Trade-offs across productivity, GHG intensity, and pollutant loads from second-generation sorghum bioenergy

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Abstract

Greenhouse gas (GHG) intensity is frequently used to assess the mitigation potential of biofuels; however, failure to quantify other environmental impacts may result in unintended consequences, effectively shifting the environmental burden of fuel production rather than reducing it. We modeled production of E85, a gasoline/ethanol blend, from forage sorghum (Sorghum bicolor cv. photoperiod LS) grown, processed, and consumed in California’s Imperial Valley in order to evaluate the influence of nitrogen (N) management on well-to-wheel (WTW) environmental impacts from cellulosic ethanol. We simulated 25 N management scenarios varying application rate, application method, and N source. Life cycle environmental impacts were characterized using the EPA’s criteria for emissions affecting the environment and human health. Our results suggest efficient use of N is an important pathway for minimizing WTW emissions on an energy yield basis. Simulations in which N was injected had the highest nitrogen use efficiency. Even at rates as high as 450 kg N ha⁻¹, injected N simulations generated a yield response sufficient to outweigh accompanying increases in most N-induced emissions on an energy yield basis. Thus, within the biofuel life cycle, trade-offs across productivity, GHG intensity, and pollutant loads may be possible to avoid at regional to global scales. However, trade-offs were seemingly unavoidable when impacts from E85 were compared to those of conventional gasoline. The GHG intensity of sorghum-derived E85 ranged from 29 to 44 g CO₂ eq MJ⁻¹, roughly 1/3 to 1/2 that of gasoline. Conversely, emissions contributing to local air and water pollution tended to be substantially higher in the E85 life cycle. These adverse impacts were strongly influenced by N management and could be partially mitigated by efficient application of N fertilizers. Together, our results emphasize the importance of minimizing on-farm emissions in maximizing both the environmental benefits and profitability of biofuels.

Keywords: air and water pollutant loads, biofuel sustainability, cellulosic ethanol, energy yield, environmental impacts, feedstock management, GHG intensity, life cycle assessment (LCA), nitrogen use efficiency

Introduction

Biofuels from cellulosic ethanol have been widely reported to have GHG intensities less than half those of conventional fuels (Schmer et al., 2008; CARB, 2009; Wang et al., 2012; Adler et al., 2012; van der Weijde et al., 2013; Murphy & Kendall, 2015; LeDuc et al., 2016). GHG intensity is determined through life cycle assessment (LCA) modeling of emissions associated with generation and use of the fuel product. Feedstock production is among the most GHG-intensive components of the biofuel life cycle (Fu et al., 2003; Adler et al., 2007, 2012; Borrión et al., 2012) and can also contribute substantially to non-GHG environmental impacts such as acidification and eutrophication of local waterways (Robertson et al., 2008; Wagner & Lewandowski, 2016). Nitrogen fertilizers are strongly linked to both increased crop yield and increased environmental impacts (von Blottnitz & Curran, 2007; Fazio & Monti, 2011; Borrión et al., 2012; Ruan et al., 2016). Thus, pursuit of high biomass yields for fuel production may occur at the expense of GHG mitigation potential and local air and water pollution. Recently, increasing attention has been drawn to non-GHG impacts, as evidence accumulates that some air and water pollutant loads from cellulosic fuels can exceed those of conventional fuels.
Exploring these trade-offs is increasingly important as cellulosic ethanol is mandated to take on a growing role in meeting the renewable energy demands of the United States (EPA, 2010; EIA, 2016).

LCA is a comprehensive, quantitative method used to evaluate sustainability metrics and frequently implemented in the assessment of alternative fuels (Cherubini et al., 2009; Guinée et al., 2011). Methodological variations in LCA are considerable; thus, the International Organization for Standardization (ISO) guidelines are frequently referenced to offer a certain degree of continuity across methods (ISO 2006a,b; Cherubini & Strømman, 2011). Most biofuel life cycles use a well-to-wheel (WTW) scope (Singh et al., 2010; Borrión et al., 2012), which includes processes inherent to generation of the fuel product, intermediary processes (e.g., transportation), and fuel combustion. System boundaries define the limits of the analysis. Second-order system boundaries are commonly employed in fuel LCAs (Borrión et al., 2012) and include upstream and downstream emissions (i.e., those occurring pre- and postuse of a product, respectively) but exclude embodied energy sources such as facilities and machinery.

Under a clearly defined scope and system boundary, a life cycle inventory (LCI) is compiled, which accounts for all of the chemical compounds consumed and emitted throughout the life cycle. The resulting chemical inventory is then used to characterize environmental impacts based on each compound’s projected influence on human health and the environment. This is accomplished by expressing each compound in equivalent units (eq) of a reference compound. Emissions are then summed and used to describe their projected contribution to a specific impact category. For instance, GHG emissions are expressed in terms of CO₂ eq based on the global warming potential of each individual GHG relative to that of CO₂. Although biofuel life cycles frequently consider only GHG emissions and energy consumption (Spatari et al., 2005; Searcy & Flynn, 2008; Stichnothe & Azapagic, 2009; Hsu et al., 2010; McKechnie et al., 2010; Stephenson et al., 2010; Zamboni et al., 2011), LCA can be used to explore a diverse range of environmental impacts (Bare et al., 2003; Brentrup et al., 2004; Hauschild et al., 2013; Jeswani et al., 2015; Mbонимпа et al., 2016; Monti et al., 2009; Sanz Requena et al., 2011; Sabrina Spatari & MacLean, 2010; Wagner & Lewandowski, 2016).

The large proportion of WTW emissions attributed to feedstock production suggests management choices can play an important role in determining pollutant loads from cellulosic fuels. In the case of annual crops, management is likely to play an especially important role as they generally sequester less carbon and have higher fertilizer demands than perennials (Monti et al., 2009; Somerville et al., 2010; Fazio & Monti, 2011; Wang et al., 2012; LeDuc et al., 2016). Increasing nitrogen (N) fertilizer rates have been shown to reduce the climate benefits associated with cellulosic fuels by increasing nitrous oxide (N₂O) emissions and can adversely impact air and water quality (Brentrup et al., 2004; Robertson et al., 2008; Luo et al., 2009; Oikawa et al., 2015a; Ruan et al., 2016). Despite the impacts of N fertilizers on the environment and the significant variability in management practices observed across growers (Baumgart-Getz et al., 2012), biofuel LCAs often assume a single scenario for agronomic feedstock production (Spatari et al., 2005, 2010; Sanderson et al., 2006; Adler et al., 2007; Fargione et al., 2010; Davis et al., 2012; Pourhashem et al., 2013; Jeswani et al., 2015; LeDuc et al., 2016). Some field studies have attempted to address this variability by examining alternate management scenarios (Lamb et al., 2003; Boehmel et al., 2008; Schmer et al., 2008, 2014; Mbонимпа et al., 2016); however, the lengthy and expensive nature of these experiments limits exploration at the field level. Coupling field data with crop models allows exploration of a large breadth of management practices in silico before further testing in a field or commercial setting.

We use a field data-driven crop model coupled with LCA modeling to explore the potential impacts of N management choices on biomass yields, GHG intensity, and local air and water pollutant loads from sorghum-derived cellulosic ethanol produced in California’s Imperial Valley. Sorghum is a heat- and drought-tolerant C₄ grass (Tonitto & Ricker-Gilbert, 2016) that thrives in the high-irradiance environment and long seasons afforded by the Imperial Valley’s mild winters (Oikawa et al., 2015b). These conditions can lead to N demands exceeding those of most biofuel crops (Fazio & Monti, 2011; Schmer et al., 2014; Ruan et al., 2016) or of sorghum grown in other parts of the United States (Haankuku et al., 2014; Hao et al., 2014; Bonin et al., 2016). We simulated contrasting N management scenarios for Imperial Valley sorghum as inputs to LCA models for sorghum-derived ethanol fuel (85% ethanol – 15% gasoline, by volume) to determine the potential range of WTW emissions associated with different feedstock production strategies. We hypothesized that increasing N application rate would mitigate environmental impacts on an energy yield basis at low-to-moderate application rates, where yield gains per kg N would be highest, but would amplify impacts at higher application rates as yield gains per kg N decline (Tilman et al., 2002). Alternatively, we hypothesized that increasing yields may be sufficient to compensate for increased emissions from N...
even at high N application rates if WTW emissions are largely derived from non-N sources. Emissions from non-N sources will decline with increasing biomass yields as these emissions are fixed and impacts are assessed on the basis of energy yield, which increases with biomass yield. As N uptake and, subsequently, yield response differ based on N source and application method, we simulated variations in both of these parameters to gain a more comprehensive understanding of nitrogen use efficiency (NUE) dynamics and associated WTW emissions.

We then investigated how substitution of conventional gasoline with sorghum-derived E85 may influence environmental impacts from the fuel sector across all nine impact categories evaluated by the U.S. Environmental Protection Agency (Bare et al., 2003). Previous work suggests that GHG intensity will be reduced for cellulosic fuels, but emissions contributing to air and water pollution may be higher (von Blottnitz & Curran, 2007; Borrion et al., 2012; Diaz-Chavez et al., 2013; da Silva et al., 2014; Mbonimpa et al., 2016; Robledo-Abad et al., 2016; Weldu & Assefa, 2016). Quantifying WTW impacts across N management scenarios and across fuel sources will identify opportunities for mitigation of adverse impacts and highlight environmental trade-offs associated with the increased use of biofuels.

Materials and methods

Three major phases of data collection and analysis were undertaken to address our objectives (Fig. 1). We used a field trial to provide data for parameterization of a crop model, which was used to simulate biomass outputs under a range of N management scenarios. Crop model outputs were used as LCA inputs for E85 fuel life cycles. A separate LCA of conventional gasoline was constructed as a reference scenario.

Field trial

Field data from in 2012 and 2014 were obtained from a 5.3-ha plot at the University of California’s Desert Research Extension Center in Holtville, Imperial Valley, CA (32°N 48′26″, 115°W 26′37.5″). The 2013 season was sacrificed to eliminate an infestation of barnyard grass (Echinochloa colona). The Imperial Valley is characterized as a high-irradiance, arid environment with hot summers, mild winters, and infrequent rainfall (Oikawa et al., 2015b). Irrigation has allowed the Imperial Valley to become a major food and feed producing region in the United States (CDFA 2015). This region is also poised to become hub for bioenergy production, with plans to build the state’s first cellulosic ethanol facility there to help meet the competitive renewable energy goals set by the state of California (CEC & CARB 2007).

Our Imperial Valley field site had deep alluvial soil, characterized as mildly alkaline, deep silty clay (pH 8.1; 42% clay, 41% silt, 16% sand). Field operations were logged by

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**Fig. 1** Major phases of data collection and analysis and their respective inputs and outputs. Outputs from the field trial were inputs to the crop model (DSSAT), and outputs from the crop model were inputs to the life cycle inventories (SimaPro). Lopez et al. (2017) provided crop coefficients and historical weather data were obtained from CIMIS. Management scenarios varied N application rate (N$_R$), N application method (N$_M$), and N source (N$_S$). Downstream emissions were determined using IPCC, EEA, Okawa, EPA, SALCA-P, AgDrift, SAEFL, EMEP, and GREET emission models.

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field managers and confirmed during frequent site visits. Following an eight-month fallow period, the soil was tilled and laser leveled on January 14, 2012. Soil nutrient analysis from spatially replicated soil samples taken January 30, 2012, showed high initial soil N levels, 186 kg N ha⁻¹. A preplant fertilizer regime of 90 kg P₂O₅ ha⁻¹ and 110 kg N ha⁻¹ as urea was implemented on February 10, 2012. On 28 February, *Sorghum bicolor* (cv. photoperiod LS, Scott Seed, Inc., Hereford, TX, US) was planted at a density of 9 individuals m⁻² on 76 cm beds. We applied supplemental N at the beginning of each growth cycle (80 kg N ha⁻¹ on 2 March, 90 kg N ha⁻¹ on 18 June, and 105 kg N ha⁻¹ on August 16, 2012) as either urea or urea ammonium nitrate (UAN). Irrigation was gravity fed via furrow flooding with scheduling based on plant need as assessed by field managers or when soil volumetric water content fell below 0.10 cm³ cm⁻³. Pesticide applications of chlorpyrifos and bromoxynil were applied on March 27, and April 30, 2012, respectively. Aboveground crop biomass was harvested three times throughout the 2012 growing season (4 June, 14 August, and 12 November) resulting in a total annual yield of 54.6 Mg dry weight (DW) ha⁻¹ (Table 1). Eddy covariance measurements were used to assess net ecosystem exchange (NEE) throughout the growing season (Oikawa et al., 2015b).

In 2014, a preplant herbicide regime of glyphosate, s-metolachlor, and atrazine was applied shortly after the field was cultivated and leveled. These efforts to reduce weed pressures delayed planting in 2014 to 4 April, allowing only two growth cycles in that year (Table 1). Four applications of urea at 90 kg N ha⁻¹ were applied throughout the 2014 growing season, including one preplant application on 25 March, two supplemental applications during the first growth cycle (14 May and 4 June), and a third supplemental application following resprouting on 18 July. Eddy covariance measurements were again recorded throughout the growing season; however, instrument failure resulted in large gaps in our 2014 NEE flux data. Thus, 2012 field data were the primary dataset used to parameterize our crop model and served as the basis for our sorghum management scenarios.

**Table 1** Agreement between modeled dry weight yields and actual dry weight yields expressed as percent difference (PD) for 2012 and 2014

| Period | Field (Mg DW ha⁻¹) | Modeled (Mg DW ha⁻¹) | Agreement (PD) |
|--------|-------------------|----------------------|----------------|
| 2012   |                   |                      |                |
| Harvest 1 | 18.363          | 18.369              | 0.03%          |
| Harvest 2 | 19.562          | 19.833              | 1.38%          |
| Harvest 3 | 16.437          | 15.874              | -3.48%         |
| Annual  | 54.635           | 54.076              | -1.03%         |
| 2014   |                   |                      |                |
| Harvest 1 | 11.584           | 11.638              | 0.47%          |
| Harvest 2 | 14.107           | 12.429              | -12.65%        |
| Annual  | 25.691           | 24.067              | -6.53%         |

**Crop modeling: parameters and adjustments**

We used 2012 field data to parameterize the Crop Environment Resource Synthesis (CERES) model for grain sorghum in DSSAT (Decision Support System for Agrotechnology Transfer v.4.5, Georgia USA; Fig. 1). DSSAT is a process-based crop modeling system that simulates soil processes, weather, and crop growth, allowing investigation of a multitude of growing conditions and management choices (Jones et al., 2003). We first constructed an *in silico* soil profile representative of our field conditions, gap-filled where necessary with DSSAT’s default soil profile for deep silty clay (Table S2). Historic (30 year) weather data for the site were compiled from nearby meteorological stations accessed through the California Irrigation Management Information System (CIMIS; Table S2 and accompanying text). Management activities simulated logged field practices in 2012.

Parameterization of the grain sorghum model to simulate our forage sorghum crop entailed several steps. We adjusted allocation to vegetative growth based on published parameter adjustments for sweet sorghum (Lopez et al., 2017). Sensitivity analyses were then used to adjust phenological parameters. We used cumulative net primary productivity (NPP) curves from eddy covariance data and field observations of phenological transitions in our parameterization (Figs S1 and S2 with details in accompanying text). Lastly, we increased the radiation use efficiency to better simulate yield outputs observed in the field (Table 1 and Fig. S1). We then modeled the 2014 growing season according to reported management practices for that year. Although eddy covariance data from 2014 were insufficient for cultivar calibration purposes, our production model for 2014 also showed reasonably good fit in terms of phenology and yield (Table 1, Fig. S2b).

Although a multiyear dataset is favorable for cultivar calibration, we used multiple growth cycles (three in 2012 and two in 2014) to compensate for the limited duration of our field experiments. Importantly, as DSSAT does not simulate resprouting postharvest, each growth cycle was modeled as a distinct planting event. We eliminated the first 14 days post-planting for secondary and tertiary growth cycles to better simulate aboveground growth following resprouting, but the model may inadequately simulate root dynamics and consequently underestimate N and water uptake. The extensive parameter adjustments required to simulate a forage sorghum would benefit from future field trials to validate the model. Our model relies on several assumptions that were not thoroughly validated. Results should be interpreted accordingly. However, the model remains a useful tool for exploring the impacts of N management on WTW environmental impacts.

**Crop modeling: scenario analyses**

We simulated 25 management scenarios varying N fertilizer application rate, application method, and source to investigate productivity and NUE dynamics (Fig. 2). In all scenarios, irrigation was simulated as furrow flooding, applied such that water was nonlimiting. Our simulated values for N application rate were based on optimal rates reported in the literature for...
rates for the secondary and tertiary growth cycles, respectively. We explored a range of 50 increments of 100 kg N ha⁻¹, and simulated applications are either broadcast without incorporation or injected at 8 cm depth. Two fertilizer types were simulated as broadcast fertilizer treatments (urea and ammonium nitrate), and three were simulated as injected (urea, anhydrous ammonia, and urea ammonium nitrate solution).

Fig. 2 Nitrogen management scenarios imposed in the DSSAT model. We varied fertilizer rate from 50 to 450 kg N ha⁻¹ in increments of 100 kg N ha⁻¹, and simulated applications are either broadcast without incorporation or injected at 8 cm depth. Two fertilizer types were simulated as broadcast fertilizer treatments (urea and ammonium nitrate), and three were simulated as injected (urea, anhydrous ammonia, and urea ammonium nitrate solution).

Management scenarios were simulated over a 30-year period using historical weather data (1983–2012) to introduce environmental variation (Table S3 and accompanying text). For all simulations, initial soil N was set to 68 kg N ha⁻¹ for the first growth cycle, a rate typical of US sorghum fields (Hao et al., 2014). Simulated residual N following the first and second harvests for each fertilizer scenario was used as initial N levels for the secondary and tertiary growth cycles, respectively.

Life cycle assessment modeling: scope and system boundaries

Life cycle inventories (LCI) were constructed using SimaPro v.8 (Pré Consultants 2013) in compliance with ISO 14040 and 14044 standards (ISO 2006a,b). We chose a well-to-wheel (WTW) scope and 1 MJ combusted energy from E₈₅ as the functional unit. An energy yield basis was selected as it allows direct comparison across energy sources (Borrion et al., 2012). Importantly, expressing emissions on an energy yield basis is most useful for assessing regional to global scale impacts and may obscure some local impacts. With the exception of select data originating from the Ecoinvent database (Wernet et al., 2016) within SimaPro v.8, we used second-order system boundaries throughout our analyses, considering all relevant material, energy, and waste flows except those of embodied energy associated with facilities and machinery (Fig. 3). The life cycle consisted of six subprocess modules: feedstock production, transportation of biomass from the farm to the conversion facility, conversion of biomass to ethanol, transportation of ethanol from the conversion facility to the refinery, blending and pumping of E₈₅ fuel, and, finally, combustion.

E₈₅ life cycle inventories: upstream flows

Chemical inventories associated with resource inputs were selected from the Ecoinvent database within SimaPro using US regional unit process data when available and European unit process data otherwise. Feedstock production considered inputs of seed, fertilizers, pesticides, and diesel fuel combusted during field operations. Pesticides were accounted for by their active ingredients. Fuel inputs were estimated for field operations reported in 2012 management logs using average fuel requirement data (Hanna, 2005). Field operations reported for 2012 were fairly consistent with typical on-farm operations, operations reported in the literature, and recommendations of university extension programs (Miller & Stroup, 2004; Haankuku et al., 2014; Hao et al., 2014; Bonin et al., 2016). For biomass and ethanol transport processes, we assumed a transport distance of 80 km (Grift et al., 2012) by truck. Refinery processes for E₈₅ fuel assumed a blend of 81% ethanol and 19% distilled petroleum, by weight, and 0.86e⁻³ kWh kg E₈₅⁻¹ electricity for pumping (Hsu et al., 2010).

Chemical inputs to the conversion process were based on near-term means of Monte Carlo simulations (Spatari et al., 2010). We assumed a relatively high conversion efficiency of 340 L ethanol Mg DW⁻¹ under dilute acid pretreatment based on a switchgrass conversion LCI model (Spatari et al., 2010) assuming NREL technology using simultaneous saccharification and cofermentation conversion processes and organic Rankine cycle energy recovery processes. The organic Rankine cycle uses excess heat from upstream reactions to vaporize organic fluids generated during the conversion process. These high-entropy, vaporized fluids are then passed through a turbine, generating electricity. The organic vapors can then be condensed back to a liquid phase and the cycle can be renewed, minimizing heat waste and maximizing electricity recovery (Laser et al., 2009; Bronnicki, 2016). This results in coproduction of electricity during cellulosic ethanol conversion.
Emissions from feedstock conversion are largely dependent on how coproducts, such as electricity, are allocated in the fuel life cycle (Pimentel & Patzek, 2005; Kaufman et al., 2010; Singh et al., 2010; Kendall & Yuan, 2013; Murphy & Kendall, 2015). We allocated electricity generated during conversion using system expansion (i.e. displacement) as ISO 14044 standards explicitly support this method (ISO 2006b). Electricity coproducts were parameterized to the United States Western Grid. Electricity generation corresponding to our biomass to ethanol conversion rate was previously determined to be 0.70 kWh/L ethanol\textsuperscript{1} (Spatari et al., 2010).

Emissions from feedstock conversion are also influenced by the assumed biomass to ethanol conversion efficiency (McKone et al., 2011; Borrion et al., 2012; Kendall & Yuan, 2013). As commercial production of cellulosic ethanol is limited, published conversion efficiencies remain uncertain (Fargione et al., 2010). Given that commercial investment would only be possible with a high ethanol yield, we assumed a conversion efficiency of 340 L ethanol Mg DW\textsuperscript{1}. Assuming a high-efficiency conversion rate also provides a more liberal estimation of conversion-induced GHG emissions. Low-efficiency conversion generates lower ethanol yields but higher electricity yields (Spatari et al., 2010). Under system expansion, displaced GHG emissions from electricity coproduction are often greater than emissions induced by cellulosic ethanol conversion processes (Pimentel & Patzek, 2005; Spatari et al., 2010). Therefore, favoring more efficient ethanol production lowers the electricity coproduct credit and, as a result, increases GHG emissions compared to less efficient conversion rates. Conversely, higher biomass demands under low-efficiency conversion required to generate the same energy outputs as high-efficiency conversion systems may inflate emissions associated with feedstock production. To evaluate the influence of conversion efficiency on overall WTW emissions and WTW emissions across N management scenarios, we constructed additional LCAs assuming a low conversion efficiency (Fig. S4 and accompanying text).

E\textsubscript{85} life cycle inventories: downstream flows

Downstream emissions were modeled for fertilizer, pesticide, and fuel inputs in all applicable life cycle subprocesses (Table 2). Importantly, while DSSAT models nitrogen cycling and associated N loss pathways, these outputs reflect the summed emissions of multiple N species and were therefore
Table 2 Downstream emissions modeled for fertilizer, pesticides, and fuel combustion

| Input          | Emission                                    | Model                     | Source                     |
|----------------|----------------------------------------------|---------------------------|---------------------------|
| Fertilizer     | N₂O*, CO₂†                                   | IPCC tier 1               | De Klein et al. (2006)    |
|                | NOₓ                                          | EEA tier 1                | Hutchings et al. (2016)   |
|                | NH₃                                          | Oikawa‡                   | Oikawa et al. (2015a)     |
|                | PO₄                                          | EPA tier 2                | Battye et al. (1994)      |
|                |                                              | SALCA-P                   | Prasuhn (2006)            |
| Pesticides     | MCPA, broxymil, chlorpyrifos                 | AgDRIFT tier 1 terrestrial§| Teske et al. (2002)       |
| Diesel and      | CO₂, CH₄, N₂O                               | IPCC tier 1               | Waldron et al. (2006)     |
| gasoline       |                                              | SAEFL tier 1              | SAEFL, (2000)             |
| E₈₅ fuel       | CO₂, CH₄, N₂O, VOCs, CO, NOₓ, SOₓ,           | EMEP tier 1               | Winther et al. (2016)     |
|                | black carbon, organic carbon, particulates    | GREET 2015§               | Burnham et al. (2006)     |

*Includes direct and indirect N₂O emissions.
†CO₂ emission model only applicable when N source is urea.
‡The Oikawa model was empirically derived based on NOx flux measurements from our field site and was used as an alternative to the generalized EEA model to calculate NOx emissions for urea and UAN fertilizer scenarios.
§AgDRIFT®; Air Resources Laboratory/NOAA, Research Triangle Park, NC, USA for pesticide deposition assuming fine particle size of applied pesticides, low boom application, and a 15.25-m buffer strip.
¶GREET 2015 ©; Argonne National Laboratory, Argonne, IL USA for a flexible fuel vehicle with AR4 global warming potential values (Forster et al., 2007), which are in alignment with the upstream values used for fuel production.

Gasoline life cycle inventory

We also conducted an LCA for conventional gasoline in order to compare its emissions to those from E₈₅ across consistent emission and characterization criteria (Fig. 1). As in our E₈₅ LCAs, this life cycle considered a WTW scope, a functional unit of 1 MJ combusted energy, and second-order system boundaries. We used a US regional unit process inventory of gasoline in the EcoInvent database in SimaPro for emissions related to fuel extraction, processing, and transportation in our gasoline LCI. Electricity required for pumping was assumed to be the same for gasoline as for E₈₅. Emissions from combustion were modeled using published petroleum emission factors (SAEFL 2000; Waldron et al., 2006) from sources consistent with those used in our E₈₅ life cycles (Table 2).

Life cycle impact assessment: characterization

Following the construction of life cycle inventories, emissions were characterized using the Tool for the Reduction and Assessment of Chemical and Other Environmental Impacts (TRACI 2 v. 3.03; Environmental Protection Agency, Washington DC, USA). TRACI characterizes midpoint impacts to the environment and human health (Bare et al., 2003). Midpoint models characterize the impacts of individual chemical compounds along that compound’s cause-and-effect chain but prior to the end point of the chain (Bare et al., 2000; Brilhuis-Meijer, 2014). For instance, if phosphorus is leached into the groundwater, it will eventually enter a body of water and, in doing so, increase the concentration of phosphorus in that water body. This increased concentration of phosphorus is the midpoint of
the cause-and-effect chain of eutrophication. A sufficiently high concentration of phosphorus can cause an algal bloom, which may result in fish die-offs. The loss of fish species would then be an end point of the cause-and-effect chain of eutrophication. While end point impacts are easier to interpret, they also have higher uncertainties (Bare et al., 2000). Further midpoint impact assessments are favorable when considering trade-offs across environmental impact categories as end point impact categories are considerably more broad and may obscure these relationships (Brilhuis-Meijer, 2014).

Nine impact categories are characterized in TRACI based on their relevance for regulatory purposes as appraised by the U.S. Environmental Protection Agency. Environmental impacts considered by TRACI are global warming, ozone depletion, smog, acidification, eutrophication, and ecotoxicity (aquatic and terrestrial). Impacts to human health are assessed in terms of carcinogens, noncarcinogens, and respiratory effects. Equivalent units and midpoint criteria for these impact categories can be found in the supporting information (Table S1). TRACI characterizes emissions contributing to each of these impact categories based on the relative potency of individual chemical compound inventoried in the life cycle in contributing to each impact (Bare et al., 2003).

Results

Crop model outputs

Yield saturation was not observed across the range of N application rates simulated in our crop model. Although yield response to N was consistently positive, the nature of this response varied considerably across fertilizer application methods and, in some instances, fertilizer sources (Fig. 4). Modeled yields from injected fertilizer scenarios varied by <1% across N sources at any given N application rate. However, among broadcast scenarios, yields varied by as much as 130% across N sources, with simulated yields from broadcast ammonium nitrate (AmNi) consistently exceeding those of broadcast urea. Simulated yields in broadcast ammonium nitrate scenarios were more similar to injected scenarios, with <18% difference in yields across the N application rates simulated. Both injected and broadcast ammonium nitrate simulations were characterized by a positive sigmoidal yield response to increasing N inputs (Fig. 4). For instance, simulated yields in injected fertilizer scenarios nearly doubled from 50 to 150 kg N ha\(^{-1}\) but increased by only 15% from 350 to 450 kg N ha\(^{-1}\). Broadcast urea simulations resulted in a weak but linear yield response to applied nitrogen that also declined with increasing N inputs (31% increase from 50 to 150 kg N ha\(^{-1}\) and 12% increase from 350 to 450 kg N ha\(^{-1}\)). This subdued response to nitrogen in broadcast urea scenarios resulted in maximum simulated yields of 21.8 Mg dry weight ha\(^{-1}\). Conversely, maximum simulated yields for broadcast ammonium nitrate and injected fertilizer scenarios were 50.4 and 59.2 Mg DW ha\(^{-1}\), respectively (Fig. 4).

Life cycle assessment: trends in emissions across N management scenarios

At any given N application rate, WTW emissions were always highest in broadcast urea scenarios (Fig. 5). Emissions tended to be lowest in injected fertilizer scenarios. Broadcast ammonium nitrate scenarios had lower emissions contributing to acidification, eutrophication, and ecotoxicity than the average emissions from injected fertilizer treatments. However, when injected scenarios were parsed by N source, only emissions from injected urea scenarios were higher than those from broadcast ammonium nitrate scenarios (Table S4).

Fig. 4  Simulated yield response to N for broadcast urea and ammonium nitrate (AmNi) treatments and injected fertilizer treatments, averaged across fertilizer sources. Error bars for broadcast scenarios depict standard deviation across simulated weather years, while error bars for injected scenarios depict combined standard deviation across weather years and fertilizer types. Model parameters were fit in MATLAB. All relationships had an \(r^2 \geq 0.94\) and \(p \leq 0.02\).
Emissions contributing to human health tended to decline or stabilize with increasing N application rate, regardless of application method or source (Fig. 5). Emissions contributing to the environment showed a more diverse response to increased N application rate. WTW emissions in broadcast urea scenarios almost always increased with increasing N inputs. Conversely, WTW emissions in broadcast ammonium nitrate and injected scenarios tended to decline or stabilize with increasing N application rate. On an energy yield basis, the most emission-conservative scenarios were injected application of anhydrous ammonia at 350 or 450 kg N ha\(^{-1}\), with differences in emissions across these scenarios varying by \(<3\%\) in all cases (Fig. 5 and Table S5). Injected UAN at 350 and 450 kg N ha\(^{-1}\) followed closely behind. Broadcast urea applied at 450 kg N ha\(^{-1}\) resulted in the highest WTW emissions per MJ energy in most impact categories (Fig. 5). Emissions contributing to noncarcinogens, respiratory effects, and ecotoxicity, however, were highest for broadcast urea applied at 50 kg N ha\(^{-1}\).

**Life cycle assessment: emissions contributing to the environment**

The carbon intensity of sorghum-derived E\(_{85}\) fuel ranged from 29 to 44 g CO\(_2\) eq MJ\(^{-1}\) across simulated feedstock production scenarios (Table S5). WTW GHG emissions in broadcast urea scenarios were 3–18% higher than in corresponding broadcast ammonium nitrate scenarios and 7–30% higher than in corresponding injected scenarios (Fig. 5a). GHGs increased by 27% and 8% with increasing N application rate in broadcast urea and ammonium nitrate scenarios, respectively, and varied by \(<5\%\) in injected scenarios. WTW emissions contributing to ozone depletion in broadcast urea scenarios were 5–19% higher than broadcast ammonium nitrate and injected scenarios (Fig. 5b). These emissions were not strongly affected by N application rate at the WTW level, increasing or decreasing by \(<8\%\) across N application rates depending on fertilizer application method and source. Emissions contributing to smog increased by 16% across N application rates in broadcast urea scenarios, varied by \(<3\%\) in ammonium nitrate scenarios, and declined by 9% in injected scenarios before roughly stabilizing at 250 kg N ha\(^{-1}\) (Fig. 5c).

Emissions contributing to acidification tended to increase with increasing N application rate regardless of fertilizer strategy (Fig. 5d). N source, however, was an important determinant of emissions contributing to acidification. These emissions increased by only 6% across N application rates in broadcast ammonium nitrate scenarios, but increased by 93% across the same range in broadcast urea scenarios. Impacts to
acidiﬁcation also varied across N sources in injected scenarios, with emissions increasing by 28% across N application rates for injected urea, decreasing by 8% for injected anhydrous ammonia, and remaining relatively stable across N application rates for UAN (Table S4). WTW emissions contributing to eutrophication were also strongly inﬂuenced by fertilizer source and application method (Fig. 5c). These emissions increased by 25% across N application rates in broadcast urea scenarios and decreased by a similar magnitude in broadcast ammonium nitrate scenarios. Emissions contributing to eutrophication also declined across N application rates in injected scenarios, but the magnitude of this response varied from 17 to 33% across N sources (Table S4). Emissions contributing to ecotoxicity consistently declined with increasing N application rate but were not substantially affected by N source or application method at the WTW level (Fig. 5).

Life cycle assessment: emissions contributing to the human health

Emissions impacting human health almost always declined with increasing N application rate (Fig. 5g–i). The only exception was carcinogenic emissions in broadcast urea scenarios, which were relatively unaffected up to 150 kg N ha\(^{-1}\) and increased by a modest 5% thereafter (Fig. 5g). Carcinogenic emissions declined from 50 to 350 kg N ha\(^{-1}\) by 13% in broadcast ammonium nitrate scenarios and by 18–29% in injected scenarios, but remained relatively stable thereafter. Noncarcinogenic emissions declined by 25%, 43%, and 49% across N application rates in broadcast urea, broadcast ammonium nitrate, and injected scenarios, respectively (Fig. 5h and Table S5). Emissions contributing to respiratory effects for these scenarios declined by 8%, 27%, and 34%, respectively.

Life cycle assessment: localized NO\(_x\) model

The Oikawa NO\(_x\) model for broadcast urea resulted in higher NO\(_x\) emissions than the tier 1 EEA model (Fig. S3). These higher NO\(_x\) emissions translated to a 12–25% increase in emissions contributing to acidification, a 2–15% increase in emissions contributing to eutrophication, and a 7–33% increase in emissions contributing to respiratory effects (Table 3). Emissions contributing to smog were most strongly affected by the assumed NO\(_x\) model, increasing by 17–113% across N application rates.

Life cycle assessment: E\(_{85}\) vs. gasoline

Relative to gasoline, sorghum-derived E\(_{85}\) reduced emissions contributing to global warming by 47–65%, to ecotoxicity by 74–79%, to carcinogenics by 92–96%, and to noncarcinogenics by 97–98% (Fig. 6). However, substitution of gasoline with E\(_{85}\) resulted in increased emissions contributing to ozone depletion by 105–132%, to acidification by 18–29%, to eutrophication by 49–141%, and to respiratory effects by 31–114% assuming the EEA NO\(_x\) model. Scenarios assuming the Oikawa NO\(_x\) model resulted in higher emissions contributing to smog, acidification, eutrophication, and respiratory effects. These emissions increased by as much as 333%, 585%, 1634%, and 183%, respectively, for E\(_{85}\) compared to gasoline (Table 3).

Discussion

Fertilizer management during feedstock production affected most pollutant loads from sorghum-derived E\(_{85}\). Increasing N inputs generated higher biomass yields (Fig. 4) but were also a major source of emissions to the environment (Fig. 5). Fertilizer application rate, application method, and source all contributed to emission intensities. Broadcast urea simulations resulted in the highest WTW emissions, with increasing N application rate tending to increase emissions. Conversely, anhydrous ammonia applied at 350–450 kg N ha\(^{-1}\) via injection resulted in the lowest WTW emissions of all scenarios simulated, suggesting the carbon intensity and pollutant loads of cellulosic fuels are not necessarily compromised by high N use at regional to global scales.

### Table 3 Percent increase in modeled WTW emissions and emissions from E\(_{85}\) relative to gasoline assuming the Oikawa NO\(_x\) model for broadcast urea scenarios in place of the EEA tier 1 NO\(_x\) model

| Impact category | N application rate (kg N ha\(^{-1}\)) | Increased WTW emissions (%) | Increased emissions relative to gasoline (%) |
|-----------------|--------------------------------------|----------------------------|---------------------------------------------|
|                 | 50 150 250 350 450                   | 50 150 250 350 450         |
| Acidification   | 12 5 7 14 25                         | 173 274 370 469 585        |
| Resp. effects   | 7 4 8 17 33                         | 146 128 133 150 183        |
| Eutrophication  | 4 2 4 8 15                          | 1133 1211 1330 1464 1634   |
| Smog            | 28 17 28 60 113                      | 125 115 146 216 333        |

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Sorghum-derived cellulosic ethanol had clear advantages over gasoline in terms of GHG intensity and several other impact categories. Emissions contributing to air and water pollution, however, tended to be substantially higher for E85 than for gasoline and were often heavily influenced by feedstock management (Fig. 6). Together, our results suggest that N management choices strongly influence life cycle trade-offs between the productivity, GHG intensity, and pollutant loads of cellulosic fuels, particularly in terms of local air and water pollution. Minimizing on-farm emissions through efficient N management should be a priority area for future field research.

**WTW emissions from E85: N application rate**

Across all impact categories, increasing N contributed to increasing emissions in absolute terms. However, assessed on an energy yield basis (MJ$^{-1}$) at the WTW scope, higher yields associated with increasing N inputs downscale these additional emissions from N. Higher yields associated with increasing N inputs also downscale emissions from non-N sources incurred during feedstock production (e.g. phosphorus, fuel) on an energy yield basis, as lesser quantities of these non-N inputs were required to generate a similar volume of E85 when N inputs were increased. Therefore, WTW impacts expressed on an energy yield basis only intensified with increasing N rate when the increase in emissions associated with additional N exceeded the decrease in emissions resulting from the corresponding yield response. Inefficient N uptake in broadcast urea simulations resulted in a modest yield response. As a result, corresponding WTW emissions tended to worsen with increasing N inputs (Figs 4 and 5). Conversely, in broadcast ammonium nitrate and injected fertilizer scenarios, simulated yield increases tended to outweigh modeled emission increases on an energy yield basis at N application rates as high as 350–450 kg N ha$^{-1}$. Our hypothesis that increasing N inputs would reduce emissions at modest fertilizer rates and increase them at higher N rates was, therefore, largely not supported by our simulations even when N constituted a major source of emissions. Emissions to several impact categories roughly stabilized at 250–350 kg N ha$^{-1}$ in injected and broadcast ammonium nitrate scenarios, increasing or decreasing by no more than 2% at 450 kg N ha$^{-1}$. This suggests that higher N application rates, which would elicit an increasingly marginal yield response, would eventually generate higher WTW emissions. However, limited field validation precludes determination of an optimal N value for Imperial Valley sorghum.

Importantly, while expressing emissions on an energy yield basis is appropriate for assessing regional to
global impacts, it can obscure impacts at the local level. In the present study, where emissions are most intensive during feedstock production, local impacts may be better characterized on a land area basis. If higher yields achieved with increasing N are not concurrent with a commensurate reduction in hectares planted, these local impacts will be intensified as N inputs increase, regardless of productivity.

**WTW emissions from E85: N application method and source**

Our analysis revealed lower emissions and higher yields with injection of N fertilizers, a win-win for both productivity and sustainability. Low NUE in broadcast urea simulations resulted in higher emissions across the board, although some impact categories were more strongly affected than others. Previous research has shown surface applications of urea result in high volatilization and denitrification losses that curtail N uptake (Linquist et al., 2012; Millar et al., 2014). Ammonium nitrate is less susceptible than urea to volatile losses during surface application, but still less efficient than injected fertilizer applications, which concentrate nutrients in the root zone (Millar et al., 2014). These differences in N accessibility and loss rates were observed across fertilizer sources and application methods in our crop model and the influence of these factors on simulated N uptake were reflected in WTW life cycles based on their yield implications (Fig. 4). However, downstream emission models largely did not account for these factors. Consequently, WTW emissions from broadcast urea scenarios presented here may be underestimated while emissions from injected scenarios may be overestimated. Our results may be similarly skewed by our model’s inability to capture the root maturation across growth cycles. In broadcast urea scenarios, where N loss primarily occurs through volatilization and uptake occurs in shallow soil layers, inadequate root development may not strongly inhibit N uptake. Uptake similarly occurs in shallow soil layers when ammonium nitrate is broadcast without incorporation. However, in injected scenarios, where N loss primarily occurs through leaching and uptake occurs at ≥8 cm depth, our model may underestimate N uptake and, consequently, NUE. Underestimation of NUE would result in overestimation of WTW emissions. Thus, the advantages of injected N fertilizers discussed here may be understated.

In injected scenarios, N source had virtually no impact on yield in our simulations, but did appear to influence emissions from several impact categories. Differences in emissions contributing to acidification, eutrophication, and carcinogenics were the most prominent (Table S4) and were all associated with source-specific emission factors for NH₃ volatilization, which are highest for urea (Battye et al., 1994). However, while these emissions factors consider N source, they do not consider N application method. Accordingly, modeled NH₃ volatilization rates for urea were the same for broadcast and injected scenarios and, as a consequence, almost certainly overestimate NH₃ emissions from injected urea (Mahler, 2001; Millar et al., 2014). Similarly, although volatilization rates for anhydrous ammonia and UAN were relatively low, these emissions may also be overestimated if emission factors assumed an unincorporated application method. Differences in emissions from injected scenarios across fertilizer sources should therefore be interpreted with caution. Along these lines, we stress the need for more refined emission factors to improve the ability to model emission outcomes associated with different fertilizer sources and application methods.

**WTW emissions from E85: GHG intensity**

The GHG intensity of sorghum-derived E85 varied by as much as 33% across N management scenarios (Fig. 5a, Table S5). Greenhouse gas emissions were roughly divided between emissions from feedstock production and postfeedstock production processes, which mitigated the impacts of nitrogen management on overall GHG intensity. Low NUE in broadcast urea simulations resulted in a weak yield response that was not sufficient to compensate for increased N₂O emissions (Figs 4 and 5a). Conversely, increased N₂O emissions from N fertilizer were largely compensated for by increased yields in injected scenarios and, to a lesser extent, in broadcast ammonium nitrate scenarios. These results contrast with recent assertions that increased N application rate compromises the GHG mitigation benefits of cellulosic fuels (Ruan et al., 2016). Although GHGs increased with N in broadcast urea scenarios, they were minimally affected by N application rate in broadcast ammonium nitrate scenarios and tended to decline slightly with increasing N application rate in injected scenarios, at least when expressed on an energy yield basis. Our results instead suggest that the effect of N on the GHG intensity of cellulosic fuels hinges on both NUE at baseline N application rates and on the degree of change in NUE as N rate increases.

Greenhouse gas emissions from N fertilizer are dominated by N₂O emissions (Adler et al., 2007; Fazio & Monti, 2011; Shcherbak et al., 2014; Ruan et al., 2016). We modeled these emissions using a tier 1 IPCC model, which, while useful for benchmarking and comparing with other research, is known to have high uncertainty (De Klein et al., 2006; Singh et al., 2010; Wang et al.,...
This model is largely based on applied N and does not distinguish between synthetic N sources, fertilizer application method, or soil properties. Given these unresolved limitations, \( \text{N}_2\text{O} \) emissions reported here may be underestimated in broadcast urea scenarios and overestimated in injected fertilizer scenarios. Although a growing body of research suggests an exponential relationship between N application rate and \( \text{N}_2\text{O} \) emissions (Hoben et al., 2011; McSwiney & Robertson, 2005; Ruan et al., 2016; Shcherbak et al., 2014; Liang, Grantz, & Jenerette, 2016) as opposed to the IPCC’s linear relationship, the assumptions of existing exponential \( \text{N}_2\text{O} \) models do not align with the observed and simulated dynamics in our system. These models assume N application rates exceeding \(-100\) kg N ha\(^{-1}\) are saturating (McSwiney & Robertson, 2005; Hoben et al., 2011; Shcherbak et al., 2014), which our field data and crop model suggest is inaccurate for Imperial Valley sorghum production. Therefore, these models may vastly overestimate emissions in our system. Further, differences in NUE across broadcast and injected treatments would likely result in different exponential responses not currently accounted for by existing exponential models. Increasing refinement of these \( \text{N}_2\text{O} \) models is an important area for future research.

**WTW emissions from E\(_{\text{E85}}\): air and water pollutant loads**

Emissions contributing to ozone depletion and ecotoxicity were largely derived from postfeedstock production processes in the \( E_{\text{E85}} \) life cycle and therefore not strongly affected by N management during feedstock production (Fig. 5b, f). Nonetheless, injected and broadcast ammonium nitrate scenarios retained slight advantages over broadcast urea scenarios. Emissions contributing to smog also tended to be dominated by postfeedstock production emissions and showed a similarly muted response to N management (Fig. 5c). However, while these emissions were only modestly affected using the EEA tier 1 emission model for \( \text{NO}_x \), emissions from broadcast urea scenarios more than doubled from 50 to 450 kg N ha\(^{-1}\) when we applied the Oikawa \( \text{NO}_x \) model (Fig. 6). As this model was derived from \( \text{NO}_x \) fluxes measured at our Imperial Valley field site following broadcast application of urea (Fig. S3), these amplified \( \text{NO}_x \) emissions are likely more accurate for our system. Unfortunately, the Oikawa \( \text{NO}_x \) model was not parameterized for broadcast ammonium nitrate or injected fertilizer applications, which remains a needed research direction.

The remaining impact categories were at least partially dominated by emissions from feedstock production. Emissions contributing to acidification, eutrophication, and carcinogenics were the most variable across N management scenarios as they were highly sensitive to nitrogen, and, subsequently, NUE (Fig. 5d, e, g). In N-inefficient broadcast urea scenarios, N was an important source of emissions. Conversely, in N-efficient broadcast ammonium nitrate and injected scenarios, emissions were predominantly from non-N sources, allowing a decline in energy yield-scaled emissions across N rates corresponding to higher simulated biomass yields. Emissions contributing to noncarcinogenics and respiratory effects were also largely derived from non-N sources and, therefore declined with increasing N across all scenarios (Fig. 5h, i).

**WTW environmental impacts across fuel sources**

GHG estimates from our LCA of gasoline were roughly 7% lower than those reported from other sources (Table S5) (Sheehan et al., 2000; CARB 2009); likely due to a difference in assumed emissions factors. Even against these conservative estimates, the carbon intensity of sorghum-derived cellulosic ethanol was, on average, less than half that of gasoline on the basis of WTW GHG emissions (34 and 84–95 g CO\(_2\) eq MJ\(^{-1}\), respectively) (Table S5). However, when evaluated across multiple impact categories, trade-offs were evident (Fig. 6). Adverse impacts to local air and water quality tended to be more severe and more variable across management scenarios than beneficial impacts to global warming, human health, and ecotoxicity. These results highlight the importance of feedstock management in determining the environmental impacts of cellulosic fuels. Notably, the potential for adverse impacts to smog was strongly influenced by our choice of \( \text{NO}_x \) model (Fig. 6). Other emission potentials may similarly be influenced by model specificity, again highlighting the importance of developing management-specific regional emission factors.

Our results are generally in agreement with those of previous studies considering non-GHG emissions. Emissions contributing to acidification and eutrophication in our model increased by several orders of magnitude for \( E_{\text{E85}} \) relative to gasoline, which is more or less in agreement with previously reported estimates for cellulosic ethanol-based fuels (von Bliotzitz & Curran, 2007; Bai et al., 2010; Borrion et al., 2012; Jeswani et al., 2015; Mboninima et al., 2016; Robledo-Abad et al., 2016; Wandel & Assefa, 2016). Importantly, emissions contributing to eutrophication may be overestimated in our model, as the SALCA-P model for phosphorus leaching does not account for low percolation rates typical of heavy clay soils found in the Imperial Valley (Prasuhn, 2006). Still, emissions derived from N and postfeedstock production practices comprise ≥50% of emissions contributing to eutrophication, suggesting eutrophication potential
would be substantially higher for sorghum-derived E85 than gasoline even in the event that no phosphorus was leached during production.

Emissions contributing to human toxicity have also been previously reported to be higher for cellulosic fuels than gasoline (von Blottnitz & Curran, 2007; Jeswani et al., 2015; Mbonimpa et al., 2016; Robledo-Abad et al., 2016; Weldu & Assefa, 2016). Although human toxicity is not specifically characterized in TRACI, several impacts to human health are. Our results show higher contributions to respiratory effects for cellulosic ethanol, but lower carcinogenic and noncarcinogenic emissions. Importantly, higher emissions contributing to smog and respiratory effects for E85 relative to gasoline may present an important trade-off for bioenergy production in the Imperial Valley, where air quality is already greatly compromised (ALA 2016). Declining local air quality may increase incidence of asthma and has been linked to increased mortality in other biofuel-producing regions (Tsao et al., 2011; Ashworth et al., 2013). While our study shows a potential reduction in emissions contributing to air and water pollution with increasing injected N inputs on an energy yield basis, recognizing that emissions will increase with increasing N inputs on a land area basis is important and may exacerbate these adverse local impacts.

Although water use impacts and land use change were not considered in this study, other studies have shown they can pose additional trade-offs for bioenergy sources (Bonsch et al., 2016). For instance, in California, water use for bioenergy can be 100–1000% higher than for gasoline (Fingerman et al., 2010) and land use impacts have been estimated to contribute an additional 10–340 g CO2 MJ−1 to bioenergy lifecycles (Plevin et al., 2010). Development and widespread implementation of standardized metrics for water and land use impacts is necessary to further evaluate these trade-offs across feedstocks and fuel technologies.

Synthesis

Coupled crop-LCA modeling systems are a useful tool for exploring multiple dimensions of the biofuel life cycle and highlighting possible pathways for emission reductions and paving the way for future field studies. When compared to gasoline, sorghum-derived cellulosic ethanol was advantageous in terms of GHG emissions and, generally, impacts to human health, but resulted in substantially higher local air and water pollutant loads. It is important to recognize the environmental trade-offs associated with alternative fuels so that adverse impacts can be avoided, or at least mitigated, whenever possible. In agreement with previous work, we found efficient application of N fertilizer to reduce environmental impacts associated with feedstock production on an energy basis (Schmer et al., 2008; Singh et al., 2010). However, we also found that high rates of N can support low GHG intensities and pollutant loads from cellulosic fuels on an energy yield basis, so long as a sufficient yield response is elicited. Meeting demands of mandates for cellulosic ethanol production (CEC & CARB 2007; EPA 2010) necessitates examination of multidimensional life cycle impacts of renewable energy production to more accurately assess their environmental impacts and to avoid solving one pollution problem at the expense of another.

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Supporting Information

Additional Supporting Information may be found online in the supporting information tab for this article:

Figure S1. Cultivar calibration and fit of modeled biomass accumulation.

Figure S2. Modeled and observed phenological transitions.

Figure S3. Cumulative and fertilizer-induced NOx fluxes using the Oikawa NOx model.

Figure S4. Influence of conversion-efficiency assumptions on WTW emissions.

Table S1. Midpoint characterization criteria in TRACI.

Table S2. Soil parameters in the DSSAT model.

Table S3. Aggregation and standardization of historical weather data.

Table S4. WTW emissions from injected nitrogen scenarios, by N source.

Table S5. Well-to-wheel GHG intensities for conventional and alternative fuel sources.