside of the US.

Our 2022_{BASE} scenario assumes that future agricultural commodity demand without additional maize stover ethanol production is met without cropland reallocation. The 2022_{CROP} Markets solution assumes no new agricultural land is added to the national inventory, but that the distribution of crops on existing NLCD delineated cropland is reallocated to meet increased demand for maize grain and stover ethanol feedstocks. The Markets solution also assumes that increasing demand for soybean and wheat derived food, oil and livestock feed is met. State-level estimates of cropland reallocation that is needed to meet this demand (given that yield trends are also met) are provided by the Markets solution, but no information is provided regarding which crop is replaced by another crop. This information is particularly important for the estimation of biogeochemical processes, soil properties, yields and environmental quality. Here, we use the reallocation hierarchy maize, soybean, sorghum, cotton, wheat, hay, alfalfa, peanuts, oats, barley, sunflower, rice, canola and Conservation Reserve Program (CRP). Process-based yield response to these shifts is highly dependent on the hierarchy structure. Although this hierarchy is reasonable for the US crop sector, alternative designs will be needed for simulations for regions outside the US. An important feature of the scenarios presented here is that cropland reallocations are performed across 20 major agricultural crops, as opposed to maize and soybean only. In the absence of policy drivers that limit farmer response to national and international market conditions, this is a more realistic description of cropland reallocation. Example reallocation calculations are provided in Supplementary Information Part II.

EPIC model simulation of yield projections

The USDA Environmental Policy Integrated Climate (EPIC) model provides agricultural management, biogeochemical and soil property information for our analysis. EPIC is a semi-empirical process-based biogeochemical model in which N and P added to, or lost from agricultural fields responds explicitly to local weather and soil conditions, farm management and land use conditions [27]. Many EPIC crop parameter values derive from the Agricultural and Management Alternative with Numerical Assessment Criteria (ALMANAC) model [28]. EPIC has been applied worldwide, and is the foundation for the field component of the Agricultural Policy/Environment Extender (APEX) model [29]. The ALMANAC, EPIC

and APEX models have been used for a wide variety of biofuels application studies e.g. [30-34]. The original EPIC software has been modified to better support linkage with regional air quality models [35]. This modified software and documentation are available as part of the Fertilizer Emission Scenario Tool for CMAQ (FEST-C). EPIC simulations are performed for 42 crop located throughout our domain (Figure 2) at a 12 km rectangular grid cell resolution (14400 ha per grid cell). Additional detail regarding the EPIC model simulation design for this application is provided in Supplementary Information Part III.

EPIC yield estimates derive from tightly coupled non-linear biogeochemical processes equations and parameters that are not easily constrained to a fixed, a priori outcome. Linkage of EPIC yield estimates to the Markets solution, then, requires development of a set of parameterizations that are consistent with the Markets model hypothetical yield trend, while remaining physically plausible. EPIC yield parameterizations rely on process-based relationships between biomass accumulation and environmental conditions/stressors, and so a technology-driven yield trend must derive from some physical process change. Modification of different process relationships, e.g., increased tolerance for high planting density or nitrogen-fixing maize, would produce a different biogeochemical system outcome and so it is critical to be explicit regarding the physical drivers of the economic model yield trend (e.g. [36]). In the future, plant physiological process models such as those contained in the Decision Support System for Agrotechnology Transfer (DSSAT) system or the Agricultural Production Systems Simulator (APSIM) [37], could help to identify plausible parameterizations. For the present application, we assume that advances in bioengineering technology will modify the partitioning of total plant biomass to harvested biomass, i.e., grain yield for each Markets solution crop. This approach is similar to that employed by Wu *et al.* [7] for maize. There are important implications of this approach for Markets solution estimates of stover production. The Markets solution assumes a 1:1 relationship between maize grain and stover increases. While this is a reasonable assumption for present-day crop varieties, in reality and as modeled here, this assumption is not necessarily supported at higher yields [38]. Another factor that can influence stover production is increasing levels of ambient CO₂. We assume here that ambient CO₂ concentrations increase from 372 ppm in 2002 to 412 ppm in 2022. This trend is based on the Mauna Loa CO₂ observed trends, 1960-current. Stockel *et al.* [39] describe the EPIC simulation of plant (biomass) increase in response to increasing CO₂ concentrations. Yield response to technology and ambient CO₂ trends are included in both 2022 future scenarios. Finally, Weather Research Forecast (WRF) simulations provide 2002 EPIC weather inputs across our domain. Weather inputs across 2002, 2022_{BASE} and 2022_{CROP} simulations are assumed to be stationary given the relatively short elapse time, i.e., [40].

Results and Discussion

Table 1 summarizes the driving Markets solution scenarios for our EPIC simulations. Most previous studies focus on land use change to meet rising feedstock demands or possible water quality consequences of increased biofuel feedstock production. Comparison of our results to findings in the existing literature is difficult because of the number of scenario variations and the unique nature of the present simulations. We begin here by considering results that focus

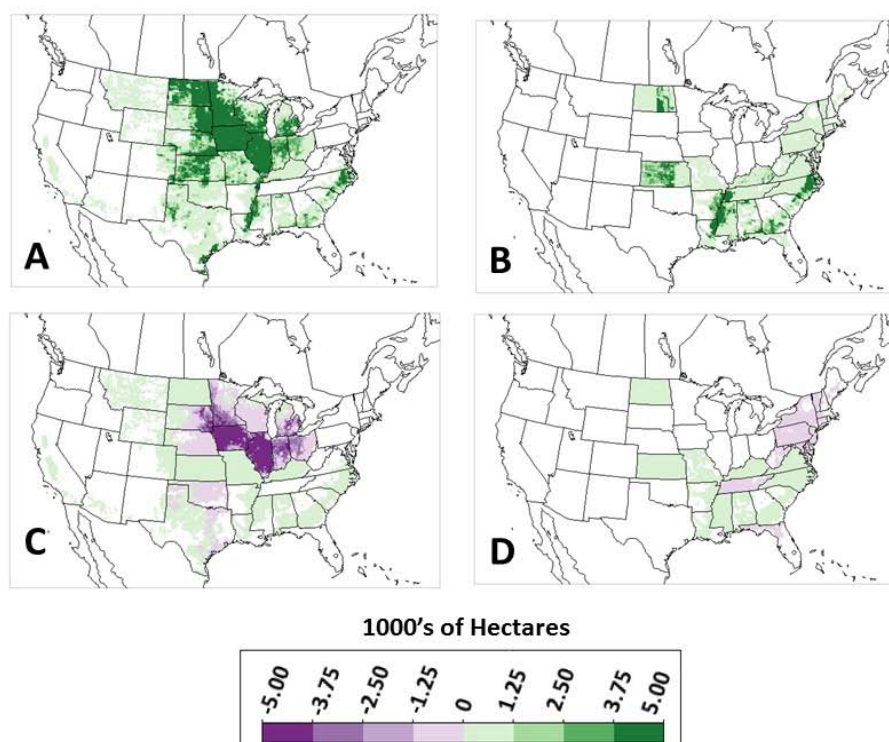


Figure 4: A) Maize cropland reallocation, B) Soybean cropland reallocation, C) Soybean cropland reallocated to Maize, D) Maize cropland reallocated to soybean. All areas are reported as hectares per simulation grid cell. Grid cell area is 14400 ha. **Note:** The lightest green plotting bin includes zero values, *i.e.*, no change.

Table 1: Biofuels simulation scenarios. Values within () are the market model solutions. Cellulose production assumes a 32 to 34% maize stover removal rate [62].

Scenario name	2002	2022 _{BASE}	2022 _{CROP}
Weather	2002	2002	2002
Technology and ambient CO ₂ trends	No	Yes	Yes
Ethanol Production (billion gallons)	Maize Grain: 2.13 Maize Cellulose: 0 Forest Cellulose: 0	Maize Grain: 12.29 Maize Cellulose: 0 Forest Cellulose: 0.25	Maize Grain: 17.97 Maize Cellulose: 8.16 Forest Cellulose: 2.41
EPIC estimated maize grain production (million metric tons)	196813 (205000)	261760	333691 (341000)
EPIC estimated maize cellulose production (million metric tons)	0	0	66.1 (80)
EPIC estimated soybean production (million metric tons)	63 (68)	73	74 (80)
EPIC estimation wheat production (million metric tons)	56 (47)	70	70 (58)

on factors related to crop feedstock production estimation, followed by metrics of water quantity and quality.

Crop production

Figure 4 summarizes our patterns of maize and soybean intensification and extensification. On a state basis, area devoted to each crop may increase or decrease, resulting in geographic changes that can produce a negligible net change at the national scale. Maize net cropland area increases by about 29% (e.g. (Figures 4A and 4D)), soybean cropland area expands by only 1% (e.g. (Figures 4B and 4C)) and wheat shows no net change (not shown). Maize cropland expansion comes at the expense (net reduction) of cotton (50%), rice (30%), grain sorghum (26%), oats (23%), barley (17%) and hay (2%) areas. The Markets solution yield trends from 2002 to 2022 range from increases of 5% for Hay up to 30% for grain corn and 35% for cotton. These trends are based on the extrapolation of historical yield trends reported by the United States Department of Agriculture.

The Market solution suggests that a yield trend of 17% for soybeans and 20% for wheat are sufficient to meet future demand without significant cropping area increases. 2022_{CROP} production includes biogeochemical and soil property responses to cropland reallocation and stover removal. In some cases, cropland reallocation generates a “yield drag” which can result when crop production moves to a location with less optimal growing conditions than previously experienced [41]. Factors contributing to reduced productivity can include higher slopes, lower organic matter, increased number of tillage operations and a shift from a broadcast crop such as hay or small grains, to a row crop such as corn or soybean, each of which can enhance soil erodibility [42,43].

The Markets solution land use change scenario as implemented here shows good agreement with current literature for the US. There is general agreement concerning observed corn/soybean area intensification, particularly in the western corn belt region (North

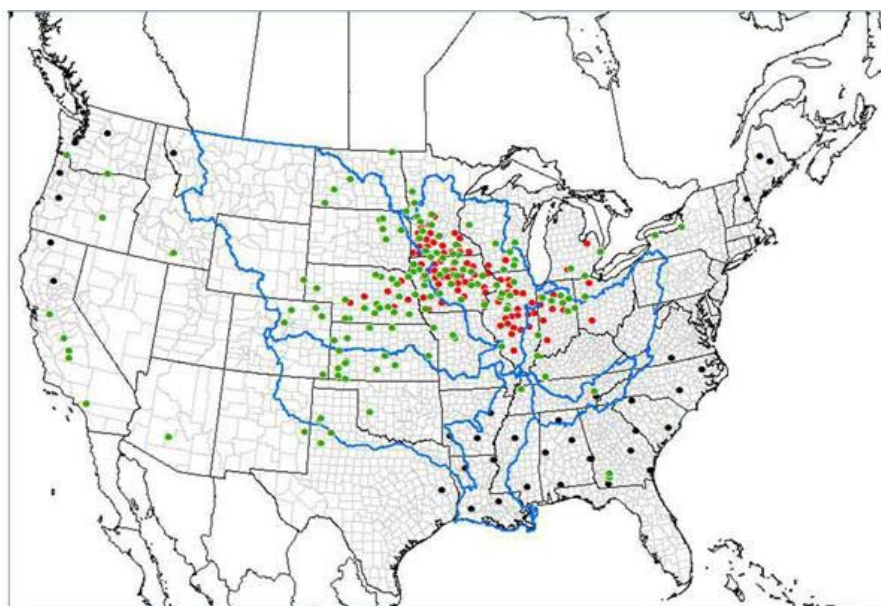


Figure 5: Projected, 2022 locations of corn starch (green circles), corn cellulose (stover) (red circles) and forest cellulose (black circles) feedstock ethanol processing facilities.

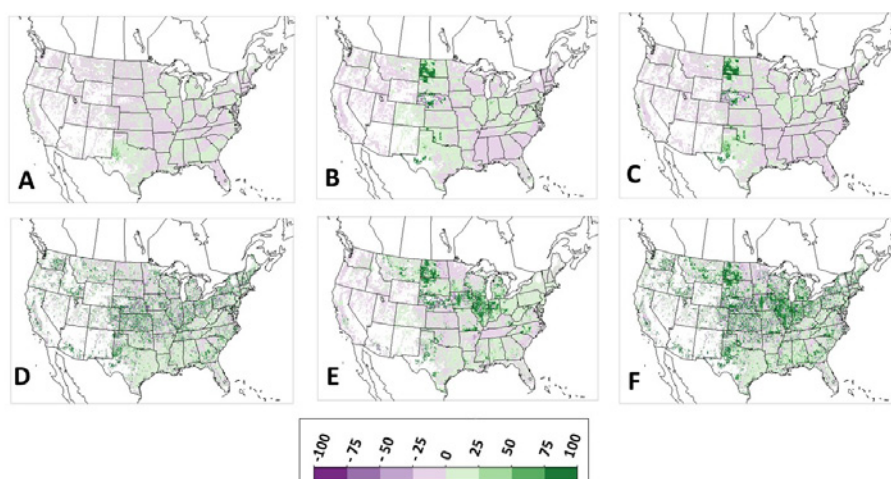


Figure 6: Percent change (%) from 2002 conditions for surface runoff attributable to A) trends only (Equation. 1), B) stover removal and cropland reallocation only (Equation. 2), C) all factors (Equation. 3), and N export attributable to D) trends only (Equation. 1), E) stover removal and cropland reallocation only (Equation. 2), and F) all factors (Equation. 3). N export includes dissolved inorganic N losses in surface and sub-surface lateral flow. Purple represents a decrease and green represents an increase. Unity values, i.e. no change are included in the lightest green bin.

Dakota, South Dakota and Montana) [44-46]. Wright *et al.* [47] and Holder *et al.* [48] suggest intensification in the central corn belt region may be concentrated around ethanol refineries. The Markets solution recognizes this tendency by “locating” new simulated refineries in areas projected to have the highest stover production (Figure 5). Greater spatial specificity than this, however, is beyond the scope of the present simulation. Wright and Wimberly [46] suggest that much of the Western Corn Belt expansion is at the expense of Conservation Reserve Program (CRP) lands. Lark *et al.* [41] perform a similar analysis covering the continental US, and areas of soybean expansion to the west and south of current centers of production agree well with our projections. Both Lark *et al.* [41] and Sayler *et al.*

[44] suggest agricultural expansion along the Gulf Coast and eastern Coastal Plain. Lark *et al.* [41] simply suggest this expansion is at the expense of “areas reserved for other uses” while Sayler *et al.* [44] suggest this expansion is at the expense of forests. Table 1 indicates that 2002 maize, soybean and wheat grain production are - 4%, - 7% and + 19% of the Markets solution respectively. We estimate that cropland reallocation for expanded biofuel production reduces our EPIC yield trend by 4% for maize grain, 2% for rice, and 10% for cotton. In spite of this yield drag effect, simulated maize, soybean and wheat production under our 2022_{CROP} scenario are - 2%, - 8% and + 21% of the a priori 2022 Markets solution. 2022_{CROP} maize stover production is - 17% of the a priori 2022 Markets solution.

Table 2: Comparison of 2022_{BASE} relative change from 2002 results (Equation for consistency with remainder of text. 1) to Wu *et al.* [7] scenario S1 and Deb *et al.* [49] scenario A2 results. 2022_{BASE} results are summarized for Upper Mississippi River Basin (UMRB), Mississippi River Basin (MRB) and United States (US) domains. N export includes removal in surface and sub-surface losses in lateral flow. P export includes removal in surface runoff only. S1 and A2 values for all but evapotranspiration represent delivery to waterbodies. EPIC scenarios represent delivery to edge-of-field.

	SI Wu <i>et al.</i> [7]	A2 Deb <i>et al.</i> [49]	2022 _{BASE} UMRB	2022 _{BASE} MRB	2022 _{BASE} US
Evapotranspiration	0.0%	+0.2 %	+0.2%	+0.2%	+0.2%
Surface Runoff	+0.3%	0.0%	-0.8%	+0.2%	0.0
Inorganic Nitrogen Application	Not reported	Not reported	+15.1%	+13.9%	+13.4%
Nitrogen Export	-5.0 %	-1.5 %	-3.3%	-0.4%	-0.6%
Sediment Export	+0.1	+1.6 %	-5.5%	-4.6%	-4.3%
Inorganic Phosphorus Application	Not reported	Not reported	+11.1%	+9.0%	+8.7%
Phosphorus Export	+0.5 %	Not reported	-0.1%	+2.6%	+2.0%
Plow Layer Organic Carbon	Not Reported	Not reported	-1.0%	-1.0%	-0.9%

Table 3: Comparison of 2022_{CROP} relative change from 2002 results (Equation 3) to Wu *et al.* [7] scenario SII-4 and Deb *et al.* [49] scenario B1 results. 2022_{BASE} results are summarized for Upper Mississippi River Basin (UMRB), Mississippi River Basin (MRB) and United States (US) domains. N export includes removal in surface and sub-surface losses in lateral flow. P export includes removal in surface runoff only. SII-4 and B1 values for all but evapotranspiration represent delivery to waterbodies. EPIC scenarios represent delivery to edge-of-field.

	SII-4 Wu <i>et al.</i> [7]	B1 Deb <i>et al.</i> [49]	2022 _{CROP} UMRB	2022 _{CROP} MRB	2022 _{CROP} US
Evapotranspiration	~ +0.1%	+2.8 %	+2.9 %	+1.4%	+1.0%
Surface Runoff	~ -0.5%	0.0%	+4.4 %	+1.1%	+0.6%
Inorganic Nitrogen Application	Not Reported	Not Reported	+24.9%	+18.0%	+15.5%
Nitrogen Export	-15.0 %	-9.1 %	+11.2 %	+5.8%	+3.9%
Sediment Export	-0.5 %	-3.1 %	+13.9 %	-0.1%	-2.2%
Inorganic Phosphorus Application	Not Reported	Not Reported	+15.3%	+12.6%	+11.6%
Phosphorus Export	-2.0 %	Not Reported	+0.4 %	+3.8%	+3.0%
Plow Layer Organic Carbon	Not Reported	Not Reported	-6.0 %	-2.6%	-1.8%

*Values are estimated from figures published in [7].

Additional results

Tables 2 and 3 and Figures 6 and 7 present our results as the response (%) or relative change of selected EPIC variables to yield and CO₂ trends alone (TR, Equation 1), response to cropland reallocation and stover removal alone (RSR, Equation 2), and response to all factors (TO, Equation 3).

$$TR = [(2022_{BASE} - 2002)/2002] * 100 \quad (1)$$

$$RSR = [(2022_{CROP} - 2022_{BASE})/2022_{BASE}] * 100 \quad (2)$$

$$TO = [(2022_{CROP} - 2002)/2002] * 100 \quad (3)$$

Tables 2 and 3 summarize our 2022_{BASE} and 2022_{CROP} results across three domains (the Upper Mississippi River Basin (UMRB), the Mississippi River Basin (MRB) and the full US (US), and compare our UMRB results to those reported by Wu *et al.* [7] and Deb *et al.* [49]. Both previous studies perform biofuel feedstock analyses for maize and soybean crops and maize stover and switchgrass biofuel feedstocks in the UMRB using the Soil Water Assessment Tool (SWAT) [50]. The SWAT field-scale biogeochemical model is similar to that of EPIC, but it lacks some biogeochemical and management detail such that identical scenario response across simulations is not to be expected. Wu *et al.* [7] focusses on nutrient response when increasing food and feed demand for maize are met by assuming a 19% technology-based yield increase. Deb *et al.* [49] focusses on

water yield response to meteorological change, and meets future maize demand through use of current high yield corn varieties and intensification, *i.e.*, movement from maize-soybean rotation to continuous maize management. Our 2022_{BASE} simulation most closely resembles the Deb *et al.* [49] A2 scenario (continuous maize, high yield) and Wu *et al.* [7] S1 scenario (increased yield, no stover harvest). The Deb *et al.* [49] B1 scenario (continuous maize, 25% stover removal) and Wu *et al.* [7] SII-4 scenario (increased yield, 24% stover removal) most closely resemble our 2022_{CROP} scenario. Significant differences between our 2022_{BASE} and 2022_{CROP} and A2, B1, S1 and SII-4 scenarios include our assumption of an increasing CO₂ trend, the explicit simulation of changing soil properties, and the use of crop extensification, *i.e.*, cropland reallocation as well as biotechnology-based yield increases across all simulated crops in order to meet future food, feedstock and energy demands.

2022_{BASE} results for selected variables are provided in (Figures 6A, 6D, 7A and 7D) and Table 2. Wu *et al.* [7] report results as total N load and Deb *et al.* [45] report results as Dissolved Inorganic Nitrogen (DIN). Neither study clearly define their metrics and so we will assume they are defined in a roughly equivalent fashion. Basin level analyses such as these usually assume that inorganic fertilizers (as opposed to animal manure) are the primary source of exported nutrients and so we will define N export as the sum of inorganic N exported in surface and sub-surface (lateral) flow, and P load is assumed to be inorganic

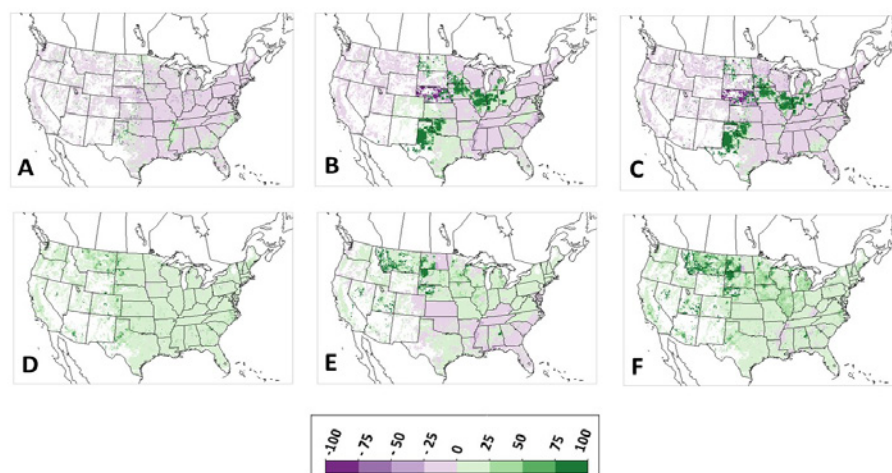


Figure 7: Percent change (%) from 2002 conditions for sediment export attributable to A) trends only (Equation. 1), B) stover removal and cropland reallocation only (Equation. 2), C) all factors (Equation. 3), and N application attributable to D) trends only (Equation. 1), E) stover removal and cropland reallocation only (Equation. 2), and F) all factors (Equation. 3). Unity values, *i.e.* no change are included in the lightest green bin.

P delivered in surface runoff only. There is good agreement among the three Table 2 UMRB results for evapotranspiration change in response to increased yields. 2022_{BASE} surface runoff, N export and sediment export results suggest reductions representing the effect of increased surface vegetation cover in response to slight ambient CO_2 increases and greater N uptake, which appear to be sufficient to overcome expected increases in response to a small reduction in plow layer organic carbon [39]. The organic carbon reduction is the product of our method of yield improvement, which assumes that a larger portion of plant N is harvested, leaving less post-harvest residue.

2022_{CROP} results for selected variables are provided in (Figures 6C, 6F, 7C and 7F) and Table 3. There is good agreement among the three Table 3 UMRB results for evapotranspiration change in response to increased yields and stover removal. Our results diverge for other Table 3 metrics primarily because of the explicit simulation of soil property changes in the 2022_{CROP} simulation. 2022_{CROP} UMRB organic carbon in the plow layer is reduced by 6.6% when cropland is reallocated across the 20 crop varieties for which Market solution projections are available and maize stover is harvested as biofuel feedstock. Reducing soil organic matter through stover removal reduces porosity in the near-surface zone and increases sealing tendencies which increase surface runoff and sediment export [51,52]. In response to this organic carbon reduction, 2022_{CROP} surface runoff, and N, sediment and P export all increase. Our results are also in agreement with the location (Illinois and Indiana) and magnitude of peak N export response to increased biofuel demand reported by Donner *et al.* [53] (Figure 6B). Although Wu *et al.* [7] suggest similar sediment export might be expected, *SII-4* results assume constant soil properties, suggest very different nutrient and sediment export outcomes, and highlight the importance of including these agroecosystem responses when evaluating biomass production alternatives. For instance, *SII-4* and B1 results suggest that water quality impairment related to N and sediment export could be reduced (N and sediment export reductions), while our 2022_{CROP} findings suggest that water quality impairment in the UMRB could be exacerbated.

Next, consider our EPIC results across UMRB, MRB and US domains. For the 2022_{BASE} scenario (Table 2, Equation 1), simulated evapotranspiration and surface runoff show little response to analysis domain extent, *i.e.*, UMRB, MRB or US. In nearly all other cases, the magnitude of variable response decreases as the domain scale increases. In the 2022_{CROP} case, even evapotranspiration and runoff follow this pattern of decreasing response. This is not surprising with our focus on maize stover harvest for biofuel feedstock and the concentration of maize production in the UMRB. These cross-scale results, however, highlight that while the bulk of the response occurs in a relatively concentrated area, cropland reallocation outside the UMRB needed to maintain food and feedstock supplies can also have important implications for environmental impairment and should not be overlooked (Figures 6,7). For instance, Table 3 suggests that sediment export reductions resulting from cropland reallocation outside the UMRB may be sufficient to offset, in a global sense, export increases within the UMRB. While our results clearly suggest the potential for significant environmental impairment challenges in the UMRB, the MRB domain is of particular interest to stakeholders concerned with the yearly development of a large area showing hypoxic conditions in the Northern Gulf of Mexico (NGM).

The development of this hypoxia is commonly attributed to nonpoint nutrient sources within the MRB, including agricultural lands. Table 3 suggests that at this scale, N export response may be about one-half that of the UMRB. The importance of this more systems-based, multi-scale approach to biofuels production assessment becomes clear when Table 3 MRB edge-of-field results are provided to a recently developed version of the Nutrient Export from WaterSheds model (NEWS2) regression-based model parameterized for the MRB, $NEWS2_{mrB}$ -DIN [10,54]. The $NEWS2_{mrB}$ -DIN simulation combined our 2022_{CROP} results with 2022 projections for additional non-agricultural N source projections such as atmospheric deposition and sewage outfalls and found that DIN export to the NGM increased by only about 4% over baseline 2002 simulated values. This is in spite of 2022_{CROP} edge-of-field N exports exceeding 11% in the UMRB alone. McCrackin *et al.* [10] directly attribute this modest MRB increase to

the assumption of higher yields driven by biotechnologically derived nutrient use efficiency improvements, which highlights the critical continuing role of agricultural and crop science to provide physically plausible estimates and physical process drivers of yield increases. In the absence of these efficiency improvements, NEWS2_{mr}-DIN DIN export from the mouth of the Mississippi River to the NGM was simulated to increase 13% over 2002 simulated values.

Conclusions

An integrated multimedia approach has been applied that combines the economic strength of energy and agricultural markets models with the physical reality of a hybrid process-based crop management model to achieve a more complete, systems-level picture of biomass feedstock production in the US. This approach facilitates more comprehensive biogeochemical accounting for potential crop intensification and extensification across 20 crops spanning the continental US. We have highlighted the continuing critical role of emerging crop science to the development of appropriate, well-defined process mechanisms of technological yield increase. In the absence of this critical knowledge, economic models may make use of weak assumptions based on historical trends (e.g., 30% maize yield increases) and static physical relationships (1:1 yield and stover increase) that can diminish the added value of such a coupled approach. Alternative assumptions will, by necessity, lead to alternative biogeochemical outcomes. We recommend that, in the future, more process-based input from crop scientists as reflected in biogeochemical process and farm management models such as EPIC and APEX be included in the determination of the joint market solution, replacing the current method of ad hoc USDA yield trends. This would also strengthen the social and environmental linkage and would reduce inconsistencies regarding agricultural commodity supplies. Our findings emphasize the potentially critical role of technology-driven yield increases and the importance of defining the mechanisms of this increase to supplement the model assessment of more traditional nitrogen management approaches [55,56]. Our results highlight that vegetation response to these technology-driven increases are part of a complex, interconnected biogeochemical system of carbon and nutrient flows that are influenced by management choices such as cropland reallocation, crop residue removal and management, and re-purposing of agricultural commodities, e.g., grain for fuel rather than food. The one biosphere systems approach described here facilitates the explicit inclusion of the economic and societal factors that influence and, in some cases, control biomass production and food supply outcomes while maintaining the process-level detail needed to reduce assessment uncertainty. This is in line with recent research suggesting the need for an improved characterization of social factors to understand their effect on yields and impacts on food supplies, ecosystems, water resources and soils and the long-term sustainability of these biomass production systems [57-59].

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