# Uncertainty in the Life Cycle Greenhouse Gas Emissions from U.S. Production of Three Bio-based Polymer Families

## SUPPORTING INFORMATION

*I. Daniel Posen*[*†,‡], *Paulina Jaramillo*[†], *W. Michael Griffin*[†]

Department of Engineering & Public Policy and Department of Civil & Environmental Engineering, Carnegie Mellon University, 5000 Forbes Avenue, Pittsburgh, Pennsylvania 15213.

*Corresponding author phone: (412) 268-2670; fax:(412) 268-3757; e-mail: daniel.posen@gmail.com

[†] Department of Engineering & Public Policy.

[‡] Department of Civil & Environmental Engineering

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# S. Supporting Information

## Contents

# S.1 Model and Data

## *S.1.1 Fossil polymer model*

As described in the main text, production of fossil polymers is modeled using data from a 2011 report for the American Chemistry Council (ACC), prepared by Franklin Associates [1]. Energy requirements and direct process emissions are reported as industry averages for each unit process. These point estimates are supplemented with full distributions previously developed by our research group for crude oil extraction and processing [2], as well as natural gas extraction and processing, along with ethane and naphtha steam cracking (for the production of olefins and pygas) [3]. Due to confidentiality requirements, the Franklin Associates report [1] suppresses details for the production of ethylene glycol, and so we model the energy demands for this step using the Ecoinvent database [4]. For several unit processes, the Franklin Associates [1] include a category for 'recovered energy.' This represents exported steam, which we assumed displaces natural gas (accounting for natural gas boiler efficiency, as per section S.1.12). In the production of benzene for PS, a portion of the feedstock is burned for energy, which Franklin Associates [1] list as a mass quantity of "internal offgas." For simplicity, we treat the direct emissions from internal offgas as methane (2.75 kg $CO_2$/kg offgas). Upstream emissions (from natural gas extraction and processing, or crude oil extraction and refining) are also accounted for on a mass basis. These internal offgas emissions are small relative to the total emissions for PS. Steam cracking is the only other process to include internal offgas use, which is accounted for as described in Posen *et al.* (2015) [3]. Table S-1 presents key parameters and distributions used in the fossil polymer model.

### *S.1.2 Land use change (LUC)*

As explained in Posen *et al.* (2015): All bio-based pathways "have the potential to cause emissions through the repurposing of land, either directly or as a consequence of indirect market forces. Such emissions may occur over the course of many years, and while there is no agreed methodology to account for their impact, LUC emissions are potentially critical to the GHG impact of bio-based products" [3]. Argonne National Laboratory's GREET model [5] includes a carbon calculator for land use change (CCLUB) tool. CCLUB models global land changes induced by the U.S. biofuel mandate [6], as predicted by the Global Trade Analysis Project (GTAP) general equilibrium model [7]. The present paper assumes that the contribution of bio-based plastics to land use change will be similar to that of biofuel production (per unit of corn or switchgrass diverted). CCLUB contains various options for modeling carbon emissions resulting from the GTAP predicted land changes.

For the base case, this paper models LUC emissions as a distribution that spans the results of the main CCLUB scenarios. Details on these scenarios can be found in the CCLUB manual [8]. For corn, the updated 2013 modeling scenario is employed. The lower bound (1.8 g $CO_2$e/MJ ethanol) comes from using the following options: CENTURY model with default parameters (annual yield increases, conventional till, 100cm soil depth considered) for domestic emissions, and the Woods Hole model for international emissions. The upper bound (15 g $CO_2$e/MJ ethanol) results from using the Winrock model for both domestic and international emissions. For switchgrass, the lower bound (-3.8 g $CO_2$e/MJ ethanol) also results from using the CENTURY model (with default parameters) for domestic emissions and the Woods Hole model for international emissions. The upper bound (31 g $CO_2$e/MJ ethanol) comes from using Woods

Hole for domestic emissions and either model (Winrock or Woods Hole) for international emissions. Using Winrock for domestic emissions would produce an even higher emissions result (94 g $CO_2$e/MJ ethanol). This estimate is excluded as it is inconsistent with other existing estimates for cellulosic crops [9], and appears to be a result of low resolution in the domestic (U.S.) model, which treats all agriculture the same, failing to account for the soil carbon sequestering properties of deep rooted systems like switchgrass [10]. Emissions per MJ ethanol are converted to emissions per kg feedstock using the ethanol yield assumed in GREET (2.79 gal/bu for corn and 80 gal / dry ton for switchgrass). Further discussion of LUC modeling choices is available in sections S.2.6 and S.2.7.

### *S.1.3 Agricultural operations*

*Corn*

The U.S. Department of Agriculture (USDA) releases periodic statistics on the amounts of fertilizer used for corn production, by state and by type (nitrogen, phosphate (as $P_2O_5$), and potash (as $K_2O$)) [11]. Using 2014 data, total fertilizer application of each type is divided by total corn production in each state for the same year [11]. The resulting estimates for each state are then weighted by that state's share of national corn production, and fitted to a continuous distribution representing the uncertainty/variability for national fertilizer use intensity. Applications of other agrochemicals ($CaCO_3$, herbicides and insecticides), and emissions from feedstock transportation are taken from GREET [5].

The amount of nitrogen in crop residue (above and below ground biomass) is calculated following the Intergovernmental Panel on Climate Change (IPCC) Guidelines for National Greenhouse Gas Inventories [12]. Using equation 11.6 of the IPCC guidelines, $Area_{(T)}$ is set to 1, $Areaburnt_{(T)}$ to 0, $Frac_{Renew(T)}$ to 1, $AG_{DM(T)}$ is fitted to a triangular distribution using table 11.2 (min: $Crop_{(T)}/1000*0.999 + 0.494$, mode: $Crop_{(T)}/1000*1.03+0.61$, max: $Crop_{(T)}/1000+0.726$), and $R_{BG\text{-}bio}$ is also fitted to a triangular distribution using table 11.2 (min: 0.163, mode: 0.22, max:0.277). For an explanation of these equations and parameters, the reader is directed to the source document [12]. $Crop_{(T)}$ represents annual crop yield in kg dry matter / ha, and is calculated as follows. Corn yield for each U.S. state is averaged across 5 years (weighted by corn production in each year), from 2010-2014 inclusive [11]. A continuous distribution is fit across these 5-year averages, weighting each state by its total corn production over the 5-year period. The resulting distribution for nitrogen in crop residue is approximately normal (mean: 9.88, stdev: 0.383) g N / kg dry corn produced.

The USDA recently reported energy use per acre of corn farming, by fuel type, for 2010 corn production [13]. We convert these values to energy use per unit of corn using the distribution for corn yield described above. Energy use is a minor contributor to the life cycle GHG emissions from corn production, and so uncertainty is not characterized further. Table S-2 presents key parameters and distributions used to model corn agriculture.

*Switchgrass*

Switchgrass is not currently grown in large quantities in the U.S., and so this study is based on prospective data. Wullschleger *et al.* (2010) [14] compiled estimates for switchgrass yield from

39 field trials (1190 observations) across the U.S. Using data read off the histogram they provide for the higher yielding lowland switchgrass variety, we find that that the yield data is best fit by a Weibull distribution. The parameters of the distribution are then adjusted to correspond to the mean (12.9 Mg/ha) and standard deviation (5.9 Mg/ha) reported by Wullschleger *et al.* (2010). The distribution is then truncated at the 95% confidence range to eliminate extreme estimates that likely do not correspond to repeatable average yields. There are no concrete guidelines for the application of nitrogen fertilizer. Wullschleger *et al.* (2010) [14] quote a 2005 article calling the issue "unsettled" and suggesting that the range is "not narrowing, nor is a central tendency developing" [15]. As a result, a wide range is appropriate; this study assumes a triangular distribution, loosely fit to the data presented in Wullschleger *et al.* (2010) [14], with mode (100 kg N/ha) set to where the authors indicate "a hint of an optimum" [14]. Using the IPCC Guidelines [16] to calculate nitrogen in crop residue, as above, results in an estimate for $N_2O$ emissions that is far higher than reported by other sources [5, 17, 18]. Thus, we instead use an estimate for above and below ground nitrogen from GREET 2014 (0.54 g nitrogen / kg switchgrass) [5] for the base case, and retain the IPCC-based distribution (mean: 17 g nitrogen / kg switchgrass) only for the sensitivity analysis. Applications of other agrochemicals ($K_2O$, $P_2O_5$, and herbicides), on farm energy use (diesel and electricity), and emissions from feedstock transportation are taken from GREET [5]. Table S-3 presents key parameters and distributions used to model switchgrass agriculture.

*Modeling common to corn and switchgrass pathways*

Emissions for the production of each agrochemical type, and $CO_2$ emissions from limestone ($CaCO_3$ application) are taken from the GREET model [5]. Nitrous oxide ($N_2O$) emissions

resulting from synthetic nitrogen fertilizer application, and from crop residue are estimated using distributions fit to the uncertainty ranges provided by the Intergovernmental Panel on Climate Change (IPCC) Guidelines for National Greenhouse Gas Inventories [12]. The combined effect of the different modes of $N_2O$ production is a mean conversion factor (from N to $N_2O$-N) of 2.2% (with a 90% confidence interval from 1.2%-3.3%) for nitrogen in synthetic fertilizer, and 1.9% (with a 90% confidence interval from 0.94%-3.0%) for nitrogen in crop residue. The means of these distributions are higher than the 'default' factors presented in the IPCC report [12] (1.2% and 1.3% respectively) or in GREET (1.5%) [5]. Sections S.2.6 and S.2.7 present results assuming a lower value of $N_2O$, consistent with IPCC default values. The higher mean employed here, in the baseline model, is a direct result of accounting for uncertainty in the default parameters. Even the upper ends of our resulting distributions are still low compared with top-down estimates of $N_2O$ emissions from agriculture [19]. Table S-4 presents key parameters and distributions related to agrochemicals and field emissions common to both feedstocks.

### *S.1.4 Corn wet milling*

The corn wet milling (CWM) process is used to separate corn grain into various valuable components, including corn starch (for use in PLA and PHB production), corn gluten meal, corn gluten feed, and corn oil. We consult multiple sources to estimate distributions for total process yield and for the mass of each co-product per unit of corn processed [5, 20-23]. Akiyama *et al.* (2003) [20] report yield on the basis of corn oil, corn meal & feed, and glucose. We divide this yield of meal & feed into separate categories of corn gluten meal and corn gluten feed, assuming the ratio between the two is as reported by other sources [21, 22]. We further assume that the glucose weight reported by Akiyama *et al.* is actually on the basis of starch produced (excluding

water added during hydrolysis), since otherwise their process implies a loss rate of over 8% - far higher than other sources indicate. Corn germ meal (which appears only in the Agri-Footprint database [21]) is treated as corn gluten feed. The resulting distributions are presented in Table S-5.

Four data sources are considered for the emissions from the wet milling process [20, 21, 23, 24]. Akiyama *et al.* (2003) [20] provide CWM primary energy use by fuel type (residual oil, natural gas, coal, electricity, others) per kg product, allocated on a mass basis. We convert this to direct energy use per kg corn processed using their assumed total product yield (98.7%) and electricity conversion efficiency (9.42 MJ / kWh), and then apply our own (stochastic) emissions factors for each fuel type. Energy listed as "others" is treated as diesel fuel. The resulting distribution is centered around 0.42 kg $CO_2$e/kg dry corn processed.

Kim and Dale (2008) [24] report CWM steam and electricity requirements (3.5kg steam and 0.7 kWh electricity), along with emissions from chemical inputs (summing to 0.042 kg $CO_2$e), per kg PHB. The authors also present the emissions from corn entering the wet mill (965 g $CO_2$e/kg PHB) and their emissions factor for corn production (219 g $CO_2$e/kg PHB) from which we estimate the total quantity of corn milled to be 4.4 kg corn / kg PHB. This value is used to convert the quantities of inputs to a per kg corn (assumed to be dry corn). Applying our own emissions factors from steam and electricity (Table S-12), and the authors' original estimates for chemical inputs, we arrive at a distribution centered on 0.32 kg $CO_2$e / kg dry corn processed.

Vink *et al*. (2015) [23] report total emissions from their CWM unit process ("dextrose production") to be 0.29 kg $CO_2$e/kg PLA (using mass allocation). They also provide the yield of PLA (10.2 kg PLA/bu corn), which we use to convert CWM emissions to a per kg corn processed basis. The authors do not present their raw data, and so we are unable to harmonize this emissions estimate using our own emissions factor. We do, however, update the global warming potential using the following method. Vink *et al*. (2015) [23] use characterization factors from CML2001 (April 2013 update), which lists methane at 25 g $CO_2$e / g $CH_4$ [25]. In a 2010 paper studying the same PLA production process [26], Vink *et al*. (2010) [26] list raw emissions of methane and $CO_2$ separated by activity type (fuel production, fuel use, transport, process and biomass). We calculate the ratio of $CH_4$ to $CO_2$ from across the fuel production, fuel use, and production process stages ($CH_4$:$CO_2$ = 0.00478:1 on a mass basis). Assuming the same ratio of gases applies to the results from Vink *et al*. (2015) [23], we calculate an multiplicative factor (centered around 1.047) by which to update the authors' GWP estimates for each production stage. This factor is stochastic due to the stochastic GWP characterization factor employed in the present study. The final distribution for CWM is centered on 0.23 kg $CO_2$e / kg dry corn processed.

Finally, the Agri-Footprint database, available in commercial SimaPro software provides emissions estimates for $CO_2$, $CH_4$ and $N_2O$ from wet mill starch production ("Maize starch, from wet milling (starch drying) at plant/US Mass") [21]. Corn farming emissions from the same database ("Maize, at farm/US Mass") are subtracted from the life cycle starch emissions, to obtain emissions unique to the wet mill unit process. The resulting emissions are adjusted for the

total CWM product yield (99.6%, based on the Agri-Footprint database) to obtain a distribution centered on 0.35 kg $CO_2$e / kg dry corn processed.

Since corn wet milling is a relatively mature technology, we assume that the different estimates above represent equivalent processes. Thus, the above estimates are combined into a single uniform distribution. The bounds of the uniform distribution are adjusted dynamically to correspond to the minimum and maximum realizations from the above distributions. Corn starch recovered from the process is assumed to be converted to glucose stoichiometrically (1.11 kg glucose / kg starch). Emissions from enzymes for starch hydrolysis are calculated based on MacLean and Spatari 2009 [27], and add approximately 13 g $CO_2$e / kg glucose. Table S-5 presents key parameters and distributions related to corn wet milling.

### *S.1.5 Corn co-product treatment*

The mass distribution of co-products from corn wet milling and corn dry milling are described in sections S.1.4 and S.1.9, respectively. These are treated alternatively by mass allocation, energy allocation, system expansion, or no allocation (i.e. co-products are ignored). The no-allocation scenario serves as an upper bound for the degree to which increased use of corn products might be responsible for an increase in emissions (i.e. if co-products go unused, or are added to the market without displacing any existing products). For the mass and energy allocation scenarios, upstream emissions (including corn production) are allocated either to starch (wet milling for PLA and PHB production) or directly to ethanol (dry milling, for bioethylene production). The energy contents of corn products are listed in Table S-14.

For the system expansion scenarios, an emissions credit is applied for displacement of existing commodities. Displacement rates are taken from the GREET 2014 model [5]. Corn gluten meal (CGM) is assumed to displace 1.53 kg corn (15.5% moisture) / kg CGM, and 0.023 kg urea / kg CGM. Corn gluten feed (CGF) and corn germ meal are assumed to displace 1 kg corn (15.5% moisture) / kg CGF and 0.015 kg urea/kg CGF. Corn oil is assumed to displace soybean oil at a rate of 1 kg soybean oil / kg corn oil. Distillers dried grains and solubles (DDGS), from dry milling, are assumed to displace 0.78 kg corn (15.5% moister) / kg DDGS, 0.31 kg soybean meal / kg DDGS and 0.023 kg urea/kg DDGS. Emissions from displaced corn are modeled as described in sections S.1.2 and S.1.3 above. Emissions from displaced urea are taken directly from GREET [5]. Emissions for displaced soy oil and soybean meal are based on GREET, but with our own distribution for $N_2O$ emissions from fertilizer and crop residue, as described in section S.1.3. GREET offers a choice of methods for treatment of soy co-products (system expansion, energy allocation, mass allocation, and economic allocation). The choice does not substantially affect the final results, and so we take an average across these models. Additional details are available in Table S-5.

### *S.1.6 Switchgrass pretreatment and saccharification*

The sugars in switchgrass are predominantly in a more recalcitrant form (cellulose) than the sugars in corn grain (starch). As a result, switchgrass must undergo a pretreatment process to activate the cellulose, followed by enzymatic hydrolysis (saccharification) to liberate the sugars. A range of pretreatment technologies have been proposed [28, 29]. Dilute acid pretreatment was

selected for this study based on its near-term potential, and high data availability [5, 17, 27, 30-32]. Emissions from chemical and enzyme inputs are calculated alternately from MacLean and Spatari (2009) [27], and from the GREET 2014 pretreatment module [5, 31]. Data in GREET is presented per ton of sugar; we convert the data to emissions per ton of feedstock input using a value of 0.53 kg sugar / kg dry switchgrass, which we calculate using the values for switchgrass composition and yield of sugars assumed in GREET (tables 1 and 4 of Adom *et al.* 2014 [31]). The resulting estimates are centered on 53 g $CO_2$e/kg dry feedstock (based on MacLean and Spatari (2009) [27]) and 93 g $CO_2$e/kg dry feedstock (based on GREET [5, 31]); the latter is stochastic due to uncertainty in GWP for $CH_4$ and $N_2O$. The present study uses these two estimates as the bounds of a uniform distribution representing emissions from switchgrass pre-treatment and saccharification.

Energy requirements for pretreatment prior to ethanol production are taken into account implicitly, as described in S.1.9. For PLA and PHB production, pretreatment energy is modeled as follows. GREET provides natural gas and electricity requirements for the production of sugar from switchgrass as a stand-alone process (5.4 MJ natural gas/kg sugar and 0.28 MJ electricity / kg sugar, respectively). These are converted to energy requirements per kg switchgrass input as above. Natural gas requirements are converted to direct steam energy, using the 80% efficiency assumed in GREET. The resulting estimates are 0.15 MJ electricity and 2.3 MJ steam. As noted in Adom *et al*. 2014 [31], the process simulations underlying the energy estimates in GREET do not account for heat integration, and should be viewed as an upper bound. To account for the potential benefits of heat integration, a second estimate of energy requirements is derived from Laser *et al.* (2009) [32]. The authors provide base-case steam and power requirements for

feedstock handling and pre-treatment as a percent of the energy in the incoming switchgrass feedstock (6.96% for steam and 0.98% for power). We convert these to energy requirements per unit mass of treated feedstock (1.3 MJ steam / kg switchgrass and 0.18 MJ electricity / kg switchgrass). These estimates are combined with those derived from GREET to arrive at uniform distributions for heat and electricity as presented in Table S-6.

We model emissions from switchgrass pretreatment and saccharification per kg feedstock and then convert to emissions per kg sugar as follow. Switchgrass composition (glucan, xylan, mannan, galactan, arbinan and lignin) is modeled as in Mullins *et al*. (2011) [33]. Mass balance is maintained by allowing the non-sugar, non-lignin portion (%w) of switchgrass to vary in function of the modeled sugar and lignin composition. Yields of sugar from cellulose and hemicellulose are split into 2 scenarios: near-term (lower) and mid-term (higher) yields, as per Spatari and MacLean (2010) [27]. For PLA and PHB, only the mid-term yield model is considered. Table S-6 presents key parameters and distributions related to switchgrass scenarios.

### *S.1.7 PLA fermentation and polymerization*

As discussed in the main text, PLA downstream production steps are split into distinct cases. These cases are described in detail below.

*Case 1*

Case 1 is based on the data provided by Groot and Boren (2010) [34]. The original paper relates to sugarcane-based PLA production in Thailand, but provides insight into chemical and energy

requirements for PLA production regardless of the original sugar source. The authors provide data on farm land allocated to PLA production (2,081 $m^2$/ metric tonne PLA) and sugarcane yield (57 tonnes/ha year), from which we calculate 11.9 tonnes of sugarcane/tonne PLA. Because land use was also partially allocated to molasses, it is necessary to de-allocate before calculating the quantity of sugar this represents. Groot and Boren (2010) assume that each metric ton of sugar is co-produced with 463 kg of molasses [34]. They perform economic allocation based on the 2006 Thai selling prices of sugar and molasses (no citation given), which we retrieve from a USDA report [35]. We calculate the allocation factor for sugar to be 89.6%, from which we calculate 13.2 kg sugarcane / kg PLA (before allocation). Finally, using data on sugar production, as reported by Groot and Boren (2010) [34] (9,653 kg sugarcane / tonne sugar), we estimate sugar input to be 1.37 kg / kg PLA.

For the actual PLA production step, Groot and Boren (2010) [34] provide data on GHG emissions from chemical production and supporting processes (lime, $H_2SO_4$, auxiliary chemicals and waste water treatment), which we use without modification (sum: 0.87 kg $CO_2$e/kg PLA). Using the authors' reported steam emissions (689 kg $CO_2$e/tonne PLA), together with their data source for boiler emissions [36], we estimate primary natural gas use to be between 9 and 10 MJ LHV / kg PLA (represented as a uniform distribution in the present study). To estimate electricity use, we start with emissions, reported by Groot and Boren (2010) [34] as 610 kg $CO_2$e/tonne PLA. Using figure 5 of that study, we estimate a change of 8.6 kg $CO_2$e/tonne PLA, for each 1 kWh change in electricity export per tonne sugarcane. Based on the allocated sugarcane input (11.9 tonne sugarcane/tonne PLA), we extrapolate that the authors' employed an electricity emissions factor of 0.72 kg $CO_2$e/ kWh. From this, we calculate process electricity

requirements to be 846 kWh electricity/tonne PLA. Applying our own emissions factors for electricity and natural gas, we estimate a distribution for PLA production (unit process) centered on 2.3 kg $CO_2$e/kg PLA (for scenarios without internal energy generation from fermentation residues)

*Cases 2-4*

Case 2 is based on data provided by Vink *et al*. (2015) [23]. The authors present data related to the corn wet mill which suggest that 10.2 kg of PLA can be produced from 14.3 kg of starch. Assuming a stoichiometric conversion from starch to sugar, we calculate a required sugar input of 1.6 kg glucose / kg PLA. The study further provides GHG estimates for each of the main production steps: lactic acid production (1.16 kg $CO_2$e / kg PLA), lactide production (0.54 kg $CO2_e$/kg PLA) and polymer production (0.20 kg $CO2_e$/kg PLA). These values are updated to reflect the GWP of methane used in this paper, as described in section S.1.4. The resulting distribution for PLA production (unit process) is centered around 2.0 kg $CO_2$e/kg PLA (for scenarios without internal energy generation from fermentation residues).

Corn Cases 3 and 4 are based on Vink *et al*. (2015) [23] for lactic acid production (as in case 2), together with data from Sakai *et al.* (2004) [37] on energy use for lactic acid polymerization (via a lactide intermediate). Sakai *et al.* (2004) estimate polymerization electricity requirements (1.71 kWh electricity / kg PLA) based on lab-scale data, which is used to parametrize case 3. They argue that their process (which also includes steps upstream of polymerization) could be improved substantially by using steam heat instead of electricity. As a bounding scenario, we model case 4, using the polymerization energy requirements of Sakai *et al.* (2004) [37],

assuming that 100% of the energy is provided by steam heat. Table S-8 presents key parameters and distributions related to PLA production cases.

### *S.1.8 PHB fermentation and recovery*

As discussed in the main text, PHB downstream production steps are split into distinct cases. These cases are described in detail below.

*Case 1*

Case 1 is based on Harding *et al.* (2007) [38]. The study is based on a prior laboratory study, with an observed polymer yield of 0.36 kg PHB/kg substrate. Harding *et al.* (2007) [38] later report sucrose requirements of 1.81 kg/kg PHB, which implies a polymer yield of 0.55 kg PHB / kg sugar. This is substantially higher than the yield from their main data source or from other studies in their literature review, and surpasses the theoretical maximum yield (0.48 kg PHB/kg sugar) discussed in Akiyama *et al.* (2003)[20]. Therefore, in the present study, we assume 0.36 kg PHB / kg sugar, which is in line with the other cases reviewed here.

Harding *et al.* (2007) [38] provide data on steam use (4.89 kg steam / kg PHB), electricity use (3.94 MJ/kg PHB), and natural gas use (2.12 MJ/kg PHB). In addition the authors provide data on hydrogen peroxide and a list of other inputs which together are responsible for 4.6% (0.12 kg $CO_2$e/kg PHB) of their reported process GHG emissions. We apply our own emissions factors for steam, electricity and natural gas, and add the emissions from other inputs to obtain a distribution centered on 2.3 kg $CO_2$e/kg PHB (for scenarios without internal energy generation from fermentation residues).

*Case 2*

Case 2 is based on case 10 presented in Akiyama *et al.* (2003) [20]. The authors report primary energy for steam and electricity, as well as energy intensity of steam and electricity production, which we use to calculate direct energy use (6.88 MJ electricity and 4.11 kg steam), to which we apply our own emissions factors. The authors also provide emissions from $NH_3$ production, cooling water, sodium dodecylsulfate (SDS) production, and NaOCl production (amounting to 0.23 kg $CO_2$e / kg PHB). We exclude their estimates of fermentation emissions (which are biogenic in origin), and emissions from glucose production (which we account for separately). Our resulting distribution is centered on 2.9 kg $CO_2$e/kg PHB (for scenarios without internal energy generation from fermentation residues).

*Case 3*

Case 3 is based on case 9 presented in Akiyama *et al.* (2003) [20]. The authors report primary energy for steam and electricity, as well as energy intensity of steam and electricity production, which we use to calculate direct energy use (4.48 MJ electricity and 3.96 kg steam), to which we apply our own emissions factors. The authors also provide emissions from $NH_3$ production, cooling water, SDS production, and NaOCl production (amounting to 0.20 kg $CO_2$e / kg PHB). As for case 2, we exclude their estimates of fermentation emissions and emissions from glucose production. Our resulting distribution is centered on 2.2 kg $CO_2$e/kg PHB (for scenarios without internal energy generation from fermentation residues).

*Case 4*

Case 4 is based on Kim and Dale (2008) [24]. The authors model a system based on no-tilled corn, and which relies heavily on renewable energy. These elements are removed for the present study. As discussed in section S.1.4, we estimate that the net process yield is 4.4 kg corn / kg PHB for the Kim and Dale (2008) study [24]. Additionally, the authors summarize corn wet mill yields ranging from 0.64 to 0.68 g glucose / g corn grain, across studies – the lower bound of which is likely from the Kim and Dale (2008) study. This implies a yield of PHB of 0.35-0.36 kg PHB/kg glucose, consistent with other details given in their SI.

The study provides details regarding the steam and electricity use for PHB production (11.5 kg steam / kg PHB and 1.2 kWh / kg PHB, respectively), to which we apply our own emissions factors. Additional emissions from water, potassium hydroxide and ammonia production (amounting to 0.25 kg $CO_2$e/kg PHB) are used without modification. Finally, the authors indicate a credit of 9.2 MJ/ kg PHB which result from the combustion of fermentation residues from corn. In the present study (corn pathway only) this is assumed to displace primary energy for steam production. Our resulting distribution (for the corn-based pathway) is centered on 3.2 kg $CO_2$e/kg PHB.

*Case 5*

Case 5 is based on Gerngross (1999) [39]. The study assumes a yield of 0.3 kg PHB / kg glucose. The author further presents data on electricity (5.3 kWh/kg PHB), steam (2.8 kg / kg PHB), and inorganic salts (0.15 kg / kg PHB). We apply our own emissions factors to the steam and electricity generation. We treat inorganic salts as their primary constituent, ammonia, with an

emissions factor (1.68 kg $CO_2$e/kg $NH_3$) taken from Akiyama *et al.* (2003)[20]. The resulting distribution is centered on 5.8 kg $CO_2$e/kg PHB (for scenarios without internal energy generation from fermentation residues).

Full distribution

The 'full distribution' scenario encompasses input parameters from each of the other five cases, as summarized in Table S-7. To account for potential correlation between steam and electricity use, the model first calculates total process energy use, without differentiating between steam and electricity. This value ranges from a low of 15 MJ/kg PHB in case 2 to a high of 35 MJ/kg PHB in case 4. A separate distribution then models the split between electricity and steam, ranging from a low of 28% steam (72% electricity) from case 5, to a high of 88% steam (12% electricity) from case 4. Table S-7 presents key parameters and distributions related to PHB production cases.

### *S.1.9 Bioethylene Production*

Bioethylene is produced via the dehydration of bioethanol. Bioethylene production from ethanol is modeled as in Posen *et al.* (2015) [3], based on Kochar *et al*. (1981) [40], Haro *et al.* (2013) [41] and Geisler *et al.* (2005) [42]. Ethylene is difficult to transport, and so it is assumed that bioethylene will be produced adjacent to conventional chemical manufacturing capabilities, rather than at the biorefinery. Emissions from ethanol production are modeled as follows.

*Corn*

Mueller and Kwik (2013) report average fuel use, electricity use, ethanol yield, and co-product yield (of dried distillers grains (DDG) and corn oil) from an assessment of over half the operating dry mill corn ethanol facilities in the United States [43]. We fit fuel use, electricity use and ethanol yield to normal distributions, assuming the same coefficients of variation as can be calculated from Mueller's 2010 report on the 2008 dry mill corn ethanol survey [44]. Reported co-product yields violate mass balance, and so we adjust these downward (dynamically) as follows. We assume that corn starch yields a 1:1 stoichiometric quantity of glucose under hydrolysis (1.11 kg glucose / kg starch), and that glucose yields a stoichiometric quantity of ethanol (0.511 kg ethanol / kg glucose [33]). Thus, the theoretical maximum yield of ethanol is 0.568 kg ethanol / kg starch (1.76 kg starch / kg ethanol). We assume that corn oil and DDG are always produced in the same ratio (0.53:15.73) as reported by Mueller and Kwik (2013) [43], in quantities set to restore mass balance on the corn feedstock, assuming 100% product yield from the dry mill. We assume that corn ethanol will be transported by truck from the Midwest to the Gulf Coast.

*Switchgrass*

Heat and electricity requirements are modeled as in Posen *et al.* (2015) [3], based on Mullins *et al.* (2011) [33]. These include energy requirements for pretreatment. Starting with sugars available after pretreatment and saccharification (section S.1.6), ethanol yield is modeled as in Spatari and MacLean (2010) [30], again following the 2 scenarios (near-term/lower yields and mid-term/higher yields) laid out by those authors. Table S-9 presents key parameters and

distributions related to bioethylene production cases. We assume that switchgrass ethanol will be transported by truck from the Southeast to the Gulf Coast.

### *S.1.10 Additional details for switchgrass scenarios*

The sugars liberated during switchgrass pretreatment and saccharification are processed into PLA, PHB or ethanol using the assumptions documented in sections S.1.7, S.1.8 and S.1.9. The use of fermentation residues as an internal energy source is a modeling decision for the switchgrass pathways. As a result, only case 1 is considered for PLA, since energy requirements are not specifically known for PLA fermentation in cases 2-4. For all PLA and PHB pathways considered, we assume that the mass yield from the mix of available switchgrass sugars is the same as the mass yield from glucose (e.g. for PLA case 1, we assume 1.37 kg sugar / kg PLA). This is a somewhat optimistic assumption, but is consistent with the prospective nature of the switchgrass pathways. For consistency with these optimistic downstream yield assumptions, PHB and PLA pathways consider only the higher yielding 'mid-term' yield of sugars from pre-treatment, discussed in section S.1.6.

In the base case, we further assume an optimistic/bounding scenario, in which all feedstock is either transformed into product (PLA, PHB or ethanol) or is available for energy generation. Based on the stoichiometry of the reactions, theoretical maximum yields are 0.800 kg PLA / kg sugar, 0.477 kg PHB / kg sugar, 0.511 kg ethanol / kg sugar. Stoichiometries for these reactions can be found in references [20, 23, 33], respectively. We use these yields to calculate quantities of unfermented monomeric sugars, which we combine with quantities of unhydrolized sugars

from pretreatment, and the non-sugar components of switchgrass. Distributions for available feedstock energy are centered on values ranging from 10.3 MJ/kg PLA (case 1), to between 41 and 58 MJ / kg PHB (bounded by cases 2 and 5), to between 25 and 75 MJ/kg ethanol (mid-term and near-term yield scenarios respectively). A less optimistic scenario for available feedstock energy is considered in S.2.7. Table S-6 presents key parameters and distributions related to switchgrass scenarios; energy densities for switchgrass components are listed in Table S-14.

We develop a number of scenarios to account for surplus biomass. These include disposal (no energy generated), steam generation, or steam and electricity generation. Scenarios are also considered both with and without credits for surplus energy (steam for the steam-only case, or electricity for the steam and electricity case). To determine plant-level energy requirements, we assume that pretreatment, fermentation and recovery (to PLA, PHB or ethanol) occur at the same facility. Ethanol dehydration to ethylene is treated as a stand-alone step. Ethylene is difficult to transport, and so it is assumed that bioethylene will be produced adjacent to conventional chemical manufacturing capabilities, rather than at the biorefinery. Nevertheless, scenarios with credit for surplus steam and electricity can be thought of as partially displacing the requirements for bioethylene production.

For steam-only cases, boiler efficiency ranges from 68% to 75% (higher heating value basis), consistent with typical biomass boilers [45-47]. For steam and electricity generation, we assume the use of a combined heat and power (CHP) plant (steam turbine) with the same boiler efficiency as above, and with generator efficiency ranging from 85% [48] to 96% [49] (modeled as a uniform distribution). When internal energy is used, we assume first that internal steam

demand (for pre-treatment and either PLA, PHB or ethanol production) is met, and then allow additional steam energy to be used for electricity generation or for export, depending on the scenario. For scenarios with electricity generation, we assume the power:heat ratio cannot exceed 1:3 (i.e. no more than 25% of the available energy may be extracted as electricity) [50]. Steam export is given an emissions credit for displaced natural gas, assuming a stochastic natural gas boiler efficiency as above. For scenarios that include electricity production, we assume first the internal electricity demands (for pretreatment and either PLA, PHB or ethanol production) are met before allowing electricity export. Exported power is given a credit for displaced electricity using the grid average electricity emissions (before line losses). Scenarios with both steam and electricity export exist when there is still leftover steam, even after accounting for process steam requirements and maximal generation of electricity. In contrast, certain scenarios have energy demands that outstrip the maximum energy provided by biomass residues. These additional energy requirements are assumed to come from conventional sources (grid electricity and natural gas fuel), with the exception of a switchgrass fuel scenario in which additional energy is provided by combustion of whole switchgrass. Combustion of whole switchgrass is assumed to take place in the same CHP plant described above. Importing switchgrass for additional energy needs is equivalent to representing lower yield scenarios, which are not modeled explicitly for PLA and PHB as they are for the 'near-term' ethanol pathway.

### *S.1.11 End of life (EOL)*

Base-case results are presented on a cradle to gate basis. They include a credit for the carbon sequestered in PLA (1.8 kg $CO_2$ / kg PLA), PHB (2.0 kg $CO_2$ / kg PHB) and bioethylene (3.1 kg

$CO_2$ / kg ethylene), determined based on the chemical formula (carbon content) of each product. EOL emissions are treated separately as additional emissions, relative to the cradle to gate baseline. We model disposal of conventional polymers (including bioethylene-based polymers) following the U.S. Environmental Protection Agency (EPA) Waste Reduction Model (WARM) [51]. Conventional polymers and PLA are assumed to be inert under landfill conditions. Thus, landfilling is assumed to generate emissions of 0.04 metric tons (Mt) $CO_2$e / short ton plastic (0.044 kg $CO_2$e/kg plastic), related only to landfill machinery and transportation of waste to the landfill [51].

For the incineration option, we assume combustion proceeds with 100% efficiency; $CO_2$ emissions are calculated based on the chemical composition of each polymer. Yu and Chen (2008) [52] provide the energy content of PHB. The energy contents of all other polymers are taken from the EPA WARM documentation [51]. The incineration facility is assumed to be equipped with energy recovery capabilities, generating electricity at a net efficiency of 17.8% [51]. We assume that electricity produced displaces grid electricity at the national average emissions factor (before line losses). Transportation of waste to the incinerator is assumed to add 0.03 Mt $CO_2$e / short ton plastic (0.033 kg $CO_2$e/kg plastic) [51].

Recycling is modeled following the EPA WARM model [51]. Estimates are available only for PET and HDPE, as these are the only polymers recycled in large quantities in the U.S. Transportation is assumed to add 0.2 Mt $CO_2$e / short ton plastic (0.22 kg $CO_2$e/kg plastic). Recycling process emissions amount to 0.35 Mt $CO_2$e/ short ton HDPE (0.39 kg $CO_2$e/kg HDPE), and 0.77 Mt $CO_2$e/ short ton PET (0.85 kg $CO_2$e/kg PET). HDPE is assumed to be

recycled with 86% efficiency (i.e. 0.86 kg product / kg waste), and to displace virgin HDPE. PET is assumed to be recycled with 89% efficiency, and to displace virgin PET. All plastics considered in this study are known to be recyclable, although potentially with some deterioration in mechanical properties [53, 54]. Thus, for all other polymers, we create scoping estimates using uniform distributions for process emissions and recycling efficiency that span the range for HDPE and PET. Each recycled plastic is given a credit for displacing virgin production of the same polymer type.

An additional option, composting, is available for PHB and PLA. Following EPA WARM, we assume that process emissions (for transportation and fuel to turn the compost pile) amount to 0.04 Mt $CO_2$e/ short ton plastic (0.44 kg $CO_2$e/kg plastic) [51]. We further assume that 90% of the carbon content of the plastic is lost as $CO_2$, resulting from 44% loss during composting, and only 18% of the remaining carbon being sequestered in soil [24]. Emissions from composting could be even higher than modeled if anaerobic conditions are present, resulting in methane emissions. Compost is frequently used as a soil amendment, and so we also considered whether compost should receive an emissions credit for displacing other product systems. After engaging in a personal correspondence with the managers of a large compost facility, we concluded that compost generally does not provide a replacement service for any existing market products. Thus, the only basis for allocation would be based on economic value; however, compost facilities typically receive tipping fees, suggesting that the waste input to these facilities have negative economic value and thus there is no appropriate allocation.

Finally, we use data relating to the anaerobic biodegradation of a PHB co-polymer (Poly(3-hydroxybutyrate-co-3-hydroxyoctanoate)) [55, 56] to estimate generation of $CO_2$ and $CH_4$ from landfilled PHB. Mineralization of PHB is modeled as a triangular distribution (min: 41.1%, mode: 42%, max: 52.5%), based on data presented in Federle (2002) [56]. Following Levis and Barlaz (2011) [55], we calculate the methane fraction of released carbon to be 56.3%, using the Buswell equation, cited in Parkin and Owen (1986) [57]. The remainder of the mineralized carbon is assumed to be generated as $CO_2$. We model oxidation of uncollected methane as a triangular distribution (min: 10%, mode: 10%, max: 40%) based on Levis and Barlaz (2011) [55]. For landfills with a gas collection system installed, we model collection efficiency as a triangular distribution (min: 59.2%, mode: 64.8%, max: 78.8%) following a range of scenarios presented in the EPA WARM documentation [51]. All collected methane is assumed to be combusted with 100% efficiency. For landfills with energy recovery in place, we assume an electricity generation efficiency of 29.2% [51]. Finally, the proportion of landfills with gas collection, and the proportion of landfills with energy recovery are modeled following Levis and Barlaz (2011) [55]. We report results for a 90% confidence interval, based on the simulation parameters described above. Key parameters and distributions related to EOL can be found in Table S-10 and Table S-11.

### *S.1.12 Fuels and electricity*

As in Posen *et al.* (2015) [3], emissions from grid electricity are modeled at the level of individual North American Reliability Corporation (NERC) regions [58], employing distributions that span the range of available literature estimates [5, 59-62]. Consistent with

existing production, [26, 63] corn-based processes are assumed to take place in the Midwest (MRO) region. Switchgrass-based processes are assumed to take place in the south/southeast region spanned by SPP, SERC and TRE reliability corporations, consistent with EPA projections [64]. We assume that conventional chemical and plastics production (as well as bioethanol dehydration to bioethylene) take place in TRE/SERC, a region that includes the U.S. gulf coast and covers a majority of U.S. payroll and jobs in plastics manufacturing and petrochemical manufacturing [65]. Electricity displaced from end of life incineration is modeled at the U.S. national average. In general, electricity emissions are modeled as delivered electricity (after line losses). When electricity is exported, displaced emissions are adjusted downward to reflect emission factors before transmission line losses. Line losses for the U.S. Eastern Interconnect are modeled as 5.82% (for switchgrass surplus electricity), and 6.18% for the U.S. national average (for end of life incineration electricity credits) [66].

Emissions from other conventional fuels are discussed in the main text. For this paper, the distribution for emissions from natural gas is modified from the original source [67] as follows. The @Risk$^{TM}$ software used in the present study does not have the ability to model a generalized extreme value distribution as recommended by Tong *et al.* (2015) [67] for upstream emissions. Instead, a Pearson V distribution provides a close fit to the original authors' recommended distribution. Further, the present paper considers large industrial facilities that would likely receive natural gas directly from transmission lines, and so we remove emissions from natural gas distribution, as fit to the parameters for distribution emissions provided in Tong *et al.* [67]. Finally, we model combustion as per the original source for Tong *et al.* [16, 67, 68].

When energy requirements are cited in terms of steam energy, we assume that steam is generated from natural gas combustion. When a data source presents only the mass of steam required, we assume it is at atmospheric pressure, with an energy content of 2.68 MJ/kg steam. Following Abrahams *et al.* (2015) [69], natural gas (HHV) boiler efficiency is modeled as a triangular distribution (min: 70%, mode: 80%, max: 94%). Biomass boilers are assumed to be between 68% and 75% efficient (HHV), for as-received (wet) biomass [45-47]. Table S-12 presents key parameters and distributions related to fuels and electricity.

### *S.1.13 Model parameters*

The following tables present a list of the key parameters for each of the models developed in this paper.

**Table S-1. Summary of key parameters for fossil polymer production**

| Parameter | Value or Distribution | Units | Source and notes |
|---|---|---|---|
| ***Upstream processes*** | | | |
| Crude oil extraction | Pearson5 (7.1, 1.7, 0.049)<br>(mean: 0.33, CI[a]: 0.18-0.65) | kg $CO_2$e / kg crude oil | Fitted to underlying model from [2] |
| Crude oil refining | Normal (0.42, 0.042) | kg $CO_2$e / kg refined product | |
| Natural gas extraction | mean: 0.25, CI[a]: 0.194, 0.345<br>(Approx: Pearson5 (14.5, 2.11, 0.098)) | kg $CO_2$e / kg wet gas | Approximate fit; actual model as described in [3] |
| Natural gas processing | mean: 0.074, CI[a]: 0.013, 0.367<br>(Approx: Pearson5 (3.25, 0.28, -0.0237)) | kg $CO_2$e / kg processed gas | |
| | | | |
| ***Ethylene glycol inputs*** | | | |
| Ethylene oxide | 0.710 | kg ethylene oxide / kg ethylene glycol | Calculated from stoichiometry |
| Electricity | 0.391 | kWh / kg ethylene glycol | [4] |
| | | | |
| ***Other unit processes*** | | | |
| Energy requirements<br>(by fuel type) | Various | Various | [1] |

**Distributions are written as: Normal (mean, stdev), Pearson5 (shape, scale, shift) – this is a Pearson type V distribution**

**(a) 95% confidence interval (CI)**

**Table S-2. Summary of key parameters for corn agriculture**

| Parameter | Value or Distribution | Units | Source and notes |
|---|---|---|---|
| ***Corn*** | | | |
| LUC emissions | Uniform (18,159) | g $CO_2$e/ kg dry corn | Based on the GREET CCLUB model [5] |
| Crop yield | Extreme value min (161, 13.9)<br>(mean: 153, CI[a]: 110,180) | bu / acre | Own analysis of USDA data [11]; used to calculate N in crop residue, and fuel use/bu |
| Nitrogen applied | Exponential (0.0391, 0.353)<br>(mean: 0.392, CI[a]: 0.35, 0.50) | kg N / bu | Own analysis of USDA data [11] |
| Phosphate applied | Triangular (0.093, 0.093, 0.23) | kg $P_2O5$ / bu | |
| Potash applied | Uniform (0.029, 0.25) | kg $K_2O$ / bu | |
| $CaCO_3$ applied | 1150 | g $CaCO_3$ / bu | [5] |
| Herbicides applied | 7 | g / bu | |
| Insecticides applied | 0.06 | g / bu | |
| Nitrogen in crop residues | approx: Normal (9.88, 3.83) | g N / kg dry corn | Based on [12]; actual distribution is described in section S.1.3. |
| Gasoline used | 1.9<br>(250) | gallons / acre<br>(MJ HHV / acre) | [13] |
| Diesel used | 5.2<br>(750) | gallons / acre<br>(MJ HHV / acre) | |
| LPG used | 1.7<br>(160) | gallons / acre<br>(MJ HHV / acre) | |
| Natural gas used | 0.2<br>(230) | MCF / acre<br>(MJ HHV / acre) | |
| Electricity used | 30.4 | kWh / acre | |
| Feedstock transportation | 410<br>0.706<br>0.007 | g $CO_2$ / bu<br>g $CH_4$ / bu<br>g $N_2O$ / bu | [5] |

**Distributions are written as: Uniform (lower, upper), Extreme value min (location, scale), Exponential (mean, shift), Triangular (lower, mode, upper), Normal (mean, standard deviation)**

**(a) 95% confidence interval (CI)**

**Table S-3. Summary of key parameters for switchgrass agriculture**

| Parameter | Value or Distribution | Units | Source and notes |
|---|---|---|---|
| LUC emissions | Uniform (-27,220) | g $CO_2$e/ kg dry SW | Based on the GREET CCLUB model [5] |
| Crop yield | Weibull (2.8, 17.4, -2.69, [3.0,25.6])<br>(mean: 12.8, CI[a]: 4, 23.4) | Mg dry matter / ha | Based on [14] |
| Nitrogen applied | Triangular (0, 100, 180) | kg N / ha | |
| Nitrogen in crop residue | 0.54 | g N / kg dry SW | [5] |
| $P_2O_5$ applied | 114<br>(0.251) | g / short ton dry SW<br>(g / kg dry SW) | [5] |
| $K_2O$ applied | 227<br>(0.125) | g / short ton dry SW<br>(g / kg dry SW) | |
| Herbicides applied | 31.8<br>(0.0351) | g / short ton dry SW<br>(g / kg dry SW) | |
| Diesel used | 18700<br>(0.218) | Btu/short ton dry SW<br>(MJ HHV / kg dry SW) | |
| Electricity used | 14500<br>(0.0169) | Btu/short ton dry SW<br>(MJ electricity / kg dry SW) | |
| Feedstock transportation | 13700<br>23.8<br>0.205<br><br>(15.1)<br>(0.0262)<br>(2.3 E-4) | g $CO_2$ / short ton dry SW<br>g $CH_4$ / short ton dry SW<br>g $N_2O$ / short ton dry SW<br><br>(g $CO_2$ / kg dry SW)<br>(g $CH_4$ / kg dry SW)<br>(g $N_2O$ / kg dry SW) | |

**Distributions are written as: Uniform (lower, upper), Weibull (shape, scale, shift, [truncation bounds]), Triangular (lower, mode, upper), Beta (α, β, [lower bound, upper bound])**

**(a) 95% confidence interval (CI)**

**Table S-4. Summary of key emission factors for agrochemicals**

| Parameter | Value or Distribution | Units | Source and notes |
|---|---|---|---|
| ***Agrochemicals*** | | | |
| Nitrogen fertilizer production | 0.465[a] | kg $CO_2$e / kg N | Calculated from [5] |
| $CaCO_3$ Production | 0.0137[a] | kg $CO_2$e / kg $CaCO_3$ | |
| $K_2O$ Production | 0.661[a] | kg $CO_2$e / kg $K_2O$ | |
| $P_2O_5$ Production | 1.53[a] | kg $CO_2$e / kg $P_2O_5$ | |
| Herbicides | 19.3[a] | kg $CO_2$e / kg herbicide | |
| Insecticides | 22.3[a] | kg $CO_2$e / kg insecticide | |
| Direct $CO_2$ emissions from $CaCO_3$ | 0.216 | kg $CO_2$ / kg $CaCO_3$ | |
| Direct $N_2O$ from synthetic fertilizer and crop residue | Triangular (0.003, 0.01, 0.03) | kg $N_2O$-N/kg N applied | [12] |
| Volatilization from synthetic fertilizer | Triangular (0.03, 0.1, 0.3) | (kg $NH_3$-N + kg $NO_x$-N) /kg N | |
| Indirect $N_2O$ from volatized N | Triangular (0.002, 0.01, 0.05) | kg $N_2O$-N / (kg $NH_3$-N + kg $NO_x$-N) | |
| Runoff/Leaching of N from synthetic fertilizer and crop residue | Triangular (0.1, 0.3, 0.8) | kg N runoff / kg N applied | |
| Indirect $N_2O$ from runoff | Triangular (0.0005, 0.0075, 0.025) | kg $N_2O$-N/kg N runoff | |

**Distributions are written as: Triangular (lower, mode, upper)**

**(a) Mean values (point estimate or distribution bounds) are shown. Actual values are stochastic due to uncertainty in GWP.**

**Table S-5. Summary of key parameters for corn wet milling and co-product treatment**

| Parameter | Value or Distribution | Units | Source and notes |
|---|---|---|---|
| Corn gluten meal yield | Triangular (0.052, 0.056, 0.068) | kg / kg dry corn processed | Lower bound: [20], upper bound: [5], modal cluster: [21-23] |
| Corn gluten feed yield | Uniform (0.21, 0.29) | kg / kg dry corn processed | Lower bound: [20], upper bound: [5] |
| Corn oil yield | Uniform (0.033, 0.054) | kg / kg dry corn processed | Lower bound: [23], upper bound: [5] |
| Total process yield | Uniform (98.7, 99.6) % | % of dry corn processed | Lower bound: [20], upper bound: [22] |
| Starch yield | approx. Triangular (0.58, 0.64, 0.70) | kg / kg dry corn processed | Not modeled directly. Calculated as remainder after co-products and losses. |
| Gross emissions | Approx. Uniform (0.23, 0.42) | kg $CO_2$e / kg dry corn processed | Bounds are adjusted dynamically based on [20, 21, 23, 24], as described in section S.1.4. |
| | | | |
| ***Emissions credit for displaced products*** | | | For the system expansion scenario only. Displacement rates are discussed in section S.1.5 |
| Soy oil | 0.74[a] | kg $CO_2$e / kg soy oil | Calculated based on [5] |
| Urea | 1.32[a] | kg $CO_2$e / kg urea | |

**Distributions are written as: Uniform (lower, upper), Triangular (lower, mode, upper).**

**(a) Mean values (point estimate or distribution bounds) are shown. Actual values are stochastic due to uncertainty in GWP, and/or $N_2O$ emission factors.**

**Table S-6. Summary of key parameters common to all switchgrass scenarios**

| Parameter | Value or Distribution | Units | Source and notes |
|---|---|---|---|
| ***Switchgrass Composition*** | | | |
| Glucan (cellulose) content | Triangular (31, 34.4, 37.2) | % | [33] |
| Xylan Content | Triangular (20.6, 23, 26) | % | |
| Mannan Content | Triangular (0.29, 0.32, 0.36) | % | |
| Galactan Content | Triangular (0.67, 1.0, 1.2) | % | |
| Arabinan Content | Uniform (2.6, 3.4) | % | |
| Lignin Content | Triangular (17.3, 21.1) | % | |
| Non-sugar, non-lignin | Mean: ~22.7 | % | Calculated based on mass balance |
| | | | |
| ***Pre-treatment and Saccharification*** | | | |
| Emissions chemicals and enzymes for pre-treatment and saccharification | Uniform (53, 93) [a] | g $CO_2$e / kg feedstock processed | Lower bound calculated based on [27]; upper bound calculated based on [5, 31] |
| Pre-treatment electricity required | Uniform (0.15, 0.18) | MJ electricity / kg feedstock processed | Bounds calculated based on [32] and [5], respectively |
| Pre-treatment steam required | Uniform (1.26, 2.28) | MJ steam / kg feedstock processed | |
| Midterm yield of sugars from cellulose and hemicellulose | 0.95 | % (molar conversion) | [30]. Used for PHB, PLA and mid-term bioethylene |
| Near-term yield of glucose from glucan | Normal (0.675, 0.038) | % (molar conversion) | [30]. Only used for near-term bioethylene scenario |
| Near-term yield of sugars from hemicellulose | Normal (0.635, 0.0097) | % (molar conversion) | |
| | | | |
| ***Internal energy use*** | | | |
| Biomass boiler | Triangular (68, 70, 74.5) | % (HHV) | Lower: [47], mode:[46], upper:[70] |
| CHP electric generator efficiency | Uniform (85,96) | % | Lower:[48], upper:[49] |
| Maximum CHP heat:power ratio | 1:3 | Ratio | [50] (value for steam turbine CHP). |

**Distributions are written as: Uniform (lower, upper), Triangular (min, mode, max), Normal (mean, stdev).**

**(a) Mean values (point estimate or distribution bounds) are shown. Actual values are stochastic due to uncertainty in GWP.**

**Table S-7. Summary of key parameters for PHB cases**

| Parameter | Value or Distribution | Units | Source and notes |
|---|---|---|---|
| | | | |
| Cradle-to-gate carbon credit (all cases) | 2.04 | kg $CO_2$ / kg PHB | Calculated from molecular formula of PHB |
| | | | |
| ***PHB Case 1*** | | | |
| PHB Yield | 0.36 | kg PHB/kg sugar | Calculated based on[38] |
| Chemical production emissions | 0.12 | kg $CO_2$e/kg PHB | |
| Electricity required | 3.94 | MJ electricity/kg PHB | |
| Steam required | 4.89 | kg / kg PHB | |
| Additional natural gas required | 2.12 | MJ / kg PHB | |
| | | | |
| ***PHB Case 2*** | | | |
| PHB Yield | 0.37 | kg PHB/kg sugar | Calculated based on [20] |
| Chemical production emissions | 0.20 | kg $CO_2$e/kg PHB | |
| Electricity required | 4.48 | MJ electricity / kg PHB | |
| Steam required | 3.96 | kg/kg PHB | |
| | | | |
| ***PHB Case 3*** | | | |
| PHB Yield | 0.3 | kg PHB/kg sugar | Calculated based on [20] |
| Chemical production emissions | 0.23 | kg $CO_2$e/kg PHB | |
| Electricity required | 6.88 | MJ electricity / kg PHB | |
| Steam required | 4.11 | kg/kg PHB | |
| | | | |
| ***PHB Case 4*** | | | |
| PHB Yield | 0.35 | kg PHB/kg sugar | Calculated based on [24] |
| Chemical production emissions | 0.25 | kg $CO_2$e/kg PHB | |
| Electricity required | 1.2 | kWh/kg PHB | |
| Steam required | 11.5 | kg / kg PHB | |
| Energy from fermentation residue (corn grain pathway only) | 9.2 | MJ / kg PHB | |
| | | | |
| | | | |

| | | | |
|---|---|---|---|
| ***PHB Case 5*** | | | |
| PHB Yield | 0.3 | kg PHB/kg sugar | [39] |
| Chemical production emissions | 0.25 | kg $CO_2$e/kg PHB | Calculated based on [39], with an emission factor from [20] |
| Electricity required | 5.32 | kWh/kg PHB | [39] |
| Steam required | 2.78 | kg / kg PHB | |
| | | | |
| ***Full distribution*** | | | |
| PHB Yield | Triangular (0.3, 0.36, 0.37) | kg PHB/kg sugar | Fit to cases 1-5 |
| Chemical production emissions | Uniform (0.12, 0.25) | kg $CO_2$e/kg PHB | |
| Total process energy | Triangular (15, 17, 35) | MJ/kg PHB | |
| Percent of process energy to steam (rest to electricity) | Triangular (28%, 88%, 88%) | % as steam | |

**Distributions are written as: Uniform (lower, upper), triangular (min, mode, max)**

**Table S-8. Summary of key parameters for PLA cases**

| Parameter | Value or Distribution | Units | Source and notes |
|---|---|---|---|
| | | | |
| Cradle-to-gate carbon credit (all cases) | -1.83 | kg $CO_2$ / kg PLA | Calculated from molecular formula of PLA |
| | | | |
| ***PLA Case 1*** | | | |
| PLA Yield | 0.72 | kg PLA/kg sugar | Calculated based on [34] |
| Chemical production emissions | 0.87 | kg $CO_2$e/kg PLA | |
| Electricity required | 3.0 | MJ electricity/kg PLA | |
| Natural gas required (when no fermentation residues are used) | Uniform (9.0, 1.0) | MJ / kg PLA | |
| | | | |
| ***PLA Cases 2-4*** | | | |
| PLA Yield | 0.64 | kg PLA/kg sugar | Calculated based on [23, 26] |
| Lactic acid production emissions | 1.04<br>0.0050 | kg $CO_2$ / kg PLA<br>kg $CH_4$ / kg PLA | |
| | | | |
| ***PLA Case 2*** | | | |
| Lactide production and polymerization emissions | 0.66<br>0.0032 | kg $CO_2$ / kg PLA<br>kg $CH_4$ / kg PLA | Calculated based on [23, 26] |
| | | | |
| ***PLA Case 3*** | | | |
| Lactide production and polymerization electricity required | 1.71 | kWh/kg PLA | [37] |
| | | | |
| ***PLA Case 4*** | | | |
| Lactide production and polymerization steam required | 6.16 | MJ / kg PLA | Based on [37] |

**Distributions are written as: Uniform (min, max)**

**Table S-9. Summary of key parameters for bioethylene pathways**

| Parameter | Value or Distribution | Units | Source and notes |
|---|---|---|---|
| | | | |
| ***Corn bioethanol*** | | | |
| Electricity use | Normal (0.75, 0.23)<br>(Normal (0.90, 0.28)) | kWh / gal EtOH<br>(MJ / kg EtOH) | Mean: [43], Stdev based on [44] |
| Fuel use | Normal (23862, 2798)<br>(Normal (8.4, 0.99)) | Btu LHV / gal EtOH<br>(MJ / kg EtOH) | |
| Ethanol yield | Normal (2.8, 0.018)<br>(Normal (0.39, 0.017) | gal EtOH / bu corn<br>(kg EtOH / kg dry corn) | |
| Transportation distance | Uniform (1000, 1800) | km | Approximate distance from existing corn ethanol refineries [63] to gulf states ethylene infrastructure [71], as per [3] |
| Truck fuel consumption | 0.0203 | L diesel / t-km | [72] |
| | | | |
| ***Corn co-products*** | | | |
| Co-product ratio from corn ethanol production | 29.7 | kg DDGS / kg corn oil | Calculated from [43]. Actual quantities determined based on mass balance per section S.1.9. |
| Emissions credit for displaced soybean meal | 0.31[a] | kg $CO_2$e / kg soybean meal | Calculated based on [5]; displacement rates are discussed in section S.1.5. |
| Emissions credit for displaced urea | 1.32[a] | kg $CO_2$e / kg urea | |
| | | | |
| ***Switchgrass bioethanol*** | | | |
| Total production energy | Uniform (0.44, 0.72)<br>(Uniform (12,19)) | MJ / MJ EtOH LHV<br>(MJ / kg EtOH) | [33] |
| Percent of energy as electricity (remainder as heat) | 10% | % | |
| Midterm ethanol yield (all sugars) | 0.95 | Fraction of theoretical | [30] |
| Near-term ethanol yield (glucose) | Normal (0.90, 0.026) | Fraction of theoretical | |

| | | | |
|---|---|---|---|
| Near-term ethanol yield (xylose) | Normal (0.70, 0.103) | Fraction of theoretical | |
| Near-term ethanol yield (other sugars) | Triangular (0, 0, 0.855) | Fraction of theoretical | |
| Transportation distance | Uniform (1000, 1800) | km | Approximate distance from projected switchgrass ethanol facilities [64] to gulf states ethylene infrastructure [71], as per [3] |
| Truck fuel consumption | 0.0203 | L diesel / t-km | [72] |
| | | | |
| ***Ethanol dehydration to ethylene*** | | | |
| Ethylene yield | Uniform (1.70, 1.74) | kg ethanol / kg ethylene | Lower:[41], upper: [40] |
| Fuel used | Lognormal (1.67, 0.611) | MJ LHV /kg ethylene | [3] based on [40, 42] |
| Electricity Used | Lognormal (1.12, 0.41) | MJ electricity/ kg ethylene | |
| Cradle-to-gate stored carbon credit | 3.14 | kg $CO_2$ / kg bioethylene | Calculated based on molecular formula |

**Distributions are written as: Normal (Mean, Stdev), Uniform (min, max), Triangular (min, mode, max)**

**(a) Mean values (point estimate or distribution bounds) are shown. Actual values are stochastic due to uncertainty in GWP, and/or $N_2O$ emission factors.**

**Table S-10. Summary of key parameters for end of life emissions estimates**

| Parameter | Value or Distribution | Units | Source and notes |
|---|---|---|---|
| ***Landfilling (all plastics)*** | | | |
| Transportation and equipment operation | 0.044 | kg $CO_2$e/kg waste | [51] |
| | | | |
| ***Landfilling (PHB only)*** | | | |
| Mineralization | Triangular (41.1, 42.0, 52.5) | % | [56] |
| Fraction of mineralized carbon to methane (rest to $CO_2$) | 56.25% | Fraction of mineralized carbon in PHB | Based on [55, 57], treated as PHB |
| Landfills with LFG collection | Triangular (60, 69, 84) | % of all landfills | [55] |
| Landfills with energy recovery | Triangular (40, 50, 66) | % of landfills with LFG collection | [55] |
| LFG collection efficiency | Triangular (59.2, 64.8, 78.8) | % of generated methane | Based on [51] |
| Oxidation of uncollected methane (to $CO_2$) | Triangular (10, 10, 40) | % of generated methane | [55] |
| Efficiency of LFG to electricity | 29.2% | % (assumed HHV) | [51] |
| | | | |
| ***Composting*** | | | |
| Reduced carbon sequestration | 89.9% | % of carbon in PHB or PLA | Based on [24]; all carbon is lost as $CO_2$ |
| Transportation and equipment operation | 0.044 | kg $CO_2$e/kg waste | [51] |
| | | | |
| ***Recycling*** | | | |
| Net recycling efficiency | 0.86 (HDPE)<br>0.89 (PET)<br>Uniform (0.86, 0.89) (Others) | kg virgin product displaced / kg waste recycled | [51] |
| Process emissions | 0.35 (HDPE)<br>0.77 (PET)<br>Uniform (0.35, 0.77) (Others) | kg $CO_2$e / kg waste | [51] |
| Transportation emissions | 0.22 | kg $CO_2$e / kg waste | [51] |
| | | | |
| ***Incineration with energy recovery*** | | | |
| Efficiency of electricity generation | 17.8% | % | [51] |
| Transportation emissions | 0.033 | kg $CO_2$e/kg waste | [51] |

**Distributions are written as: Triangular (lower, mode, upper), Uniform (min, max)**

**Table S-11. Summary of key plastics carbon content and energy density (for incineration modeling)**

| Plastic | Carbon content based on stoichiometry (kg $CO_2$ / kg plastic) | Energy content (MJ / kg plastic) | Source for energy content |
|---|---|---|---|
| HDPE | 3.1 | 46.5 | [51] |
| LDPE | 3.1 | 46.3 | |
| LLDPE | 3.1 | 46.4 | |
| PP | 3.1 | 46.4 | |
| PET | 2.3 | 24.7 | |
| GPPS | 3.4 | 41.9 | |
| HIPS | 3.4 | 41.9 | |
| PVC | 1.4 | 18.4 | |
| PLA | 1.8 | 19.4 | |
| PHB (treated as PHB) | 2.0 | 24.1 | [52] |

**Table S-12. Boiler efficiencies, and emission factors for fuels and electricity.**

| Parameter | Value | Units | Source and notes |
|---|---|---|---|
| ***Fuel Emissions*** | | | |
| Gasoline life cycle emissions | Log-logistic† (2.2, 0.2, 80) | g $CO_2$e/MJ (LHV) | [2] |
| Diesel life cycle emissions | Log-logistic† (2.3, 0.2, 82) | g $CO_2$e/ MJ (LHV) | |
| Residual fuel life cycle emissions | Log-logistic† (2.3, 0.3, 83) | g $CO_2$e/ MJ (LHV) | |
| LPG life cycle emissions | Log-logistic† (2.1, 0.2, 77) | g $CO_2$e/ MJ (LHV) | |
| Coal life cycle emissions | Log-logistic (3.05, 0.14, 74) | g $CO_2$e/ MJ (HHV) | [73] |
| Natural gas: all upstream emissions (including distribution) | Pearson5 (7.66, 54.9, -0.306, [0, ∞])<br>Pearson5 (4.14, 0.232, 0.179, [0, ∞]) | g $CO_2$ / MJ (LHV)<br>g $CH_4$ / MJ (LHV) | Approximate fit to results from [67] |
| Natural gas distribution | Triangular (0.047, 0.06, 0.073) | g $CH_4$ / MJ (LHV) | Approximate fit to results from [67] |
| Natural gas combustion emissions | Triangular (54.3, 56.1, 58.3)<br>Triangular (3E-4, 1E-4, 3E-3)<br>Triangular (3E-5, 1E-4, 3E-4) | g $CO_2$ / MJ (LHV)<br>g $CH_4$ / MJ (LHV)<br>g $N_2O$ / MJ (LHV) | [16] (original source for [67]). |
| | | | |
| ***Boiler efficiencies*** | | | |
| Natural gas boiler | Triangular (70%, 80%, 94%) | % (HHV) | [69] |
| Biomass boiler | Triangular (68%, 70%, 74.5%) | % (HHV) | Lower: [47], mode:[46], upper:[70] |
| | | | |
| ***Electricity Emissions*** | | | |
| U.S. average electricity | Uniform (163, 208)[a] | g $CO_2$e/MJ | Lower bound: [74], upper bound: [75] |
| MRO electricity | Uniform (197, 313)[a] | g $CO_2$e/MJ | Lower bound: [74]; upper bound: [60] |
| TRE electricity (encompasses SERC as well) | Uniform (164, 220)[a] | g $CO_2$e/MJ | Lower bound from [74] for TRE. Upper bound from [59]. |

**Distributions are written as: Uniform (min, max), Triangular (lower, mode, upper), Normal (mean, standard deviation), Log-logistic† (location of the underlying logistic, scale of the underlying logistic, shift), Lognormal (mean of the lognormal distribution, standard deviation of the lognormal distribution, shift), Pearson5 (shape, scale, shift, [truncation bounds]) – this is a Pearson type V distribution.**

**(a) Mean values (point estimate or distribution bounds) are shown. Actual values are stochastic due to uncertainty in GWP.**

**Table S-13. Global warming potentials.**

| Parameter | Value | Units | Source |
|---|---|---|---|
| ***Global warming potentials*** | | | |
| $CH_4$ GWP | Normal (36, 8.5) | g $CO_2$e / g $CH_4$ | [76, 77] |
| $N_2O$ GWP | Normal (298, 52.5) | g $CO_2$e / g $N_2O$ | |

**Table S-14. Energy and mass densities used throughout this paper**

| ***Liquids*** Item | LHV Energy Density (btu/gal) | HHV Energy Density (btu/gal) | Mass Density |
|---|---|---|---|
| Gasoline | 112,194[a] | 120,439[a] | 2,836[a] g/gal |
| Diesel/distillate | 128,450[a] | 137,380[a] | 3,167[a] g/gal |
| Residual Fuel Oil | 140,353[a] | 150,110[a] | 3,752[a] g/gal |
| Ethanol | 76,330[a] | 84,530[a] | 2,988[a] g/gal |

| ***Gasses*** Item | LHV Energy Density (btu/ft$^3$) | HHV Energy Density (btu/ft$^3$) | Mass Density |
|---|---|---|---|
| Natural gas | 983[a] | 1,089[a] | 22[a] g/ft$^3$ |
| Methane | 962[a] | 1,068[a] | 20.3[a] g/ft$^3$ |
| Hydrogen | 290[a] | 343[a] | 2.55[a] g/ft$^3$ |

| ***Solids*** Item | HHV Energy Density (MJ/kg) | ***Solids*** Item | HHV Energy Density (MJ/kg) |
|---|---|---|---|
| Glucan/Cellulose | 16.9[b] | Glucose | 15.6[c] |
| Xylan | 17.4[b] | Xylose | 15.6[c] |
| Mannan | 16.6[b] | Mannose | 15.6[c] |
| Galactan | 17.2[b] | Galactose | 15.5[c] |
| Arabinan | 16.9[b] | Arabinose | 15.6[c] |
| Lignin | 25.1[b] | Non-sugar, non-lignin switchgrass components | 11.8[b] |
| Corn grain | 19.2[a] | Coal | 24.0[a] |
| Corn gluten meal | Triangular (21.2, 23.1, 24.1)[d] | Switchgrass | 18.1[a] |
| Corn gluten feed | Triangular (18.3, 18.8, 19.5)[d] | | |
| Corn oil | 39.1 | | |
| Corn starch | Triangular (17.1, 17.4, 17.9)[d] | | |
| Corn DDGS | Triangular (19.9, 21.4, 23)[d] | | |

**(a) Based on GREET 2013 or GREET 2014 [5, 74]**
**(b) Calculated from [47]**
**(c) [78]**
**(d) [79]**
**(e) [21]**

## S.2 Additional Results and Sensitivity Analysis

### *S.2.1 Numerical GHG emission results for upstream operations (agriculture and corn wet milling)*

**Table S-15. Modeled greenhouse gas emissions (mean and 95% confidence interval) from corn production, excluding carbon uptake credit (kg $CO_2$e / kg dry corn),**

| Emissions category | Mean | 2.5% | 97.5% |
|---|---|---|---|
| Land use change | 0.089 | 0.022 | 0.16 |
| Fertilizer production | 0.10 | 0.085 | 0.12 |
| Farm energy use | 0.044 | 0.036 | 0.060 |
| Field emissions (from fertilizer and crop residue) | 0.28 | 0.13 | 0.51 |
| Other (pesticides and feedstock transportation) | 0.027 | 0.026 | 0.027 |
| Total | 0.54 | 0.36 | 0.79 |
| Approximate distribution: Gamma (shape = 9.97, scale = 0.036, shift = 0.185) | | | |

**Table S-16. Modeled greenhouse gas emissions (mean and 95% confidence interval) for corn glucose production via wet milling (with system expansion), excluding carbon uptake credit (kg $CO_2$e / kg glucose)**

| Emissions category | Mean | 2.5% | 97.5% |
|---|---|---|---|
| Upstream (corn production) | 0.76 | 0.50 | 1.12 |
| Wet milling (gross emissions) | 0.46 | 0.32 | 0.62 |
| Co-product credit (system expansion) | -0.27 | -0.40 | -0.18 |
| Enzyme production | 0.013 | 0.012 | 0.014 |
| Total | 0.96 | 0.71 | 1.25 |
| Approximate distribution: Weibull (shape = 3.15, scale = 0.455, shift = 0.553) | | | |

**Table S-17 Modeled greenhouse gas emissions (mean and 95% confidence interval) from switchgrass production, excluding carbon uptake credit (kg $CO_2$e / kg dry switchgrass),**

| Emissions category | Mean | 2.5% | 97.5% |
|---|---|---|---|
| Land use change | 0.097 | -0.021 | 0.21 |
| Fertilizer production | 0.043 | 0.008 | 0.13 |
| Farm energy use | 0.022 | 0.021 | 0.024 |
| Field emissions (from fertilizer and crop residue) | 0.097 | 0.015 | 0.31 |
| Other (pesticides and feedstock transportation) | 0.016 | 0.016 | 0.017 |
| Total | 0.28 | 0.085 | 0.59 |
| Approximate distribution: Lognormal (mean = 0.28, stdev = 0.12, shift = -0.1) | | | |

### *S.2.2 Graphical results for Switchgrass PHB cases 1-5*

The main text presents only results of the 'full distribution' case for switchgrass PHB. Figure S-1 presents a full set of results for cases 1-5.

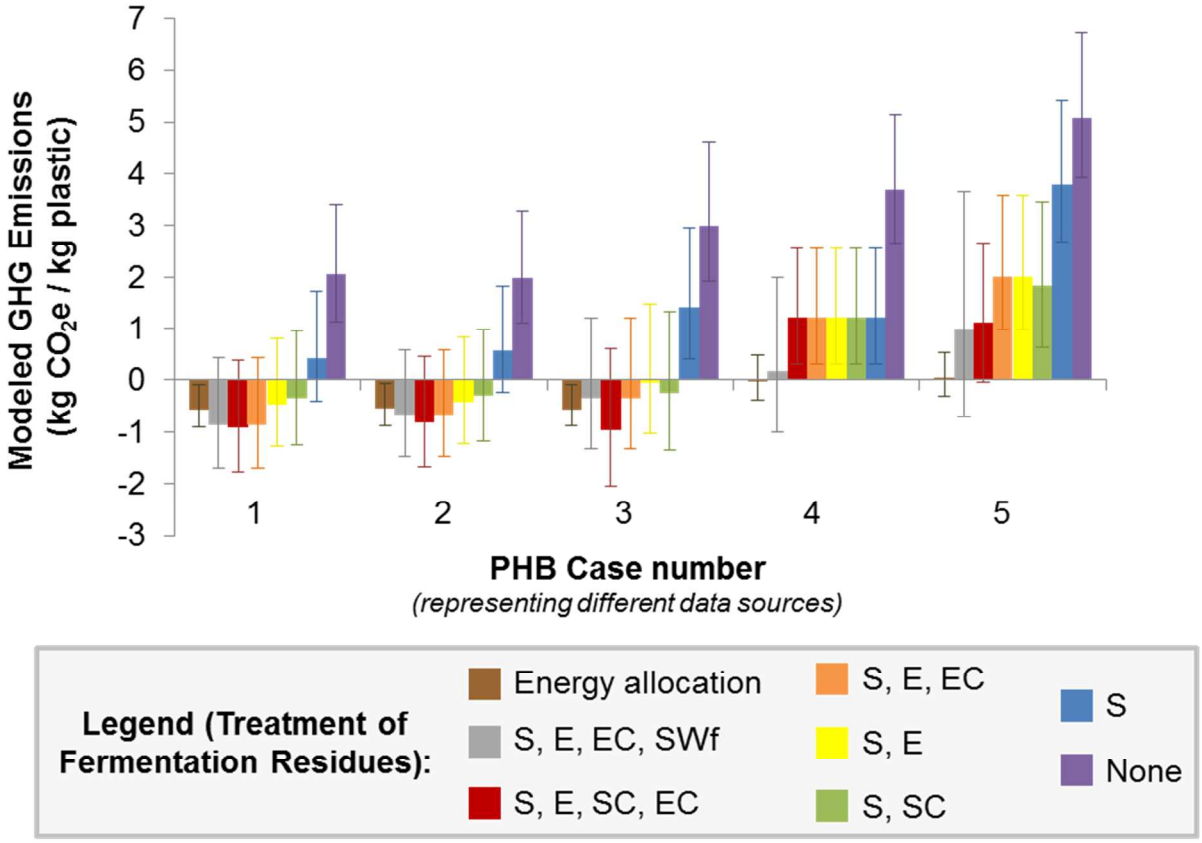


**Figure S-1 Cradle-to-gate greenhouse gas emissions for switchgrass-based PHB (cases 1-5). Error bars span 95% of simulations. The legend refers to the assumptions about the use (or allocation) of unfermented residues: S = steam, E = electricity, C = emission credit applied for surplus steam (SC) and/or electricity (EC) when available, SWf = balance of energy (when needed) from switchgrass combustion, Energy allocation = no direct use of fermentation residues, but emissions allocated to residue and PHB on the basis of energy content.**

### *S.2.3 Numerical GHG emission results for cradle-to-gate polymer production pathways*

**Table S-18. Modeled greenhouse gas emissions (mean and 95% confidence interval) from fossil polymer production with conventional energy, under different input assumptions (kg $CO_2$e / kg plastic)**

| Scenario | Plastic | Mean | 2.5% | 97.5% |
|---|---|---|---|---|
| **Base-Case (Hydrogen from stream cracking treated by system expansion)** | HDPE | 1.43 | 0.97 | 1.93 |
| | LDPE | 1.70 | 1.22 | 2.22 |
| | LLDPE | 1.44 | 0.97 | 1.93 |
| | PP | 1.49 | 1.10 | 1.92 |
| | PET | 2.34 | 2.14 | 2.60 |
| | PS (GPPS) | 3.08 | 2.75 | 3.49 |
| | HIPS | 3.05 | 2.71 | 3.47 |
| | PVC | 2.14 | 1.88 | 2.46 |
| **Hydrogen from steam cracking combusted for energy** | HDPE | 1.67 | 1.28 | 2.12 |
| | LDPE | 1.94 | 1.54 | 2.41 |
| | LLDPE | 1.67 | 1.29 | 2.12 |
| | PP | 1.70 | 1.37 | 2.10 |
| | PET | 2.39 | 2.19 | 2.64 |
| | PS (GPPS) | 3.20 | 2.89 | 3.59 |
| | HIPS | 3.18 | 2.87 | 3.58 |
| | PVC | 2.25 | 2.01 | 2.54 |
| **Hydrogen from steam cracking treated by mass allocation** | HDPE | 2.12 | 1.74 | 2.56 |
| | LDPE | 2.41 | 2.00 | 2.87 |
| | LLDPE | 2.13 | 1.75 | 2.58 |
| | PP | 2.07 | 1.73 | 2.46 |
| | PET | 2.47 | 2.27 | 2.73 |
| | PS (GPPS) | 3.42 | 3.11 | 3.83 |
| | HIPS | 3.41 | 3.09 | 3.82 |
| | PVC | 2.46 | 2.20 | 2.77 |

**Table S-19. Modeled greenhouse gas emissions (mean and 95% confidence interval) from corn-based PHB polymer production (kg $CO_2$e / kg plastic)**

| Treatment of corn co-products | Case # | Mean | 2.5% | 97.5% |
|---|---|---|---|---|
| **System expansion** | 1 | 2.92 | 2.14 | 3.84 |
| | 2 | 2.74 | 1.96 | 3.64 |
| | 3 | 4.02 | 3.02 | 5.15 |
| | 4 | 3.86 | 2.98 | 4.86 |
| | 5 | 6.88 | 5.39 | 8.48 |
| **Mass allocation** | 1 | 2.48 | 1.81 | 3.27 |
| | 2 | 2.30 | 1.64 | 3.08 |
| | 3 | 3.48 | 2.63 | 4.47 |
| | 4 | 3.41 | 2.65 | 4.27 |
| | 5 | 6.35 | 4.96 | 7.82 |
| **Energy allocation** | 1 | 2.29 | 1.67 | 3.03 |
| | 2 | 2.12 | 1.50 | 2.85 |
| | 3 | 3.26 | 2.46 | 4.19 |
| | 4 | 3.22 | 2.49 | 4.04 |
| | 5 | 6.13 | 4.77 | 7.55 |
| **No allocation** | 1 | 3.68 | 2.70 | 4.89 |
| | 2 | 3.48 | 2.51 | 4.65 |
| | 3 | 4.93 | 3.71 | 6.40 |
| | 4 | 4.63 | 3.57 | 5.90 |
| | 5 | 7.80 | 6.12 | 9.64 |

**Table S-20. Modeled greenhouse gas emissions (mean and 95% confidence interval) from switchgrass-based PHB polymer production (kg $CO_2$e / kg plastic)**

| Treatment of fermentation residues | Case # | Mean | 2.5% | 97.5% |
|---|---|---|---|---|
| **None** | 1 | 2.05 | 1.14 | 3.37 |
| | 2 | 1.98 | 1.11 | 3.26 |
| | 3 | 3.00 | 1.92 | 4.58 |
| | 4 | 3.69 | 2.67 | 5.11 |
| | 5 | 5.08 | 3.93 | 6.71 |
| | Full distribution | 3.02 | 1.55 | 4.96 |
| **Steam for internal use only (S)** | 1 | 0.42 | -0.41 | 1.70 |
| | 2 | 0.57 | -0.24 | 1.82 |
| | 3 | 1.42 | 0.42 | 2.97 |
| | 4 | 1.22 | 0.33 | 2.54 |
| | 5 | 3.78 | 2.68 | 5.38 |
| | Full distribution | 1.20 | -0.22 | 3.18 |
| **Steam for internal use and with system expansion credit for surplus (S, SC)** | 1 | -0.36 | -1.23 | 0.94 |
| | 2 | -0.31 | -1.16 | 0.96 |
| | 3 | -0.25 | -1.33 | 1.32 |
| | 4 | 1.22 | 0.33 | 2.54 |
| | 5 | 1.83 | 0.65 | 3.42 |
| | Full distribution | 0.40 | -1.04 | 2.31 |
| **Steam and electricity for internal use only (S, E)** | 1 | -0.47 | -1.28 | 0.81 |
| | 2 | -0.42 | -1.22 | 0.82 |
| | 3 | -0.06 | -1.04 | 1.48 |
| | 4 | 1.22 | 0.33 | 2.54 |
| | 5 | 2.01 | 0.98 | 3.55 |
| | Full distribution | 0.14 | -1.07 | 1.93 |
| **Steam and electricity, with system expansion credits for surplus electricity (S, E, EC)** | 1 | -0.87 | -1.69 | 0.42 |
| | 2 | -0.67 | -1.47 | 0.57 |
| | 3 | -0.34 | -1.33 | 1.20 |
| | 4 | 1.22 | 0.33 | 2.54 |
| | 5 | 2.01 | 0.98 | 3.55 |
| | Full distribution | -0.01 | -1.54 | 1.89 |
| **Steam and electricity, with system expansion credits for both surplus electricity and surplus steam (S, E, SC, EC)** | 1 | -0.92 | -1.78 | 0.37 |
| | 2 | -0.82 | -1.68 | 0.45 |
| | 3 | -0.97 | -2.06 | 0.61 |
| | 4 | 1.22 | 0.33 | 2.54 |
| | 5 | 1.10 | -0.02 | 2.66 |
| | Full distribution | -0.15 | -1.67 | 1.79 |

| | | | | |
|---|---|---|---|---|
| **Energy allocation** | 1 | -0.57 | -0.90 | -0.10 |
| | 2 | -0.55 | -0.88 | -0.08 |
| | 3 | -0.56 | -0.88 | -0.10 |
| | 4 | -0.02 | -0.38 | 0.48 |
| | 5 | 0.05 | -0.30 | 0.53 |
| | Full distribution | -0.32 | -0.82 | 0.35 |
| **Steam and electricity, with system expansion credits for surplus electricity (when available, and balance of energy (when needed) from switchgrass combustion and (S, E, EC, SWf)** | 1 | -0.87 | -1.69 | 0.42 |
| | 2 | -0.67 | -1.47 | 0.57 |
| | 3 | -0.34 | -1.33 | 1.20 |
| | 4 | 0.16 | -0.99 | 1.98 |
| | 5 | 0.97 | -0.71 | 3.65 |
| | Full distribution | -0.48 | -1.54 | 0.91 |

**Table S-21. Modeled greenhouse gas emissions (mean and 95% confidence interval) from corn-based PLA polymer production (kg $CO_2$e / kg plastic)**

| Scenario | Case # | Mean | 2.5% | 97.5% |
|---|---|---|---|---|
| **System expansion** | 1 | 1.81 | 1.38 | 2.30 |
| | 2 | 1.65 | 1.22 | 2.13 |
| | 3 | 2.45 | 1.85 | 3.09 |
| | 4 | 1.37 | 0.94 | 1.85 |
| **Mass allocation** | 1 | 1.59 | 1.21 | 2.01 |
| | 2 | 1.40 | 1.04 | 1.82 |
| | 3 | 2.20 | 1.65 | 2.78 |
| | 4 | 1.12 | 0.76 | 1.53 |
| **Energy allocation** | 1 | 1.50 | 1.14 | 1.90 |
| | 2 | 1.30 | 0.96 | 1.68 |
| | 3 | 2.10 | 1.57 | 2.65 |
| | 4 | 1.01 | 0.68 | 1.40 |
| **No allocation** | 1 | 2.19 | 1.67 | 2.80 |
| | 2 | 2.08 | 1.54 | 2.71 |
| | 3 | 2.87 | 2.18 | 3.65 |
| | 4 | 1.79 | 1.26 | 2.43 |

**Table S-22. Modeled greenhouse gas emissions (mean and 95% confidence interval) from switchgrass-based PLA polymer production, case 1 (kg $CO_2$e / kg plastic).**

| Treatment of fermentation residues | Mean | 2.5% | 97.5% |
|---|---|---|---|
| **None** | 1.31 | 0.87 | 1.97 |
| **S** | 0.41 | 0.00 | 1.04 |
| **S, SC** | 0.31 | -0.12 | 0.94 |
| **S, E** | 0.20 | -0.31 | 0.86 |
| **S, E, EC** | 0.20 | -0.31 | 0.86 |
| **S, E, SC, EC** | 0.20 | -0.31 | 0.86 |
| **Energy Allocation** | -0.19 | -0.43 | 0.14 |
| **S, E, EC, SWf** | -0.02 | -0.57 | 0.85 |

**Treatment of fermentation residues refer to scenarios for the use (or allocation) of unfermented residues: S = steam, E = electricity, C = emission credit applied for surplus steam (SC) and/or electricity (EC) when available, SWf = balance of energy (when needed) from switchgrass combustion, Energy allocation = no direct use of fermentation residues, but emissions allocated to residue and PHB on the basis of energy content**

**Table S-23. Modeled greenhouse gas emissions (mean and 95% confidence interval) from polymers produced using corn bioethylene (kg $CO_2$e / kg plastic)**

| Treatment of corn co-products | Plastic | Mean | 2.5% | 97.5% |
|---|---|---|---|---|
| **System Expansion** | HDPE | 0.84 | 0.07 | 1.79 |
| | LDPE | 1.10 | 0.30 | 2.08 |
| | LLDPE | 0.84 | 0.06 | 1.79 |
| | PET | 2.24 | 2.00 | 2.53 |
| | PS (GPPS) | 2.90 | 2.54 | 3.34 |
| | HIPS | 2.89 | 2.53 | 3.32 |
| | PVC | 1.87 | 1.47 | 2.36 |
| **Mass Allocation** | HDPE | -0.15 | -0.72 | 0.55 |
| | LDPE | 0.09 | -0.50 | 0.81 |
| | LLDPE | -0.16 | -0.73 | 0.54 |
| | PET | 2.06 | 1.85 | 2.31 |
| | PS (GPPS) | 2.61 | 2.30 | 3.00 |
| | HIPS | 2.61 | 2.30 | 3.01 |
| | PVC | 1.42 | 1.11 | 1.81 |
| **Energy Allocation** | HDPE | 0.13 | -0.51 | 0.88 |
| | LDPE | 0.37 | -0.28 | 1.16 |
| | LLDPE | 0.12 | -0.52 | 0.88 |
| | PET | 2.11 | 1.89 | 2.37 |
| | PS (GPPS) | 2.69 | 2.37 | 3.09 |
| | HIPS | 2.69 | 2.37 | 3.09 |
| | PVC | 1.55 | 1.21 | 1.96 |
| **No Allocation** | HDPE | 1.50 | 0.55 | 2.68 |
| | LDPE | 1.77 | 0.80 | 2.97 |
| | LLDPE | 1.51 | 0.55 | 2.70 |
| | PET | 2.36 | 2.09 | 2.67 |
| | PS (GPPS) | 3.10 | 2.70 | 3.59 |
| | HIPS | 3.07 | 2.68 | 3.55 |
| | PVC | 2.18 | 1.70 | 2.77 |

**Table S-24. Modeled greenhouse gas emissions (mean and 95% confidence interval) from polymers produced using switchgrass bioethylene with near-term yield (kg $CO_2$e / kg plastic)**

| Treatment of fermentation residues | Plastic | Mean | 2.5% | 97.5% |
|---|---|---|---|---|
| None | HDPE | 3.33 | 1.33 | 6.26 |
| | LDPE | 3.64 | 1.58 | 6.62 |
| | LLDPE | 3.35 | 1.33 | 6.31 |
| | PET | 2.69 | 2.27 | 3.26 |
| | PS (GPPS) | 3.64 | 2.97 | 4.56 |
| | HIPS | 3.58 | 2.94 | 4.45 |
| | PVC | 3.01 | 2.07 | 4.37 |
| Steam for internal use only (S) | HDPE | 1.43 | -0.39 | 4.32 |
| | LDPE | 1.70 | -0.16 | 4.64 |
| | LLDPE | 1.43 | -0.40 | 4.35 |
| | PET | 2.34 | 1.96 | 2.90 |
| | PS (GPPS) | 3.08 | 2.46 | 3.96 |
| | HIPS | 3.05 | 2.46 | 3.89 |
| | PVC | 2.14 | 1.28 | 3.48 |
| Steam for internal use and with system expansion credit for surplus (S, SC) | HDPE | -3.1 | -5.5 | -0.1 |
| | LDPE | -3.0 | -5.4 | 0.1 |
| | LLDPE | -3.2 | -5.6 | -0.1 |
| | PET | 1.5 | 1.1 | 2.1 |
| | PS (GPPS) | 1.7 | 1.0 | 2.6 |
| | HIPS | 1.8 | 1.1 | 2.6 |
| | PVC | 0.1 | -1.0 | 1.4 |
| Steam and electricity for internal use only (S, E) | HDPE | 0.92 | -0.89 | 3.79 |
| | LDPE | 1.18 | -0.67 | 4.12 |
| | LLDPE | 0.92 | -0.91 | 3.82 |
| | PET | 2.25 | 1.87 | 2.81 |
| | PS (GPPS) | 2.92 | 2.32 | 3.81 |
| | HIPS | 2.91 | 2.33 | 3.75 |
| | PVC | 1.91 | 1.05 | 3.25 |
| Steam and electricity, with system expansion credits for surplus electricity (S, E, EC) | HDPE | -1.92 | -3.83 | 0.91 |
| | LDPE | -1.71 | -3.67 | 1.16 |
| | LLDPE | -1.95 | -3.88 | 0.92 |
| | PET | 1.73 | 1.33 | 2.28 |
| | PS (GPPS) | 2.08 | 1.46 | 2.97 |
| | HIPS | 2.12 | 1.52 | 2.96 |
| | PVC | 0.61 | -0.29 | 1.91 |
| Steam and electricity, with system expansion credits for both surplus electricity and surplus steam (S, E, SC, EC) | HDPE | -4.4 | -7.0 | -1.4 |
| | LDPE | -4.2 | -6.9 | -1.2 |
| | LLDPE | -4.5 | -7.1 | -1.4 |
| | PET | 1.3 | 0.8 | 1.9 |
| | PS (GPPS) | 1.3 | 0.6 | 2.3 |
| | HIPS | 1.4 | 0.7 | 2.3 |
| | PVC | -0.5 | -1.7 | 0.8 |

**Table S-25. Modeled greenhouse gas emissions (mean and 95% confidence interval) from polymers produced using switchgrass bioethylene with mid-term yield (kg $CO_2$e / kg plastic)**

| Treatment of fermentation residues | Plastic | Mean | 2.5% | 97.5% |
|---|---|---|---|---|
| None | HDPE | 1.93 | 0.61 | 3.69 |
| | LDPE | 2.21 | 0.86 | 4.00 |
| | LLDPE | 1.94 | 0.61 | 3.72 |
| | PET | 2.43 | 2.12 | 2.83 |
| | PS (GPPS) | 3.22 | 2.74 | 3.85 |
| | HIPS | 3.19 | 2.72 | 3.79 |
| | PVC | 2.37 | 1.73 | 3.21 |
| Steam for internal use only (S) | HDPE | 0.03 | -1.03 | 1.65 |
| | LDPE | 0.27 | -0.81 | 1.92 |
| | LLDPE | 0.02 | -1.05 | 1.66 |
| | PET | 2.09 | 1.82 | 2.45 |
| | PS (GPPS) | 2.66 | 2.25 | 3.23 |
| | HIPS | 2.66 | 2.26 | 3.20 |
| | PVC | 1.50 | 0.98 | 2.26 |
| Steam for internal use and with system expansion credit for surplus (S, SC) | HDPE | -0.5 | -1.8 | 1.2 |
| | LDPE | -0.3 | -1.6 | 1.5 |
| | LLDPE | -0.5 | -1.8 | 1.2 |
| | PET | 2.0 | 1.7 | 2.4 |
| | PS (GPPS) | 2.5 | 2.0 | 3.1 |
| | HIPS | 2.5 | 2.1 | 3.1 |
| | PVC | 1.3 | 0.6 | 2.0 |
| Steam and electricity for internal use only (S, E) | HDPE | -0.42 | -1.49 | 1.20 |
| | LDPE | -0.18 | -1.28 | 1.46 |
| | LLDPE | -0.43 | -1.52 | 1.21 |
| | PET | 2.01 | 1.74 | 2.37 |
| | PS (GPPS) | 2.53 | 2.11 | 3.09 |
| | HIPS | 2.54 | 2.13 | 3.08 |
| | PVC | 1.30 | 0.76 | 2.06 |
| Steam and electricity, with system expansion credits for surplus electricity (S, E, EC) | HDPE | -0.93 | -2.26 | 0.89 |
| | LDPE | -0.70 | -2.05 | 1.15 |
| | LLDPE | -0.95 | -2.28 | 0.88 |
| | PET | 1.92 | 1.61 | 2.30 |
| | PS (GPPS) | 2.38 | 1.91 | 2.99 |
| | HIPS | 2.40 | 1.94 | 2.98 |
| | PVC | 1.06 | 0.43 | 1.90 |
| Steam and electricity, with system expansion credits for both surplus electricity and surplus steam (S, E, SC, EC) | HDPE | -1.0 | -2.3 | 0.9 |
| | LDPE | -0.7 | -2.1 | 1.1 |
| | LLDPE | -1.0 | -2.4 | 0.9 |
| | PET | 1.9 | 1.6 | 2.3 |
| | PS (GPPS) | 2.4 | 1.9 | 3.0 |
| | HIPS | 2.4 | 1.9 | 3.0 |
| | PVC | 1.0 | 0.4 | 1.9 |

### *S.2.4 Cradle-to-gate comparison to original data sources*

GHG emission results from the present study often differ from the results reported by the authors of the original data sources used to parametrize each PLA and PHB case. Table S-26 shows a breakdown of these differences for corn PLA, and Table S-27 shows a breakdown of these differences for corn PHB. Both tables include commentary on the reasons for these differences.

The model for bioethylene is an updated version of the one published by Posen *et al.* (2015) [3], and follows a similar model structure. Emissions from corn bioethylene are lower in the present paper due primarily to a lower estimate for LUC emissions. Differences in emissions for switchgrass bioethylene are generally due to updates to the pre-treatment module, different ethanol yield scenarios, and more detailed modeling of scenarios for energy generation from fermentation residues. Posen *et al.* (2015) [3] also estimated emissions from production of bio-LDPE in Brazil, using sugarcane as a feedstock (mean: -1.3 kg $CO_2$e / kg LDPE), which is similar to results from the more optimistic switchgrass bio-LDPE scenarios in the present paper. Likewise, results from the more optimistic switchgrass bio-HDPE scenarios in the present paper are in the same range as emissions previously reported for Braskem's bio-HDPE production using Brazilian sugarcane (-2.15 kg $CO_2$e / kg HDPE) [80]. Braskem is currently among the largest producers of bioethylene based plastics [81].

**Table S-26. Comparison of life cycle corn PLA emissions between this study (mean results) and original data sources. All values in kg $CO_2$e/kg PLA. The column heading F&P stands for fermentation and polymerization. The column heading $CO_2$ credit refers to the $CO_2$ absorbed during agriculture, and then sequestered in the plastic. Abbreviations used in the row headings refer to system expansion (SE) and mass allocation (MA). All studies include the same credit of 1.8 kg $CO_2$/kg PLA to arrive at the total cradle-to-gate emissions value. Differences in upstream emissions between cases from this study are due to different product yields.**

| | Upstream | | | F&P | $CO_2$ Credit | Total | Comments |
|---|---|---|---|---|---|---|---|
| | *Corn production* | *Wet milling* | *Co-product credit* | | | | |
| **Groot *et al.* (2010) [34]** | 0.1 (sugarcane, not corn) | | | 2.2 | -1.8 | 0.502 | Groot *et al.* (2010) [34] is based on production from sugarcane in Thailand, and so upstream results are not comparable. Minor differences in F&P are due to the use of an updated GWP characterization factor for $CH_4$ emissions, and small differences in natural gas and electricity emission factors. |
| **This study, case 1 (SE)** | 1.0 | 0.64 | -0.37 | 2.3 | -1.8 | 1.8 | |
| | | | | | | | |
| **Vink *et al.* (2015) [23] (MA)** | 0.25 | 0.29 | - | 1.9 | -1.8 | 0.62 | Vink *et al.* (2015) [23] do not include emissions from land use change (which adds 0.12 kg $CO_2$e/kg PLA). Beyond this, that study provides insufficient data to compare corn production emissions. Vink *et al.* (2015) provides the lower bound for the distribution of wet milling emissions employed in this study. Other estimates are 44%, 54% and 90% higher, respectively. Small differences in wet milling and F&P are also due to the updated GWP characterization factor for $CH_4$ emissions used in this study. |
| **This study, case 2 (MA)** | 0.77 | 0.48 | - | 2.0 | -1.8 | 1.4 | |
| **This study, case 2 (SE)** | 1.2 | 0.7 | -0.42 | 2.0 | -1.8 | 1.6 | The original data source (Vink *et al.* 2015) uses mass allocation, which is more favorable to PLA than system expansion. |
| | | | | | | | |
| **Sakai *et al.* (2004) [37]** | - | - | - | - | - | - | Cases 3 and 4 are also based on Vink *et al.* (2015) [23], but use Sakai *et al.* (2004) [37] for polymerization energy requirements. Sakai *et al.* (2004) [37] do not report GHG emissions. |
| **This study, case 3 (SE)** | Same as case 2 | | | 2.8 | -1.8 | 2.4 | |
| **This study, case 4 (SE)** | Same as case 2 | | | 1.7 | -1.8 | 1.4 | |

**Table S-27. Comparison of life cycle corn PHB emissions between this study (mean results) and original data sources. All values in kg $CO_2$e/kg PHB (or PHA). The column heading F&R stands for fermentation and recovery. The column heading $CO_2$ credit refers to the $CO_2$ absorbed during agriculture, and then sequestered in the plastic. Abbreviations used in the row headings refer to system expansion (SE) and mass allocation (MA). Differences in upstream emissions between cases from this study are due to different product yields.**

| | Upstream | | | F&R | $CO_2$ credit | Total | Comments |
|---|---|---|---|---|---|---|---|
| | *Corn production* | *Wet milling* | *Co-product credit* | | | | |
| **Harding *et al.* (2007) [38]** | - | - | - | - | ? | 1.96 or 2.6 | Harding et al. (2007) [38] is based on production from sugarcane in South Africa, and so results are not comparable to this study. The authors report conflicting values (1.96 and 2.6) for total emissions in different parts of the paper without explanation. |
| **This study, case 1 (SE)** | 2.1 | 1.3 | -0.76 | 2.3 | -2.05 | 2.9 | |
| | | | | | | | |
| **Akiyama *et al.* (2003) [20] case 9 (MA)** | 0.4 | 1.0 | - | 1.87 | -2.8 | 0.48 | Akiyama *et al.* (2003) [20] use a lower emissions factor for electricity, and some fuels. Further, they do not appear to account for emissions from LUC. Other differences in agricultural emissions likely stem from different assumptions regarding fertilizer use and/or $N_2O$ emissions rate. Akiyama *et al.* (2003) provide the upper bound for the distribution of emissions from wet milling employed in this study. Differences in F&R are primarily due to different electricity emissions factors. Akiyama *et al.* (2003) apply an emissions credit directly to $CO_2$ sequestered in glucose, which surpasses the sum of $CO_2$ released during fermentation and stored in PHB. No explanation is given. |
| **This study, case 2 (MA)** | 1.3 | 0.8 | - | 2.2 | -2.05 | 2.3 | |
| **This study, case 2 (SE)** | 2.1 | 1.3 | -0.74 | 2.2 | -2.05 | 2.7 | |
| | | | | | | | |
| **Akiyama *et al.* (2003) [20] case 10 (MA)** | 0.5 | 1.2 | - | 2.31 | -2.7 | 1.39 | |
| **This study, case 3 (MA)** | 1.6 | 1.0 | - | 2.9 | -2.05 | 3.5 | |
| **This study, case 3 (SE)** | 2.5 | 1.6 | -0.9 | 2.9 | -2.05 | 4.0 | |
| | | | | | | | |
| **Kim and Dale (2008) [24] (SE)** | 0.97 | 0.06 | -0.45 | 0.33 | -2.05 | -2.3 | Kim and Dale (2008) [24] also include emissions from collection of stover (0.25) and a credit for using fermentation residues (-1.4) (not shown in table). Kim and Dale (2008) assume slightly lower fertilizer application rates with slightly higher yields, and more favorable tillage practices than we do, while excluding other emissions from LUC. Most of the energy used in their wet milling and F&R processes is generated in a CHP power plant by combustion of corn stover, with the remainder from wind power. Our model assumes the process will use conventional energy sources. Finally, they assume corn fermentation residues are used to displace coal in a CHP plant, whereas we assume these residues displace only natural gas for steam generation. |
| **This study, case 4 (SE)** | 2.1 | 1.3 | -0.77 | 3.2 | -2.05 | 3.8 | |
| | | | | | | | |
| **Gerngross (1999) [39]** | - | - | - | - | - | - | Gerngross (1999) [39] does not report GHG emissions |
| **This study, case 5 (SE)** | 2.5 | 1.6 | -0.9 | 5.7 | -2.05 | 6.9 | |

### *S.2.5 Graphical results for polymer life cycle GHG emissions, including EOL*

Figure 6 in the main text presents the difference in emissions that result from switching from fossil-based polymers to each of the main corn-based or switchgrass-based production pathways, on a cradle to gate basis. The following figures similarly present the difference in emissions between fossil-based and bio-based polymers, but accounting for end of life (EOL) emissions. Figure S-2 presents alternate EOL scenarios for PHB pathways. Panels a), b) and c) present the optimistic case for corn PHB (case 2, system expansion). Only when fossil plastics and PHB are both incinerated (panel c) is there any probability that corn PHB will have lower emissions than any fossil polymer. Panels d), e) and f) present the 'full distribution' case for switchgrass, assuming fermentation residues are used to generate steam and electricity, and applying a system expansion credit for surplus electricity. Even under this relatively optimistic scenario for the treatment of fermentation residues, landfilled PHB likely has higher emissions than all fossil polymers (panel d), and composted PHB has approximately comparable emissions to most fossil polymers (panel e). When both PHB and fossil polymers are incinerated, however, switchgrass PHB results in lower GHG emissions than all fossil polymers, with probability approaching 1 (panel f).

Figure S-3 presents alternate EOL scenarios for PLA pathways. Panels a), b) and c) present the results for corn PLA (case 1, system expansion). The landfill scenario (panel a) is equivalent to the cradle to gate model, since landfill emissions are the same for both PLA and fossil plastics. Composted corn PLA (panel b) has higher emissions than all fossil plastics. Under an

incineration scenario (panel c), corn PLA offers slightly greater GHG reductions than in the cradle to gate model. This is because incineration increases the emissions from fossil polymers by more than the emissions from PLA. Panels d), e) and f) present the results for switchgrass PLA (case 1), assuming fermentation residues are used to generate steam and electricity, and applying a system expansion credit for surplus electricity. Under a landfill or incineration scenario (panels d and f), PLA has lower emissions than all fossil plastics with probability approaching 1. When switchgrass PLA is composted (and fossil plastics are landfilled), however, there is only a low chance (<40%) that PLA has lower life cycle emissions than LDPE, HDPE or PP. Finally, bioethylene based polymers are identical to their fossil counterparts, so EOL scenarios do not affect the comparison between the two.

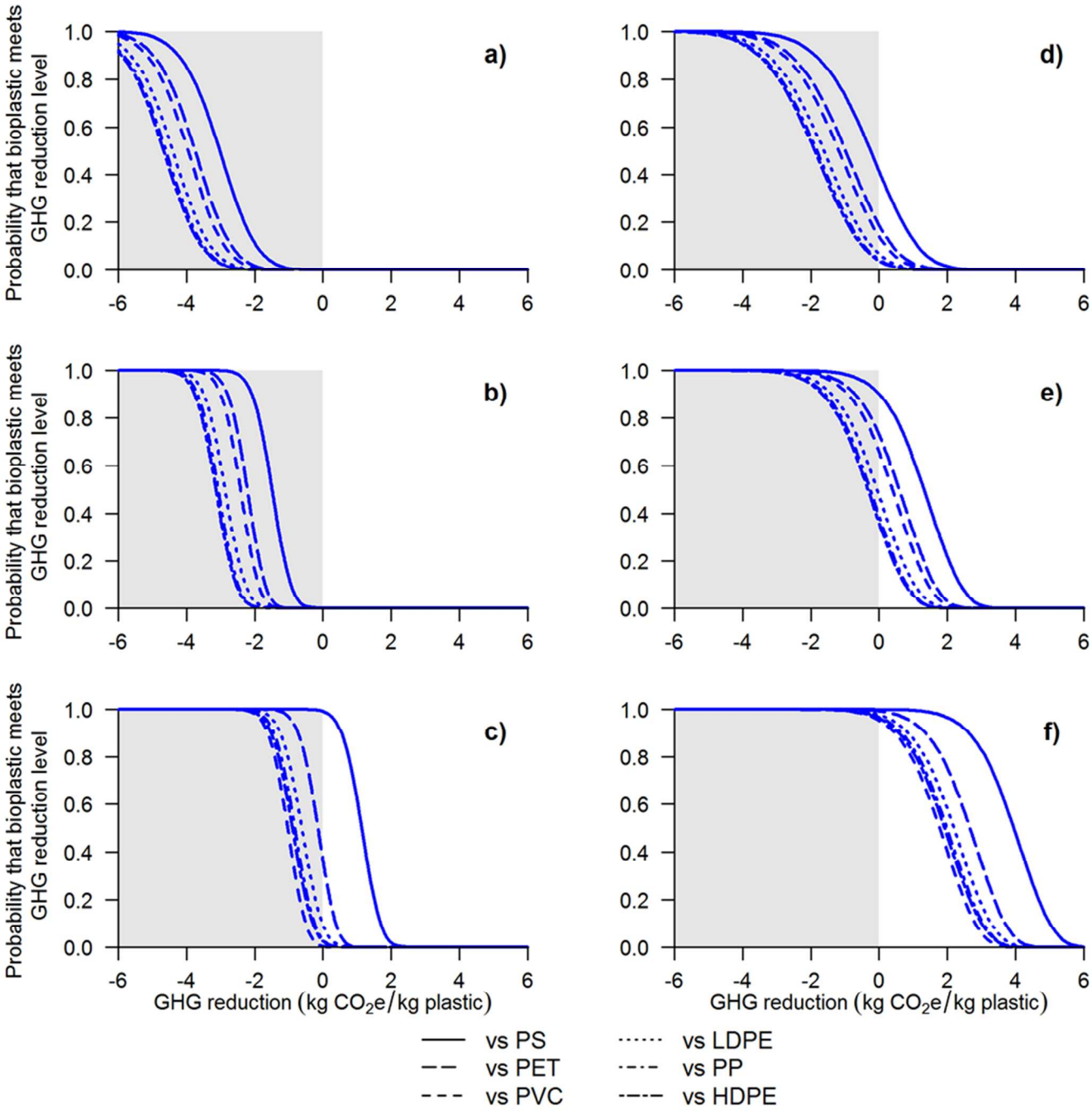


**Figure S-2. Difference in GHG emissions between PHB and fossil plastics. Positive numbers (white background) indicate the bioplastic has lower GHG emissions than the fossil plastic. Negative numbers (gray background) indicate the bioplastic has higher GHG emissions than the fossil plastic. Panels a), b) and c) represent corn PHB (optimistic: case 2, system expansion), under landfill, compost or incineration scenarios, respectively. Panels d), e) and f) represent switchgrass PHB (full distribution), under landfill, compost or incineration scenarios, respectively. All switchgrass cases include generation of steam and electricity from unfermented switchgrass, together with a system expansion credit for surplus electricity, when available. Within a panel, each line represents a different fossil plastic for comparison. For the PHB landfill and compost scenarios (panels a), b), d) and e)), the model assumes fossil plastics are landfilled. For the PHB incineration scenario (panels c) and f)), the model assumes fossil plastics are also incinerated.**

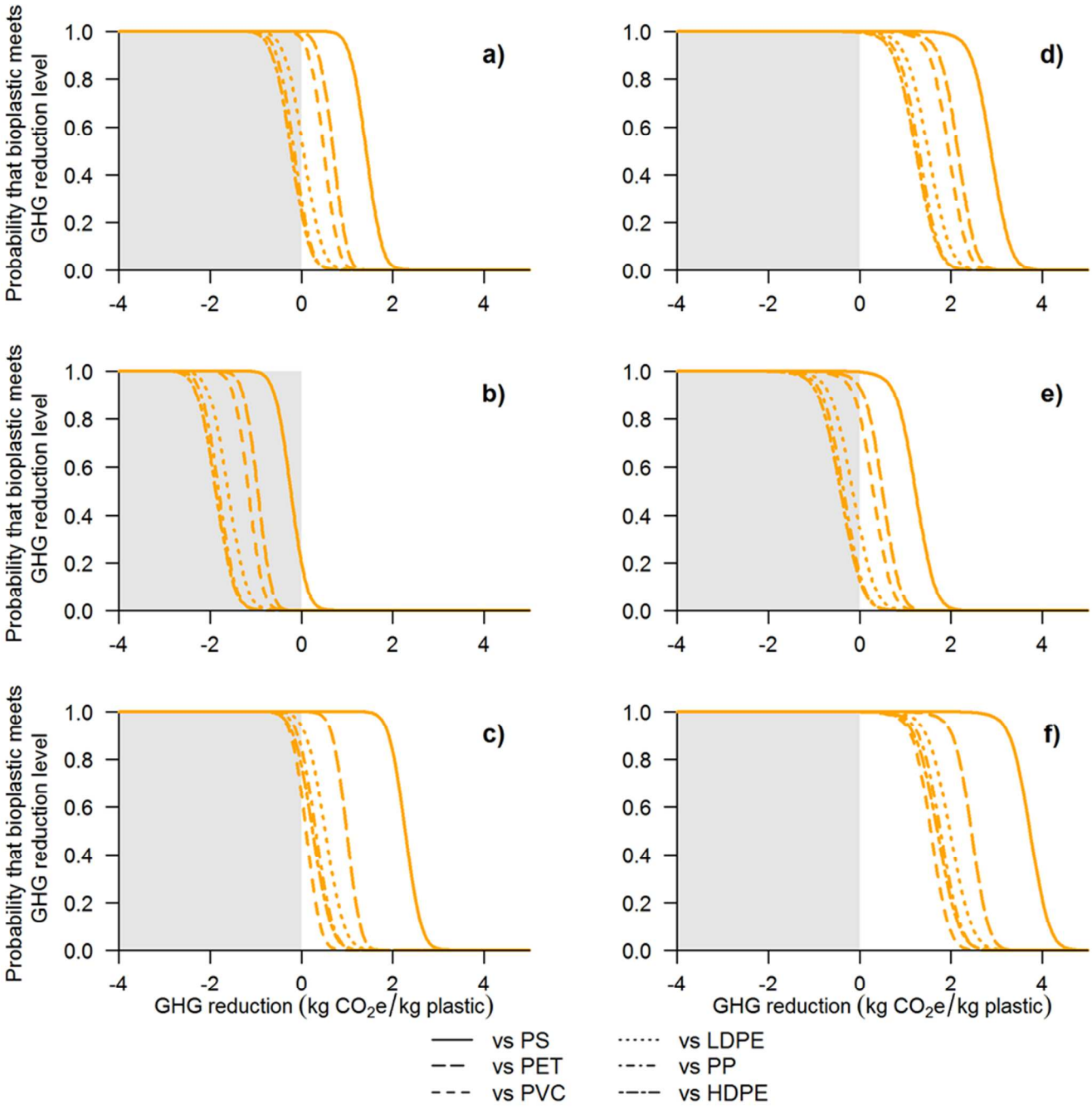


**Figure S-3. Difference in GHG emissions between PLA and fossil plastics. Positive numbers indicate PLA has lower GHG emissions than the fossil plastic. Negative numbers (gray background) indicate PLA has higher GHG emissions than the fossil plastic. Panels a), b) and c) represent corn PLA (baseline: case 2, system expansion), under landfill, compost or incineration scenarios, respectively. Panels d), e) and f) represent switchgrass PLA (case 2), under landfill, compost or incineration scenarios, respectively. Switchgrass cases include generation of steam and electricity from unfermented residues, plus a system expansion credit for surplus electricity, when available. Within a panel, each line represents a different fossil plastic for comparison. For the PLA landfill and compost scenarios (panels a), b), d) and e)), the model assumes fossil plastics are landfilled. For the PLA incineration scenario (panels c) and f)), the model assumes fossil plastics are also incinerated.**

### *S.2.6 Numerical results for GHG savings from corn bioplastics, with additional scenarios*

The following tables (Table S-28 to Table S-32) present results for the difference in GHG emissions between select corn bioplastic pathways and fossil plastics, on a cradle to gate basis, under a range of different modeling assumptions. Pathways correspond to those singled out in the main text: the optimistic scenario for corn PHB (case 2), the baseline scenario for corn PLA (case 2), and the model for corn bioethylene based polymers. Both corn co-products and fossil polymer hydrogen co-product are treated by system expansion.

Table S-28 shows baseline results, corresponding to figure 6 of the main text. As discussed in section S.1.3, this paper uses a $N_2O$ emissions factors for applied nitrogen in agriculture that is higher than the default value from the IPCC guidelines [12]. Thus, Table S-29 presents results assuming a lower (deterministic) $N_2O$ emissions factor of 1.325% for all applied nitrogen, calculated using the IPCC methodology [12]. Finally, to account for deep uncertainty in emissions from land use change (LUC), this section includes results from 3 alternate LUC scenarios. Table S-30 presents results assuming there are no LUC emissions – this serves as a lower bound. Table S-31 presents results using a distribution for corn LUC emissions approximately fit to the results from the 'food consumption not fixed' scenario reported by Plevin *et al*. (2015) [82]. The distribution we employ is lognormal with mean = 24.4 and stdev = 7.5; this fits the 95% confidence interval reported by Plevin *et al*. (2015) [82]. Finally, Table S-32 presents results for a 'high LUC' scenario, of 1 kg $CO_2$e / kg dry corn, which corresponds approximately to 100 g $CO_2$e / MJ ethanol.

**Table S-28. Difference in GHG emissions (mean and 95% confidence interval) between bioplastics and fossil plastics, on a cradle to gate basis (kg $CO_2$e/kg plastic). Positive numbers indicate the bioplastic has lower GHG emissions than the fossil plastic. The table also shows the probability that the bioplastic has lower GHG emissions than the fossil plastic (P>0). Fossil plastics are all modeled using system expansion for hydrogen co-product. This table presents baseline results, corresponding to figure 6 of the main text.**

| Bio-plastic | Fossil Plastic | Mean | 2.5% | 97.5% | P(>0) |
|---|---|---|---|---|---|
| **Corn PHB (optimistic, case 2, system expansion) (Base model)** | HDPE | -1.30 | -2.25 | -0.40 | 0.3% |
| | LDPE | -1.03 | -1.99 | -0.13 | 1.2% |
| | PP | -1.24 | -2.17 | -0.37 | 0.3% |
| | PET | -0.39 | -1.26 | 0.40 | 18% |
| | PS | 0.34 | -0.57 | 1.18 | 78% |
| | PVC | -0.59 | -1.47 | 0.20 | 8% |
| **Corn PLA (baseline, case 2, system expansion) (Base model)** | HDPE | -0.22 | -0.85 | 0.40 | 24% |
| | LDPE | 0.05 | -0.59 | 0.69 | 56% |
| | PP | -0.16 | -0.75 | 0.42 | 30% |
| | PET | 0.69 | 0.20 | 1.15 | 100% |
| | PS | 1.42 | 0.88 | 1.98 | 100% |
| | PVC | 0.49 | -0.01 | 0.97 | 97% |
| **Corn Ethylene (system expansion) (Base model)** | HDPE | 0.59 | -0.45 | 1.50 | 88% |
| | LDPE | 0.60 | -0.45 | 1.52 | 88% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.11 | -0.08 | 0.27 | 88% |
| | PS | 0.17 | -0.13 | 0.44 | 88% |
| | PVC | 0.27 | -0.20 | 0.69 | 88% |

**Table S-29. Difference in GHG emissions (mean and 95% confidence interval) between bioplastics and fossil plastics, on a cradle to gate basis (kg CO2e/kg plastic). Positive numbers indicate the bioplastic has lower GHG emissions than the fossil plastic. The table also shows the probability that the bioplastic has lower GHG emissions than the fossil plastic (P>0). Fossil plastics are all modeled using system expansion for hydrogen co-product. This table presents results assuming a lower $N_2O$ emissions factor (1.325%) for applied fertilizer and crop residue.**

| Bio-plastic | Fossil Plastic | Mean | 2.5% | 97.5% | P(>0) |
|---|---|---|---|---|---|
| **Corn PHB (optimistic, case 2, system expansion) (low $N_2O$ emissions)** | HDPE | -1.04 | -1.88 | -0.25 | 0.5% |
| | LDPE | -0.78 | -1.61 | 0.02 | 2.9% |
| | PP | -0.98 | -1.77 | -0.23 | 0.5% |
| | PET | -0.13 | -0.83 | 0.53 | 37% |
| | PS | 0.60 | -0.14 | 1.31 | 94% |
| | PVC | -0.33 | -1.05 | 0.33 | 18.0% |
| **Corn PLA (baseline, case 2, system expansion) (low $N_2O$ emissions)** | HDPE | -0.07 | -0.62 | 0.50 | 39% |
| | LDPE | 0.20 | -0.36 | 0.78 | 74% |
| | PP | -0.01 | -0.51 | 0.52 | 48% |
| | PET | 0.84 | 0.47 | 1.23 | 100% |
| | PS | 1.57 | 1.13 | 2.08 | 100% |
| | PVC | 0.64 | 0.24 | 1.06 | 100% |
| **Corn Ethylene (system expansion) (low $N_2O$ emissions)** | HDPE | 0.92 | 0.19 | 1.64 | 99% |
| | LDPE | 0.93 | 0.19 | 1.67 | 99% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.17 | 0.03 | 0.30 | 99% |
| | PS | 0.27 | 0.06 | 0.49 | 99% |
| | PVC | 0.42 | 0.09 | 0.75 | 99% |

**Table S-30. Difference in GHG emissions (mean and 95% confidence interval) between bioplastics and fossil plastics, on a cradle to gate basis (kg CO2e/kg plastic). Positive numbers indicate the bioplastic has lower GHG emissions than the fossil plastic. The table also shows the probability that the bioplastic has lower GHG emissions than the fossil plastic (P>0). Fossil plastics are all modeled using system expansion for hydrogen co-product. This table presents results assuming there are no emissions from land use change (LUC).**

| Bio-plastic | Fossil Plastic | Mean | 2.5% | 97.5% | P(>0) |
|---|---|---|---|---|---|
| **Corn PHB (optimistic, case 2, system expansion) (No LUC)** | HDPE | -1.06 | -2.03 | -0.19 | 0.8% |
| | LDPE | -0.79 | -1.77 | 0.08 | 3.9% |
| | PP | -1.00 | -1.94 | -0.16 | 0.9% |
| | PET | -0.15 | -1.01 | 0.61 | 38% |
| | PS | 0.58 | -0.32 | 1.38 | 90% |
| | PVC | -0.35 | -1.23 | 0.42 | 21% |
| **Corn PLA (baseline, case 2, system expansion) (No LUC)** | HDPE | -0.08 | -0.72 | 0.54 | 40% |
| | LDPE | 0.19 | -0.45 | 0.81 | 72% |
| | PP | -0.02 | -0.61 | 0.55 | 47% |
| | PET | 0.83 | 0.35 | 1.27 | 100% |
| | PS | 1.56 | 1.02 | 2.10 | 100% |
| | PVC | 0.63 | 0.12 | 1.10 | 99% |
| **Corn Ethylene (system expansion) (No LUC)** | HDPE | 0.90 | -0.09 | 1.75 | 96% |
| | LDPE | 0.91 | -0.09 | 1.78 | 96% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.16 | -0.02 | 0.32 | 96% |
| | PS | 0.27 | -0.03 | 0.52 | 96% |
| | PVC | 0.41 | -0.04 | 0.80 | 96% |

**Table S-31. Difference in GHG emissions (mean and 95% confidence interval) between bioplastics and fossil plastics, on a cradle to gate basis (kg CO2e/kg plastic). Positive numbers indicate the bioplastic has lower GHG emissions than the fossil plastic. The table also shows the probability that the bioplastic has lower GHG emissions than the fossil plastic (P>0). Fossil plastics are all modeled using system expansion for hydrogen co-product. This table presents results assuming higher land use change (LUC) as modeled by Plevin *et al.* (2015)[82]**

| Bio-plastic | Fossil Plastic | Mean | 2.5% | 97.5% | P(>0) |
|---|---|---|---|---|---|
| **Corn PHB (optimistic, case 2, system expansion) (LUC from Plevin *et al.* 2015)** | HDPE | -1.76 | -2.81 | -0.79 | 0.1% |
| | LDPE | -1.49 | -2.54 | -0.52 | 0.2% |
| | PP | -1.69 | -2.72 | -0.77 | 0.1% |
| | PET | -0.84 | -1.82 | 0.02 | 3% |
| | PS | -0.11 | -1.11 | 0.78 | 42% |
| | PVC | -1.05 | -2.03 | -0.18 | 0.8% |
| **Corn PLA (baseline, case 2, system expansion) (LUC from Plevin *et al.* 2015)** | HDPE | -0.48 | -1.15 | 0.18 | 8% |
| | LDPE | -0.21 | -0.90 | 0.46 | 26% |
| | PP | -0.42 | -1.06 | 0.19 | 9% |
| | PET | 0.43 | -0.12 | 0.93 | 94% |
| | PS | 1.16 | 0.56 | 1.75 | 100% |
| | PVC | 0.23 | -0.33 | 0.74 | 80% |
| **Corn Ethylene (system expansion) (LUC from Plevin *et al.* 2015)** | HDPE | 0.01 | -1.15 | 0.99 | 52% |
| | LDPE | 0.01 | -1.17 | 1.01 | 52% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.00 | -0.21 | 0.18 | 52% |
| | PS | 0.00 | -0.34 | 0.29 | 52% |
| | PVC | 0.00 | -0.53 | 0.45 | 52% |

**Table S-32. Difference in GHG emissions (mean and 95% confidence interval) between bioplastics and fossil plastics, on a cradle to gate basis (kg CO2e/kg plastic). Positive numbers indicate the bioplastic has lower GHG emissions than the fossil plastic. The table also shows the probability that the bioplastic has lower GHG emissions than the fossil plastic (P>0). Fossil plastics are all modeled using system expansion for hydrogen co-product. This table presents results assuming a high value for land use change (1 kg $CO_2$e / kg corn)**

| Bio-plastic | Fossil Plastic | Mean | 2.5% | 97.5% | P(>0) |
|---|---|---|---|---|---|
| **Corn PHB (optimistic, case 2, system expansion) (High LUC)** | HDPE | -3.77 | -4.76 | -2.89 | 0.0% |
| | LDPE | -3.51 | -4.49 | -2.62 | 0.0% |
| | PP | -3.71 | -4.66 | -2.86 | 0.0% |
| | PET | -2.86 | -3.74 | -2.09 | 0% |
| | PS | -2.13 | -3.04 | -1.32 | 0% |
| | PVC | -3.06 | -3.95 | -2.28 | 0.0% |
| **Corn PLA (baseline, case 2, system expansion) (High LUC)** | HDPE | -1.64 | -2.29 | -1.02 | 0% |
| | LDPE | -1.38 | -2.02 | -0.74 | 0% |
| | PP | -1.58 | -2.18 | -1.01 | 0% |
| | PET | -0.73 | -1.22 | -0.29 | 0% |
| | PS | 0.00 | -0.55 | 0.54 | 50% |
| | PVC | -0.93 | -1.45 | -0.46 | 0% |
| **Corn Ethylene (system expansion) (High LUC)** | HDPE | -2.58 | -3.58 | -1.72 | 0% |
| | LDPE | -2.63 | -3.65 | -1.75 | 0% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | -0.47 | -0.65 | -0.31 | 0% |
| | PS | -0.76 | -1.06 | -0.51 | 0% |
| | PVC | -1.18 | -1.64 | -0.79 | 0% |

### *S.2.7 Numerical results for GHG savings from switchgrass bioplastics, with additional scenarios*

The following tables (Table S-33 to Table S-42) present results for the difference in GHG emissions between select switchgrass bioplastic pathways and fossil plastics, on a cradle to gate basis, under a range of different modeling assumptions. Fossil polymer hydrogen co-product is treated by system expansion.

Table S-33 shows baseline results, corresponding to figure 6 of the main text. Table S-34 shows results assuming that fermentation residues are only used to generate steam for the fermentation and recovery process. Table S-35 shows results assuming there is no use of fermentation residues. As discussed in section S.1.3, this paper uses a $N_2O$ emissions factors for applied nitrogen in agriculture that is higher than the default value from the IPCC guidelines [12]. Thus, Table S-36 presents results assuming a lower (deterministic) $N_2O$ emissions factor of 1.325% for all applied nitrogen, calculated from the IPCC methodology [12]. To account for deep uncertainty in emissions from land use change (LUC), this section includes results from 2 alternate LUC scenarios. Table S-37 presents results assuming there are no LUC emissions – this serves as a lower bound. Table S-38 presents results using a high estimate for LUC emissions (670 g $CO_2e$ / kg dry switchgrass), based on the Winrock scenario from the GREET CCLUB model [5], as discussed in section S.1.2. As explained in section S.1.10, the baseline model assumes that all switchgrass is either transformed into product, or available for energy recovery (as fermentation residues). Table S-39 presents results, assuming that only the non-soluble

portion of the switchgrass lignin (95% of the lignin) is available for energy recovery, as per GREET 2014 [5, 31].

As explained in section S.1.3, using the IPCC guidelines [16] to calculate nitrogen in switchgrass crop residue, results in an estimate for $N_2O$ emissions that is far higher than reported by other sources [5, 17, 18]. Thus, the baseline model used an estimate for above and below ground nitrogen from GREET 2014 (0.54 g nitrogen / kg switchgrass) [5]. Table S-40 presents results using the IPCC-based distribution (mean: 17g N / kg switchgrass). This value of crop residue is calculated as follows: From equation 11.6 of the IPCC guidelines [16]:

$$F_{CR} = Crop * (area - area\ burnt * C_f) * Frac_{Renew} * [R_{AG} * N_{AG} * (1 - Frac_{remove}) + R_{BG} * N_{BG}],$$

Where:

$AG_{DM}$ = Crop/1000*slope + intercept (from table 11.2)

$R_{AG} = AG_{DM} * 1000 / Crop$ = slope + intercept

$R_{BG} = R_{BG\text{-}BIO} * [(AG_{DM} * 1000 + Crop) / Crop] = R_{BG\text{-}BIO} * [slope + intercept + 1]$

The resulting equation for nitrogen in crop residue per kg dry switchgrass is:

$$F_{CR} / Crop = (area - area\ burnt * C_f) * Frac_{Renew} * [(slope + intercept) * N_{AG} * (1 - Frac_{remove}) + (R_{BG\text{-}BIO} * (slope + intercept + 1)) * N_{BG}],$$

These variables are all defined in the IPCC source document [16]. We use the following values:

- Area = 1
- Area burnt = 0
- $Frac_{renew}$ = 1
- Slope = triangular (min = 0.15, mode = 0.3, max = 0.45) (based on table 11.2)
- Intercept = 0
- $N_{AG}$ = 0.015 kg N / kg d.m. (table 11.2)
- $Frac_{remove}$ = 0
- $R_{BG\text{-}BIO}$ = triangular (min = 0.4, mode = 0.8, max = 1.2) (based on table 11.2)
- $N_{BG}$ = 0.012 kg N / kg d.m. (table 11.2)

Table S-41 presents results for a scenario with higher switchgrass crop yield: triangular distribution with min = 10, mode = 15, max = 30 (Mg dry matter / ha), based on the mid-term scenario of Spatari and MacLean (2010) [17]. Finally, Table S-42 presents results for a scenario in which switchgrass crop yield and applied nitrogen fertilizer are perfectly correlated (correlation coefficient of 1)

**Table S-33. Difference in GHG emissions (mean and 95% confidence interval) between bioplastics and fossil plastics, on a cradle to gate basis (kg CO2e/kg plastic). Positive numbers indicate the bioplastic has lower GHG emissions than the fossil plastic. The table also shows the probability that the bioplastic has lower GHG emissions than the fossil plastic (P>0). Fossil plastics are all modeled using system expansion for hydrogen co-product. Switchgrass fermentation residues are used to generate steam, and electricity, with surplus electricity receiving a system expansion credit. This table presents baseline results, consistent with figure 6 of the main text.**

| Bio-plastic | Fossil Plastic | Mean | 2.5% | 97.5% | P(>0) |
|---|---|---|---|---|---|
| **Switchgrass PHB (full distribution, S, E, EC) (Base model)** | HDPE | 1.44 | -0.57 | 3.03 | 93% |
| | LDPE | 1.71 | -0.30 | 3.31 | 96% |
| | PP | 1.51 | -0.50 | 3.06 | 94% |
| | PET | 2.36 | 0.38 | 3.86 | 99% |
| | PS | 3.09 | 1.07 | 4.64 | 100% |
| | PVC | 2.15 | 0.17 | 3.68 | 98% |
| **Switchgrass PLA (case 1, S, E, EC) (Base model)** | HDPE | 1.23 | 0.42 | 1.97 | 100% |
| | LDPE | 1.50 | 0.68 | 2.25 | 100% |
| | PP | 1.29 | 0.52 | 1.97 | 100% |
| | PET | 2.14 | 1.46 | 2.71 | 100% |
| | PS | 2.87 | 2.13 | 3.52 | 100% |
| | PVC | 1.94 | 1.23 | 2.54 | 100% |
| **Switchgrass ethylene plastics (near-term ethanol yield, S, E, EC) (Base model)** | HDPE | 3.35 | 0.46 | 5.33 | 98% |
| | LDPE | 3.41 | 0.47 | 5.43 | 98% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.61 | 0.08 | 0.97 | 98% |
| | PS | 0.99 | 0.14 | 1.58 | 98% |
| | PVC | 1.54 | 0.21 | 2.44 | 98% |
| **Switchgrass ethylene plastics (mid-term ethanol yield, S, E, EC) (Base model)** | HDPE | 2.36 | 0.48 | 3.79 | 99% |
| | LDPE | 2.40 | 0.48 | 3.85 | 99% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.43 | 0.09 | 0.69 | 99% |
| | PS | 0.70 | 0.14 | 1.12 | 99% |
| | PVC | 1.08 | 0.22 | 1.73 | 99% |

**Table S-34. Difference in GHG emissions (mean and 95% confidence interval) between bioplastics and fossil plastics, on a cradle to gate basis (kg CO2e/kg plastic). Positive numbers indicate the bioplastic has lower GHG emissions than the fossil plastic. The table also shows the probability that the bioplastic has lower GHG emissions than the fossil plastic (P>0). Fossil plastics are all modeled using system expansion for hydrogen co-product. Switchgrass fermentation residues are used to generate steam only.**

| Bio-plastic | Fossil Plastic | Mean | 2.5% | 97.5% | P(>0) |
|---|---|---|---|---|---|
| **Switchgrass PHB (full distribution, S)** | HDPE | 0.23 | -1.85 | 1.74 | 64% |
| | LDPE | 0.50 | -1.58 | 2.01 | 73% |
| | PP | 0.29 | -1.75 | 1.77 | 66% |
| | PET | 1.14 | -0.88 | 2.58 | 89% |
| | PS | 1.87 | -0.17 | 3.35 | 96% |
| | PVC | 0.94 | -1.08 | 2.39 | 85% |
| **Switchgrass PLA (case 1, S)** | HDPE | 1.02 | 0.25 | 1.67 | 99% |
| | LDPE | 1.29 | 0.51 | 1.96 | 100% |
| | PP | 1.09 | 0.36 | 1.69 | 99% |
| | PET | 1.94 | 1.28 | 2.41 | 100% |
| | PS | 2.67 | 1.97 | 3.25 | 100% |
| | PVC | 1.74 | 1.05 | 2.26 | 100% |
| **Switchgrass ethylene plastics (near-term ethanol yield, S)** | HDPE | 0.00 | -2.93 | 1.90 | 55% |
| | LDPE | 0.00 | -2.98 | 1.93 | 55% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.00 | -0.53 | 0.34 | 55% |
| | PS | 0.00 | -0.87 | 0.56 | 55% |
| | PVC | 0.00 | -1.34 | 0.87 | 55% |
| **Switchgrass ethylene plastics (mid-term ethanol yield, S)** | HDPE | 1.40 | -0.25 | 2.58 | 96% |
| | LDPE | 1.43 | -0.26 | 2.62 | 96% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.26 | -0.05 | 0.47 | 96% |
| | PS | 0.42 | -0.08 | 0.76 | 96% |
| | PVC | 0.64 | -0.12 | 1.18 | 96% |

**Table S-35. Difference in GHG emissions (mean and 95% confidence interval) between bioplastics and fossil plastics, on a cradle to gate basis (kg CO2e/kg plastic). Positive numbers indicate the bioplastic has lower GHG emissions than the fossil plastic. The table also shows the probability that the bioplastic has lower GHG emissions than the fossil plastic (P>0). Fossil plastics are all modeled using system expansion for hydrogen co-product. Switchgrass fermentation residues are not used.**

| Bio-plastic | Fossil Plastic | Mean | 2.5% | 97.5% | P(>0) |
|---|---|---|---|---|---|
| **Switchgrass PHB (full distribution, none)** | HDPE | -1.59 | -3.59 | -0.06 | 2.0% |
| | LDPE | -1.32 | -3.32 | 0.22 | 5.3% |
| | PP | -1.53 | -3.52 | 0.00 | 2% |
| | PET | -0.68 | -2.62 | 0.79 | 23% |
| | PS | 0.05 | -1.90 | 1.55 | 56% |
| | PVC | -0.88 | -2.82 | 0.59 | 16% |
| **Switchgrass PLA (case 1, none)** | HDPE | 0.12 | -0.64 | 0.76 | 65% |
| | LDPE | 0.39 | -0.38 | 1.04 | 87% |
| | PP | 0.18 | -0.55 | 0.78 | 73% |
| | PET | 1.03 | 0.37 | 1.51 | 99% |
| | PS | 1.76 | 1.07 | 2.31 | 100% |
| | PVC | 0.83 | 0.16 | 1.32 | 99% |
| **Switchgrass ethylene plastics (near-term ethanol yield, none)** | HDPE | -1.90 | -4.88 | 0.15 | 3.8% |
| | LDPE | -1.93 | -4.96 | 0.15 | 3.8% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | -0.35 | -0.89 | 0.03 | 3.8% |
| | PS | -0.56 | -1.44 | 0.04 | 3.8% |
| | PVC | -0.87 | -2.23 | 0.07 | 3.8% |
| **Switchgrass ethylene plastics (mid-term ethanol yield, none)** | HDPE | -0.49 | -2.25 | 0.88 | 28% |
| | LDPE | -0.50 | -2.29 | 0.90 | 28% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | -0.09 | -0.41 | 0.16 | 28% |
| | PS | -0.15 | -0.67 | 0.26 | 28% |
| | PVC | -0.23 | -1.03 | 0.40 | 28% |

**Table S-36. Difference in GHG emissions (mean and 95% confidence interval) between bioplastics and fossil plastics, on a cradle to gate basis (kg CO2e/kg plastic). Positive numbers indicate the bioplastic has lower GHG emissions than the fossil plastic. The table also shows the probability that the bioplastic has lower GHG emissions than the fossil plastic (P>0). Fossil plastics are all modeled using system expansion for hydrogen co-product. Switchgrass fermentation residues are used for steam and electricity, with a system expansion credit for surplus electricity generation. This table presents results assuming a lower $N_2O$ emissions factor (1.325%) for applied fertilizer and crop residue.**

| Bio-plastic | Fossil Plastic | Mean | 2.5% | 97.5% | P(>0) |
|---|---|---|---|---|---|
| **Switchgrass PHB (full distribution, S, E, EC) (Low $N_2O$)** | HDPE | 1.61 | -0.26 | 3.13 | 96% |
| | LDPE | 1.87 | 0.00 | 3.41 | 98% |
| | PP | 1.67 | -0.19 | 3.17 | 96% |
| | PET | 2.52 | 0.69 | 3.96 | 100% |
| | PS | 3.25 | 1.40 | 4.73 | 100% |
| | PVC | 2.32 | 0.49 | 3.77 | 99% |
| **Switchgrass PLA (case 1, S, E, EC) (Low $N_2O$)** | HDPE | 1.31 | 0.58 | 2.01 | 100% |
| | LDPE | 1.57 | 0.84 | 2.29 | 100% |
| | PP | 1.37 | 0.70 | 2.01 | 100% |
| | PET | 2.22 | 1.65 | 2.75 | 100% |
| | PS | 2.95 | 2.32 | 3.56 | 100% |
| | PVC | 2.02 | 1.42 | 2.58 | 100% |
| **Switchgrass ethylene plastics (near-term ethanol yield, S, E, EC) (Low $N_2O$)** | HDPE | 3.70 | 1.56 | 5.49 | 100% |
| | LDPE | 3.77 | 1.59 | 5.59 | 100% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.67 | 0.28 | 1.00 | 100% |
| | PS | 1.09 | 0.46 | 1.62 | 100% |
| | PVC | 1.69 | 0.71 | 2.51 | 100% |
| **Switchgrass ethylene plastics (mid-term ethanol yield, S, E, EC) (Low $N_2O$)** | HDPE | 2.56 | 0.94 | 3.88 | 100% |
| | LDPE | 2.60 | 0.96 | 3.95 | 100% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.47 | 0.17 | 0.70 | 100% |
| | PS | 0.76 | 0.28 | 1.15 | 100% |
| | PVC | 1.17 | 0.43 | 1.78 | 100% |

**Table S-37. Difference in GHG emissions (mean and 95% confidence interval) between bioplastics and fossil plastics, on a cradle to gate basis (kg CO2e/kg plastic). Positive numbers indicate the bioplastic has lower GHG emissions than the fossil plastic. The table also shows the probability that the bioplastic has lower GHG emissions than the fossil plastic (P>0). Fossil plastics are all modeled using system expansion for hydrogen co-product. Switchgrass fermentation residues are used for steam and electricity, with a system expansion credit for surplus electricity generation. This table presents results assuming there are no emissions from land use change (LUC)**

| Bio-plastic | Fossil Plastic | Mean | 2.5% | 97.5% | P(>0) |
|---|---|---|---|---|---|
| **Switchgrass PHB (full distribution, S, E, EC) (No LUC)** | HDPE | 1.87 | -0.06 | 3.33 | 97% |
| | LDPE | 2.14 | 0.20 | 3.60 | 98% |
| | PP | 1.93 | 0.02 | 3.35 | 98% |
| | PET | 2.78 | 0.89 | 4.15 | 100% |
| | PS | 3.52 | 1.62 | 4.92 | 100% |
| | PVC | 2.58 | 0.71 | 3.96 | 99% |
| **Switchgrass PLA (case 1, S, E, EC) (No LUC)** | HDPE | 1.43 | 0.68 | 2.09 | 100% |
| | LDPE | 1.70 | 0.94 | 2.38 | 100% |
| | PP | 1.49 | 0.78 | 2.10 | 100% |
| | PET | 2.34 | 1.70 | 2.83 | 100% |
| | PS | 3.07 | 2.39 | 3.66 | 100% |
| | PVC | 2.14 | 1.48 | 2.67 | 100% |
| **Switchgrass ethylene plastics (near-term ethanol yield, S, E, EC) (No LUC)** | HDPE | 4.26 | 1.62 | 5.75 | 99% |
| | LDPE | 4.34 | 1.64 | 5.85 | 99% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.77 | 0.29 | 1.05 | 99% |
| | PS | 1.26 | 0.48 | 1.70 | 99% |
| | PVC | 1.95 | 0.74 | 2.63 | 99% |
| **Switchgrass ethylene plastics (mid-term ethanol yield, S, E, EC) (No LUC)** | HDPE | 2.88 | 1.13 | 4.03 | 100% |
| | LDPE | 2.93 | 1.15 | 4.10 | 100% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.52 | 0.21 | 0.73 | 100% |
| | PS | 0.85 | 0.33 | 1.19 | 100% |
| | PVC | 1.32 | 0.52 | 1.85 | 100% |

**Table S-38. Difference in GHG emissions (mean and 95% confidence interval) between bioplastics and fossil plastics, on a cradle to gate basis (kg CO2e/kg plastic). Positive numbers indicate the bioplastic has lower GHG emissions than the fossil plastic. The table also shows the probability that the bioplastic has lower GHG emissions than the fossil plastic (P>0). Fossil plastics are all modeled using system expansion for hydrogen co-product. Switchgrass fermentation residues are used for steam and electricity, with a system expansion credit for surplus electricity generation. This table presents results assuming a higher value of land use change (LUC) as per the Winrock scenario in the GREET CCLUB model [5].**

| Bio-plastic | Fossil Plastic | Mean | 2.5% | 97.5% | P(>0) |
|---|---|---|---|---|---|
| **Switchgrass PHB (full distribution, S, E, EC) (High LUC)** | HDPE | -1.09 | -2.99 | 0.33 | 9% |
| | LDPE | -0.83 | -2.72 | 0.61 | 18% |
| | PP | -1.03 | -2.93 | 0.37 | 10% |
| | PET | -0.18 | -2.05 | 1.16 | 45% |
| | PS | 0.55 | -1.34 | 1.94 | 76% |
| | PVC | -0.38 | -2.24 | 0.97 | 36% |
| **Switchgrass PLA (case 1, S, E, EC) (High LUC)** | HDPE | 0.04 | -0.71 | 0.69 | 56% |
| | LDPE | 0.30 | -0.45 | 0.97 | 82% |
| | PP | 0.10 | -0.60 | 0.69 | 64% |
| | PET | 0.95 | 0.30 | 1.42 | 99% |
| | PS | 1.68 | 0.99 | 2.25 | 100% |
| | PVC | 0.75 | 0.08 | 1.27 | 98% |
| **Switchgrass ethylene plastics (near-term ethanol yield, S, E, EC) (High LUC)** | HDPE | -2.01 | -4.77 | -0.56 | 0% |
| | LDPE | -2.05 | -4.86 | -0.57 | 0% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | -0.37 | -0.87 | -0.10 | 0% |
| | PS | -0.59 | -1.41 | -0.16 | 0% |
| | PVC | -0.92 | -2.18 | -0.26 | 0% |
| **Switchgrass ethylene plastics (mid-term ethanol yield, S, E, EC) (High LUC)** | HDPE | -0.69 | -2.42 | 0.46 | 17% |
| | LDPE | -0.70 | -2.47 | 0.47 | 17% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | -0.13 | -0.44 | 0.08 | 17% |
| | PS | -0.20 | -0.72 | 0.14 | 17% |
| | PVC | -0.32 | -1.11 | 0.21 | 17% |

**Table S-39. Difference in GHG emissions (mean and 95% confidence interval) between bioplastics and fossil plastics, on a cradle to gate basis (kg CO2e/kg plastic). Positive numbers indicate the bioplastic has lower GHG emissions than the fossil plastic. The table also shows the probability that the bioplastic has lower GHG emissions than the fossil plastic (P>0). Fossil plastics are all modeled using system expansion for hydrogen co-product. Switchgrass fermentation residues are used for steam and electricity, with a system expansion credit for surplus electricity generation. This table presents results assuming only the lignin portion of switchgrass is available for energy recovery.**

| Bio-plastic | Fossil Plastic | Mean | 2.5% | 97.5% | P(>0) |
|---|---|---|---|---|---|
| **Switchgrass PHB (full distribution, S, E, EC) (Lignin only for energy recovery)** | HDPE | 0.22 | -1.78 | 1.77 | 63% |
| | LDPE | 0.49 | -1.51 | 2.05 | 73% |
| | PP | 0.28 | -1.69 | 1.81 | 66% |
| | PET | 1.13 | -0.82 | 2.60 | 90% |
| | PS | 1.87 | -0.11 | 3.38 | 97% |
| | PVC | 0.93 | -1.03 | 2.42 | 86% |
| **Switchgrass PLA (case 1, S, E, EC) (Lignin only for energy recovery)** | HDPE | 0.93 | 0.15 | 1.60 | 99% |
| | LDPE | 1.19 | 0.41 | 1.88 | 100% |
| | PP | 0.99 | 0.26 | 1.61 | 99% |
| | PET | 1.84 | 1.19 | 2.33 | 100% |
| | PS | 2.57 | 1.87 | 3.16 | 100% |
| | PVC | 1.64 | 0.97 | 2.17 | 100% |
| **Switchgrass ethylene plastics (near-term ethanol yield, S, E, EC) (Lignin only for energy recovery)** | HDPE | 1.89 | -0.97 | 3.78 | 94% |
| | LDPE | 1.92 | -0.99 | 3.85 | 94% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.34 | -0.18 | 0.69 | 94% |
| | PS | 0.56 | -0.29 | 1.12 | 94% |
| | PVC | 0.86 | -0.44 | 1.73 | 94% |
| **Switchgrass ethylene plastics (mid-term ethanol yield, S, E, EC) (Lignin only for energy recovery)** | HDPE | 1.78 | -0.12 | 3.40 | 97% |
| | LDPE | 1.81 | -0.12 | 3.46 | 97% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.32 | -0.02 | 0.62 | 97% |
| | PS | 0.53 | -0.04 | 1.00 | 97% |
| | PVC | 0.82 | -0.06 | 1.56 | 97% |

**Table S-40. Difference in GHG emissions (mean and 95% confidence interval) between bioplastics and fossil plastics, on a cradle to gate basis (kg CO2e/kg plastic). Positive numbers indicate the bioplastic has lower GHG emissions than the fossil plastic. The table also shows the probability that the bioplastic has lower GHG emissions than the fossil plastic (P>0). Fossil plastics are all modeled using system expansion for hydrogen co-product. Switchgrass fermentation residues are used for steam and electricity, with a system expansion credit for surplus electricity generation. This table presents results assuming a higher value for switchgrass crop residue, as per IPCC guidelines [12].**

| Bio-plastic | Fossil Plastic | Mean | 2.5% | 97.5% | P(>0) |
|---|---|---|---|---|---|
| **Switchgrass PHB (full distribution, S, E, EC) (High crop residue)** | HDPE | 0.80 | -1.37 | 2.51 | 80% |
| | LDPE | 1.07 | -1.11 | 2.79 | 86% |
| | PP | 0.86 | -1.31 | 2.54 | 82% |
| | PET | 1.71 | -0.43 | 3.36 | 95% |
| | PS | 2.45 | 0.27 | 4.11 | 98% |
| | PVC | 1.51 | -0.63 | 3.17 | 93% |
| **Switchgrass PLA (case 1, S, E, EC) (High crop residue)** | HDPE | 0.93 | 0.03 | 1.72 | 98% |
| | LDPE | 1.20 | 0.29 | 2.01 | 99% |
| | PP | 0.99 | 0.13 | 1.73 | 99% |
| | PET | 1.84 | 1.03 | 2.48 | 100% |
| | PS | 2.57 | 1.73 | 3.28 | 100% |
| | PVC | 1.64 | 0.82 | 2.31 | 100% |
| **Switchgrass ethylene plastics (near-term ethanol yield, S, E, EC) (High crop residue)** | HDPE | 2.00 | -1.38 | 4.38 | 91% |
| | LDPE | 2.03 | -1.40 | 4.46 | 91% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.36 | -0.25 | 0.80 | 91% |
| | PS | 0.59 | -0.41 | 1.29 | 91% |
| | PVC | 0.91 | -0.63 | 2.00 | 91% |
| **Switchgrass ethylene plastics (mid-term ethanol yield, S, E, EC) (High crop residue)** | HDPE | 1.59 | -0.53 | 3.21 | 94% |
| | LDPE | 1.62 | -0.54 | 3.27 | 94% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.29 | -0.10 | 0.58 | 94% |
| | PS | 0.47 | -0.16 | 0.95 | 94% |
| | PVC | 0.73 | -0.24 | 1.47 | 94% |

**Table S-41. Difference in GHG emissions (mean and 95% confidence interval) between bioplastics and fossil plastics, on a cradle to gate basis (kg CO2e/kg plastic). Positive numbers indicate the bioplastic has lower GHG emissions than the fossil plastic. The table also shows the probability that the bioplastic has lower GHG emissions than the fossil plastic (P>0). Fossil plastics are all modeled using system expansion for hydrogen co-product. Switchgrass fermentation residues are used for steam and electricity, with a system expansion credit for surplus electricity generation. This table presents results assuming a higher value for switchgrass crop yield, as per Spatari and MacLean (2010) [17].**

| Bio-plastic | Fossil Plastic | Mean | 2.5% | 97.5% | P(>0) |
|---|---|---|---|---|---|
| **Switchgrass PHB (full distribution, S, E, EC) (High crop yield)** | HDPE | 1.68 | -0.11 | 3.15 | 97% |
| | LDPE | 1.95 | 0.16 | 3.42 | 98% |
| | PP | 1.74 | -0.02 | 3.17 | 97% |
| | PET | 2.59 | 0.86 | 3.98 | 100% |
| | PS | 3.32 | 1.56 | 4.74 | 100% |
| | PVC | 2.39 | 0.65 | 3.80 | 100% |
| **Switchgrass PLA (case 1, S, E, EC) (High crop yield)** | HDPE | 1.34 | 0.67 | 2.03 | 100% |
| | LDPE | 1.61 | 0.93 | 2.31 | 100% |
| | PP | 1.40 | 0.79 | 2.03 | 100% |
| | PET | 2.25 | 1.75 | 2.77 | 100% |
| | PS | 2.98 | 2.40 | 3.59 | 100% |
| | PVC | 2.05 | 1.51 | 2.60 | 100% |
| **Switchgrass ethylene plastics (near-term ethanol yield, S, E, EC) (High crop yield)** | HDPE | 3.86 | 2.14 | 5.53 | 100% |
| | LDPE | 3.93 | 2.18 | 5.63 | 100% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.70 | 0.39 | 1.01 | 100% |
| | PS | 1.14 | 0.63 | 1.64 | 100% |
| | PVC | 1.77 | 0.98 | 2.53 | 100% |
| **Switchgrass ethylene plastics (mid-term ethanol yield, S, E, EC) (High crop yield)** | HDPE | 2.65 | 1.21 | 3.91 | 100% |
| | LDPE | 2.70 | 1.23 | 3.98 | 100% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.48 | 0.22 | 0.71 | 100% |
| | PS | 0.78 | 0.36 | 1.16 | 100% |
| | PVC | 1.21 | 0.55 | 1.79 | 100% |

**Table S-42. Difference in GHG emissions (mean and 95% confidence interval) between bioplastics and fossil plastics, on a cradle to gate basis (kg CO2e/kg plastic). Positive numbers indicate the bioplastic has lower GHG emissions than the fossil plastic. The table also shows the probability that the bioplastic has lower GHG emissions than the fossil plastic (P>0). Fossil plastics are all modeled using system expansion for hydrogen co-product. Switchgrass fermentation residues are used for steam and electricity, with a system expansion credit for surplus electricity generation. This table presents results assuming crop yield and nitrogen application are perfectly correlated.**

| Bio-plastic | Fossil Plastic | Mean | 2.5% | 97.5% | P(>0) |
|---|---|---|---|---|---|
| **Switchgrass PHB (full distribution, S, E, EC) (Correlated N and yield)** | HDPE | 1.56 | -0.24 | 3.00 | 96% |
| | LDPE | 1.83 | 0.03 | 3.28 | 98% |
| | PP | 1.62 | -0.15 | 3.03 | 96% |
| | PET | 2.47 | 0.74 | 3.83 | 100% |
| | PS | 3.20 | 1.45 | 4.60 | 100% |
| | PVC | 2.27 | 0.53 | 3.64 | 99% |
| **Switchgrass PLA (case 1, S, E, EC) (Correlated N and yield)** | HDPE | 1.28 | 0.63 | 1.95 | 100% |
| | LDPE | 1.55 | 0.89 | 2.24 | 100% |
| | PP | 1.34 | 0.74 | 1.96 | 100% |
| | PET | 2.19 | 1.71 | 2.70 | 100% |
| | PS | 2.92 | 2.37 | 3.51 | 100% |
| | PVC | 1.99 | 1.48 | 2.53 | 100% |
| **Switchgrass ethylene plastics (near-term ethanol yield, S, E, EC) (Correlated N and yield)** | HDPE | 3.59 | 2.05 | 5.17 | 100% |
| | LDPE | 3.66 | 2.08 | 5.27 | 100% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.65 | 0.37 | 0.94 | 100% |
| | PS | 1.06 | 0.61 | 1.53 | 100% |
| | PVC | 1.65 | 0.94 | 2.37 | 100% |
| **Switchgrass ethylene plastics (mid-term ethanol yield, S, E, EC) (Correlated N and yield)** | HDPE | 2.50 | 1.09 | 3.72 | 100% |
| | LDPE | 2.54 | 1.11 | 3.78 | 100% |
| | PP | #N/A | #N/A | #N/A | #N/A |
| | PET | 0.45 | 0.20 | 0.68 | 100% |
| | PS | 0.74 | 0.32 | 1.10 | 100% |
| | PVC | 1.14 | 0.50 | 1.70 | 100% |

### *S.2.8 Sensitivity to displacement rates*

The comparative analysis presented in Figure 6 of the main text assumed that 1 kg of each bio-based plastic can displace 1 kg of each fossil-based plastic (i.e. 1:1 displacement). While this assumption is valid for bioethylene plastics, it may not be appropriate for PLA and PHB. Figure S-4 to Figure S-7 consider a range of displacement rates for each of the main PLA and PHB scenarios presented in Figure 6 of the main text. We define the 'displacement rate' as the quantity of fossil plastic displaced by a unit of mass bioplastic. For example, a displacement rate of 0.8 implies that 1 kg of bioplastic can displace 0.8 kg of fossil plastic (on a physical basis – not accounting for indirect market interactions). For each pair of figures, the left figure shows the proportion of model runs in which the bioplastic achieves a net GHG reduction over the displaced quantity of fossil plastic. The right figure shows the corresponding mean GHG reduction, per kg of bioplastic, displacing different quantities of each fossil plastic (negative values imply that switching to the bioplastic results in a net increase in GHG emissions). As for figure 6 in the main text, the figures below present a baseline scenario for corn PLA (case 2, system expansion), an optimistic scenario for corn PHB (case 2, system expansion), and somewhat optimistic scenarios for switchgrass-based plastics that include the generation of steam and electricity from fermentation residues, along with a credit for the sale of surplus electricity.

Unsurprisingly, the effect of displacement rate on mean emission reductions is more important for high emission fossil plastics, like PS, than it is for low emission fossil plastics like HDPE and LDPE. In addition, Figure S-4 (left) shows that corn PLA continues to have a high chance

(>80%) of reducing emissions compared to high emission polymers (PS, PET, PVC) for moderate displacement rates (> ~0.8), but that large displacement rates (>1.3) would be necessary to have the same confidence (>80%) that corn PLA can achieve reductions relative to HDPE or LDPE. Figure S-5 (left) shows that even in the optimistic scenario, corn PHB requires displacement rates in excess of 1.3 to have a high level of confidence (>80%) that there will be a reduction in emissions compared to any plastic other than PS. Finally Figure S-6 and Figure S-7 show that switchgrass PLA and PHB can reduce emissions relative to fossil polymers for a wide range of displacement rates. This is due to the fact that the selected switchgrass pathways exhibit cradle-to-gate GHG emissions that are already close to 0, even before displacing any fossil plastic.

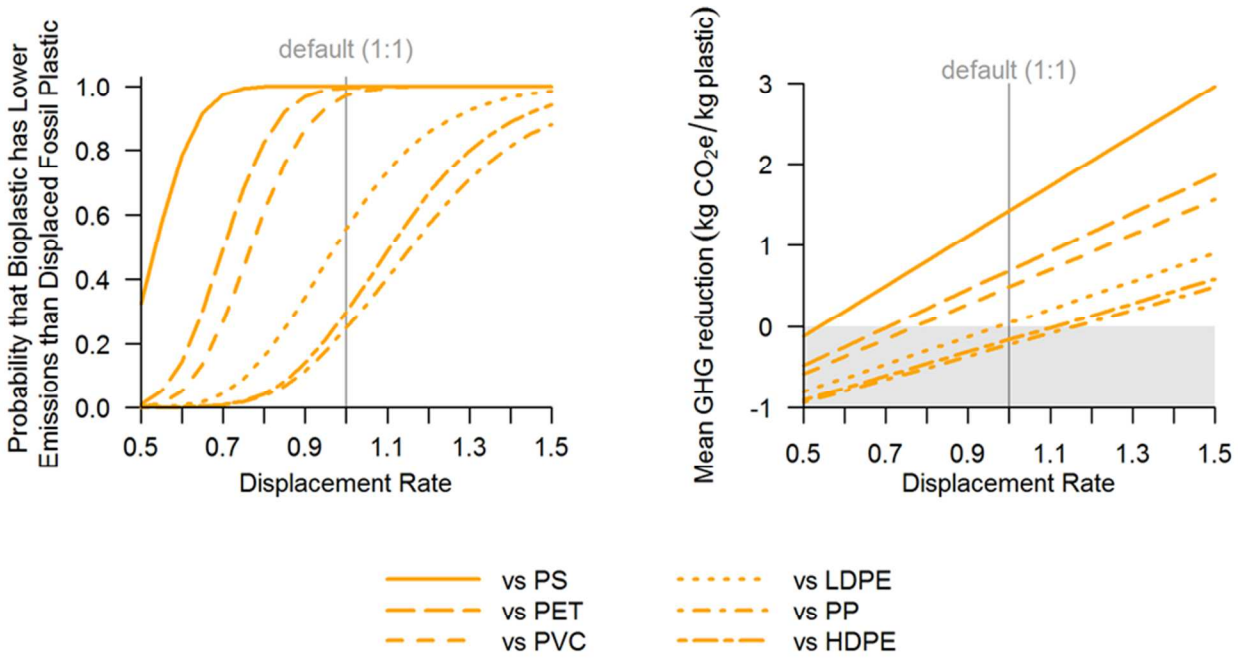


**Figure S-4. Sensitivity of cradle-to-gate net emissions from corn PLA (baseline case 2, system expansion) to fossil plastic displacement rate. The x-axis in each figure corresponds to the quantity of fossil plastic displaced by 1 mass unit of PLA. The left figure shows the probability that 1 kg corn PLA has lower GHG emissions than the displaced quantity of each fossil plastic. The right figure shows the mean GHG emissions**

**reduction achieved by 1 kg corn PLA (negative values imply that switching to the bioplastic increases emissions). Both figures show a line at the default 1:1 displacement rate.**

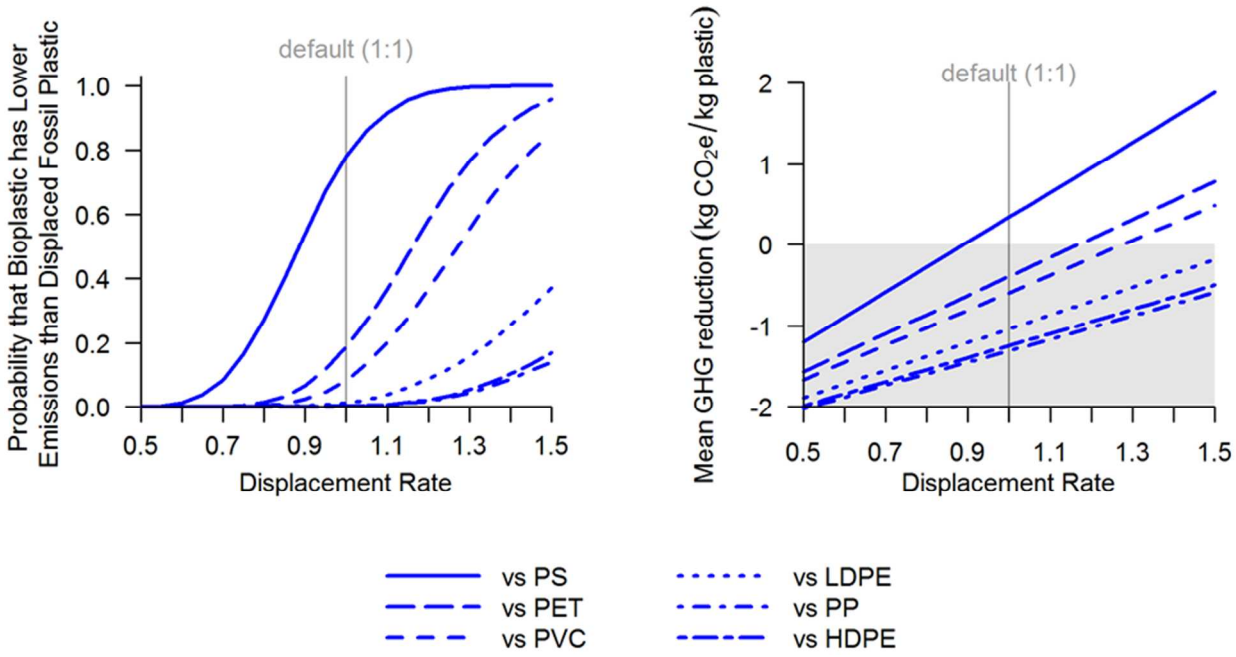


**Figure S-5. Sensitivity of cradle-to-gate net emissions from corn PHB (optimistic, case 2, system expansion) to fossil plastic displacement rate. The x-axis in each figure corresponds to the quantity of fossil plastic displaced by 1 mass unit of PHB. The left figure shows the probability that 1 kg corn PHB has lower GHG emissions than the displaced quantity of each fossil plastic. The right figure shows the mean GHG emissions reduction achieved by 1 kg corn PHB (negative values imply that switching to the bioplastic increases emissions). Both figures show a line at the default 1:1 displacement rate.**

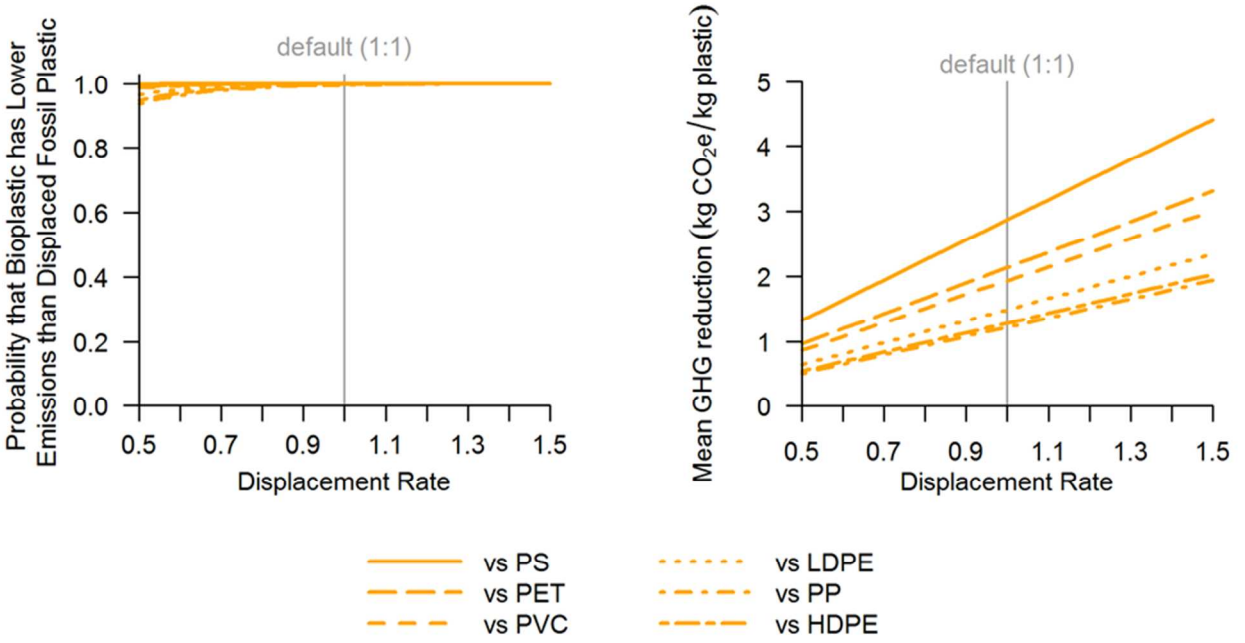


**Figure S-6. Sensitivity of cradle-to-gate net emissions from switchgrass PLA (case 1, S, E, EC) to fossil plastic displacement rate. The x-axis in each figure corresponds to the quantity of fossil plastic displaced by 1 mass unit of PLA. The left figure shows the probability that 1 kg corn PLA has lower GHG emissions than the displaced quantity of each fossil plastic. The right figure shows the mean GHG emissions reduction achieved by 1 kg corn PLA. Both figures show a line at the default 1:1 displacement rate.**

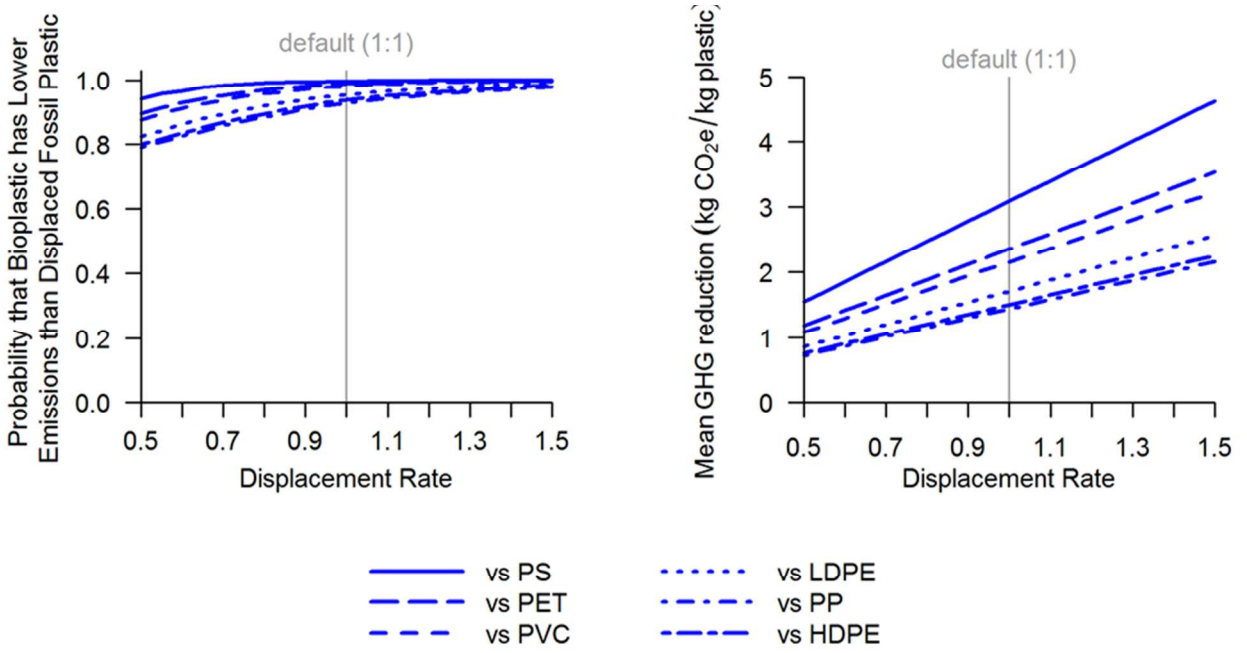


**Figure S-7. Sensitivity of cradle-to-gate net emissions from switchgrass PHB (full distribution, S, E, EC) to fossil plastic displacement rate. The x-axis in each figure corresponds to the quantity of fossil plastic displaced by 1 mass unit of PHB. The left figure shows the probability that 1 kg corn PHB has lower GHG emissions than the displaced quantity of each fossil plastic. The right figure shows the mean GHG emissions reduction achieved by 1 kg corn PHB. Both figures show a line at the default 1:1 displacement rate.**

### *S.2.9 Sensitivity to omitted stages*

As noted in the main text, our model excludes emissions from downstream processing and transportation. Table S-43 explores the sensitivity of the main bio-based plastic pathways (those presented in figure 6 of the main paper) to these additional stages. For each bio-based plastic, the table shows how much additional road transport, ship transport, downstream process heat or downstream process electricity would have to be applied to that plastic (relative to its fossil counterparts) for its mean GHG emissions to be the same as the mean emissions for each fossil plastic. Negative values imply that the bio-based plastic would have to undergo less transportation or downstream processing energy than its fossil counterpart to achieve equal GHG emissions. For this analysis, we assume that road transportation is carried out with a diesel powered single unit truck (0.0203 L diesel/t-km [72], resulting in mean emissions of 0.072 g $CO_2$e/kg-km), ship transportation is carried out via ocean freighter (0.00493 L residual fuel oil/t-km [83], resulting in mean emissions of 0.019 g $CO_2$e/kg-km), process heat is provided by natural gas (mean: 64 g $CO_2$e/MJ HHV as parametrized in Table S-12), and process electricity is generated with the U.S. average emissions factor (mean: 0.19 g $CO_2$e/MJ, per Table S-12). The results in each column of the table are separate from one another. For example, corn PLA would have the same mean GHG emissions as PET if PLA were transported 9,600 km further than PET by truck, *or* if PLA were shipped 36,000 km further than PET, *or* if product forming from PLA required 11 MJ/kg more process heat than from PET, *or* if product forming from PLA required 3.7 more MJ of process electricity than from PET. For reference, the U.S. is approximately 4,000 km across (East/West) and 2,500 km long (North/South). The shipping distance from Brazil (a major producer of bio-based plastics from sugarcane) to the U.S. is approximately 10,000 km [84]. Very few entries in the table are within these ranges.

**Table S-43. Sensitivity of main pathways to omitted stages. The table shows the additional road transport distance, additional ship transport distance, additional process heat requirements or additional process electricity requirements (per kg plastic) that (individually) would make each bio-based plastic have the same mean GHG emissions as each fossil-based plastic. Negative values imply that the bio-based plastic would have to undergo less transportation or downstream processing energy than its fossil counterpart to achieve equal mean GHG emissions.**

| BioPlastic | Plastic | Road transport (km) | Ship transport (km) | Process heat (MJ) | Process electricity (MJ elec) |
|---|---|---|---|---|---|
| **Corn PLA (baseline: case 2, system expansion)** | HDPE | -3,000 | -11,000 | -3.4 | -1.2 |
| | LDPE | 680 | 2,500 | 0.8 | 0.3 |
| | LLDPE | -3,000 | -11,000 | -3.4 | -1.2 |
| | PP | -2,200 | -8,200 | -2.5 | -0.9 |
| | PET | 9,600 | 36,000 | 11 | 3.7 |
| | PS (GPPS) | 20,000 | 74,000 | 22 | 7.7 |
| | HIPS | 19,000 | 72,000 | 22 | 7.5 |
| | PVC | 6,800 | 25,000 | 8 | 2.7 |
| **Switchgrass PLA (case 1, S, E, EC)** | HDPE | 17,000 | 64,000 | 19 | 6.6 |
| | LDPE | 21,000 | 78,000 | 23 | 8.1 |
| | LLDPE | 17,000 | 64,000 | 19 | 6.6 |
| | PP | 18,000 | 67,000 | 20 | 7.0 |
| | PET | 30,000 | 110,000 | 33 | 12 |
| | PS (GPPS) | 40,000 | 150,000 | 45 | 15 |
| | HIPS | 39,000 | 150,000 | 44 | 15 |
| | PVC | 27,000 | 100,000 | 30 | 10 |
| **Corn PHB (optimistic: case 2, system expansion)** | HDPE | -18,000 | -67,000 | -20 | -7.0 |
| | LDPE | -14,000 | -54,000 | -16 | -5.6 |
| | LLDPE | -18,000 | -67,000 | -20 | -7.0 |
| | PP | -17,000 | -64,000 | -19 | -6.7 |
| | PET | -5,400 | -20,000 | -6.1 | -2.1 |
| | PS (GPPS) | 4,700 | 18,000 | 5.3 | 1.8 |
| | HIPS | 4,400 | 16,000 | 4.9 | 1.7 |
| | PVC | -8,200 | -31,000 | -9.2 | -3.2 |
| **Switchgrass PHB (full distribution, S, E, EC)** | HDPE | 20,000 | 75,000 | 22 | 7.8 |
| | LDPE | 24,000 | 89,000 | 27 | 9 |
| | LLDPE | 20,000 | 75,000 | 23 | 7.8 |
| | PP | 21,000 | 78,000 | 23 | 8.1 |
| | PET | 33,000 | 120,000 | 37 | 13 |
| | PS (GPPS) | 43,000 | 160,000 | 48 | 17 |
| | HIPS | 42,000 | 160,000 | 48 | 16 |
| | PVC | 30,000 | 110,000 | 34 | 12 |
| **Corn Ethylene (System expansion)** | HDPE | 8,200 | 30,000 | - | - |
| | LDPE | 8,300 | 31,000 | - | - |
| | LLDPE | 8,300 | 31,000 | - | - |
| | PET | 1,500 | 5,500 | - | - |

| | | | | | |
|---|---|---|---|---|---|
| | PS (GPPS) | 2,400 | 9,000 | - | - |
| | HIPS | 2,300 | 8,400 | - | - |
| | PVC | 3,700 | 14,000 | - | - |
| **Switchgrass ethylene (near-term, S, E, EC)** | HDPE | 46,000 | 170,000 | - | - |
| | LDPE | 47,000 | 180,000 | - | - |
| | LLDPE | 47,000 | 170,000 | - | - |
| | PET | 8,400 | 31,000 | - | - |
| | PS (GPPS) | 14,000 | 51,000 | - | - |
| | HIPS | 13,000 | 48,000 | - | - |
| | PVC | 21,000 | 79,000 | - | - |
| **Switchgrass ethylene (mid-term, S, E, EC)** | HDPE | 33,000 | 120,000 | - | - |
| | LDPE | 33,000 | 120,000 | - | - |
| | LLDPE | 33,000 | 120,000 | - | - |
| | PET | 5,900 | 22,000 | - | - |
| | PS (GPPS) | 9,700 | 36,000 | - | - |
| | HIPS | 9,100 | 34,000 | - | - |
| | PVC | 15,000 | 56,000 | - | - |

### *S.2.10 Uncertainty importance analysis*

Figure S-8 to Figure S-14 present top contributors to uncertainty for select bio-polymer production pathways. The main text includes a discussion of key observations.

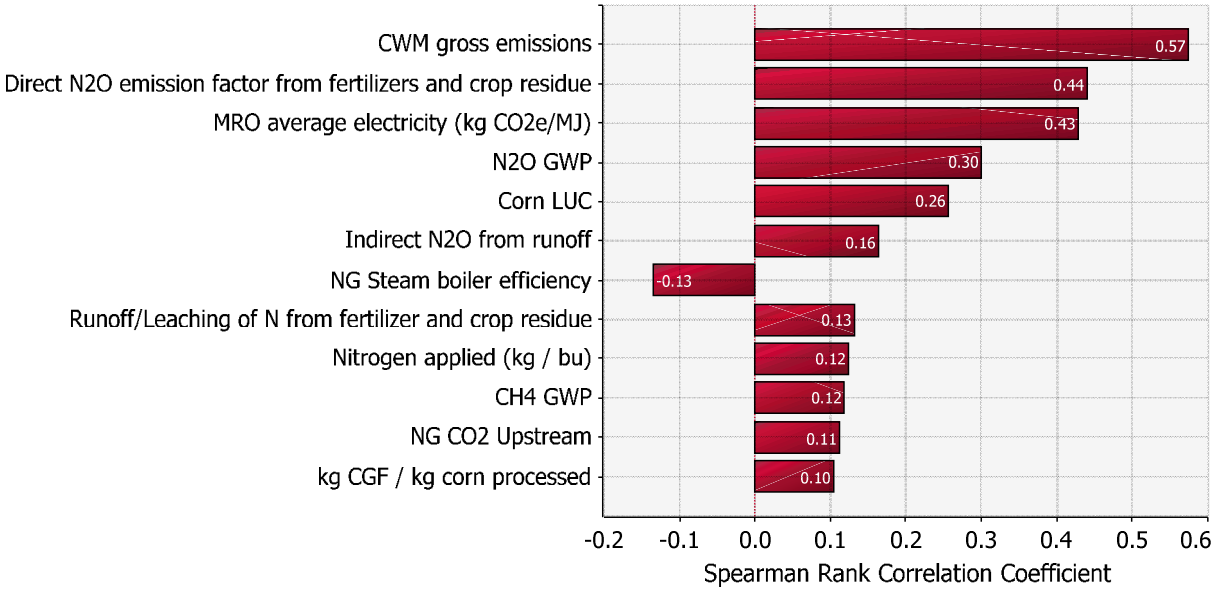


**Figure S-8. Spearman rank correlation coefficient for top contributors to uncertainty in the life cycle GHG emissions for corn PHB (case 2, system expansion)**

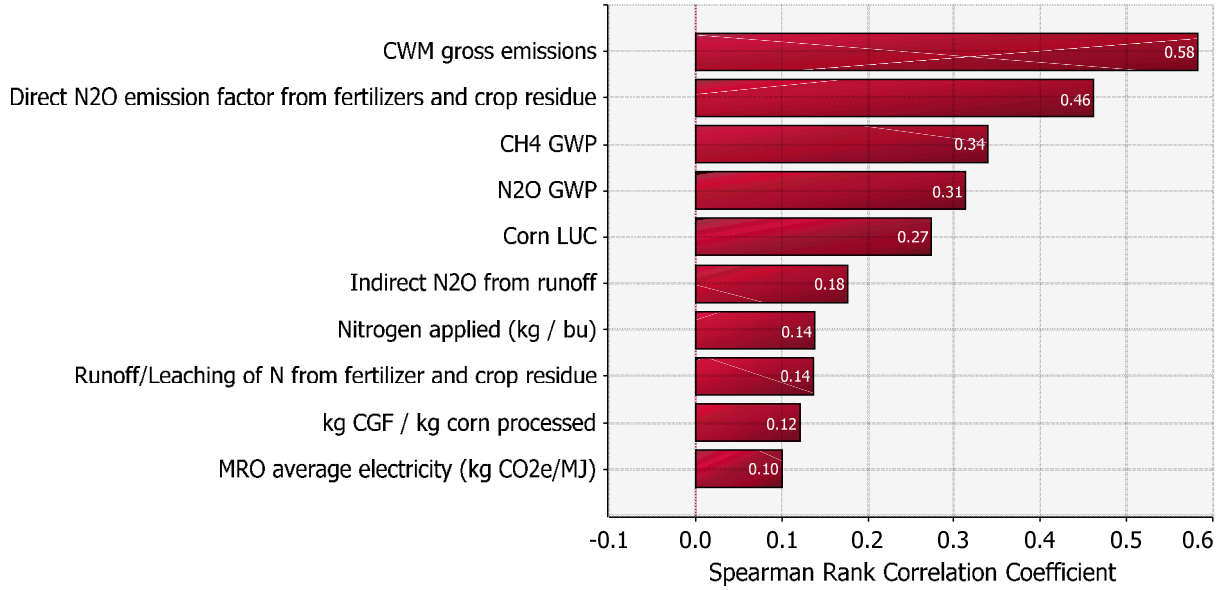


**Figure S-9. Spearman rank correlation coefficient for top contributors to uncertainty in the life cycle GHG emissions for corn PLA (case 2, system expansion)**

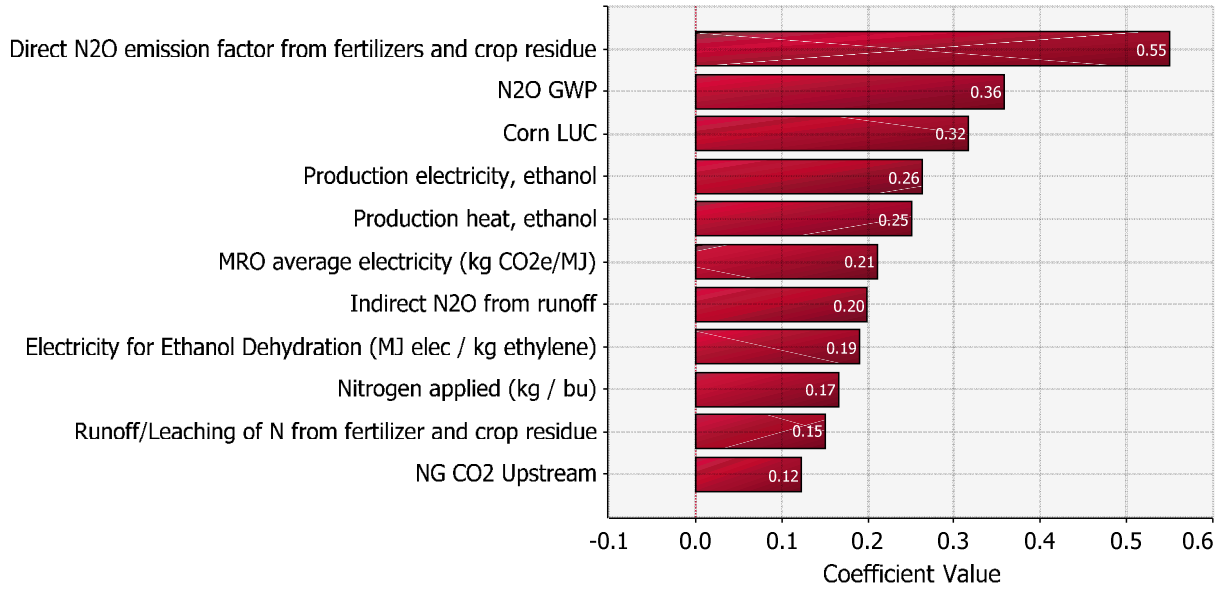


**Figure S-10. Spearman rank correlation coefficient for top contributors to uncertainty in the life cycle GHG emissions for corn ethylene (system expansion)**

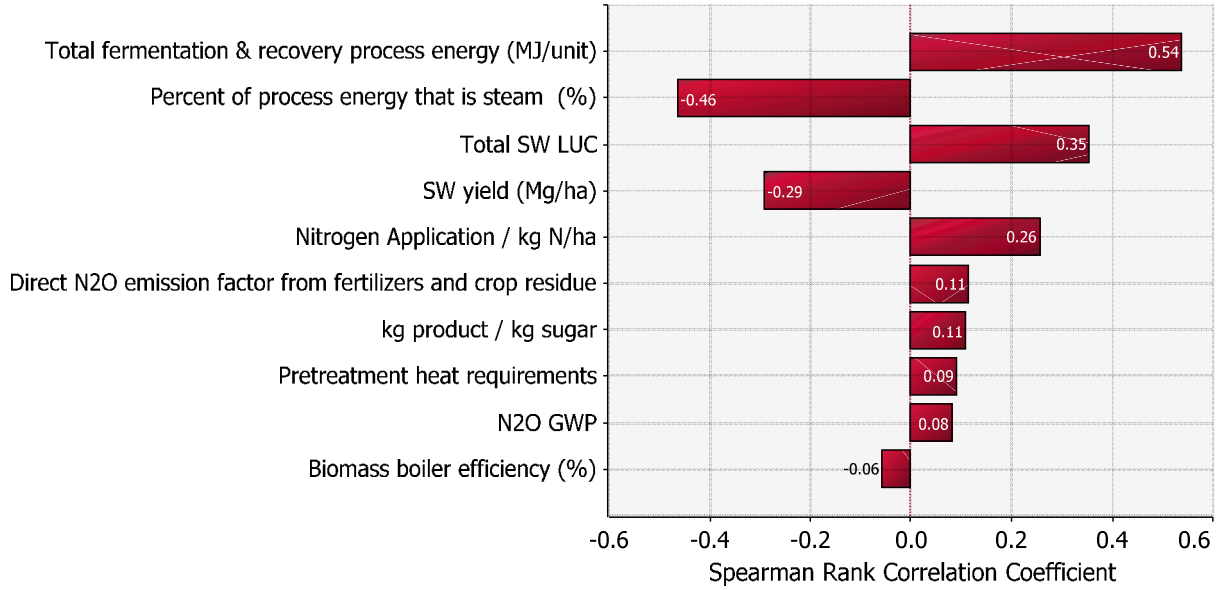


**Figure S-11. Spearman rank correlation coefficient for top contributors to uncertainty in the life cycle GHG emissions for switchgrass PHB (full distribution, using fermentation residues for steam and electricity, and including a system expansion credit for surplus electricity)**

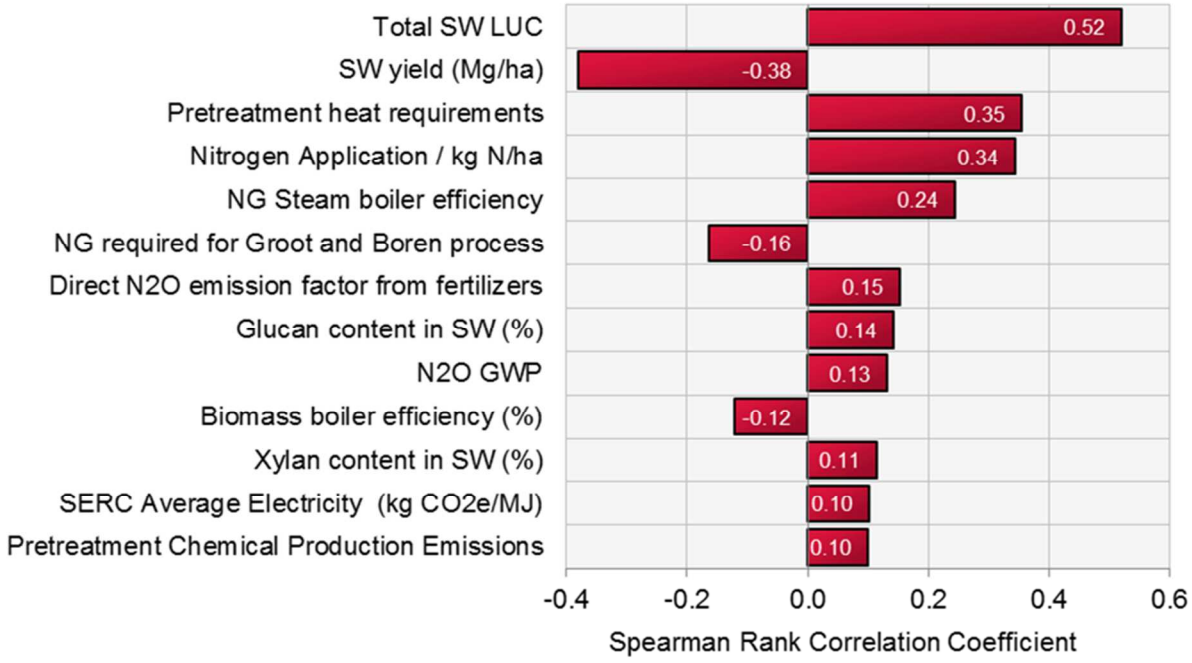


**Figure S-12. Spearman rank correlation coefficient for top contributors to uncertainty in the life cycle GHG emissions for switchgrass PLA (case 1, using fermentation residues for steam and electricity, and including a system expansion credit for surplus electricity)**

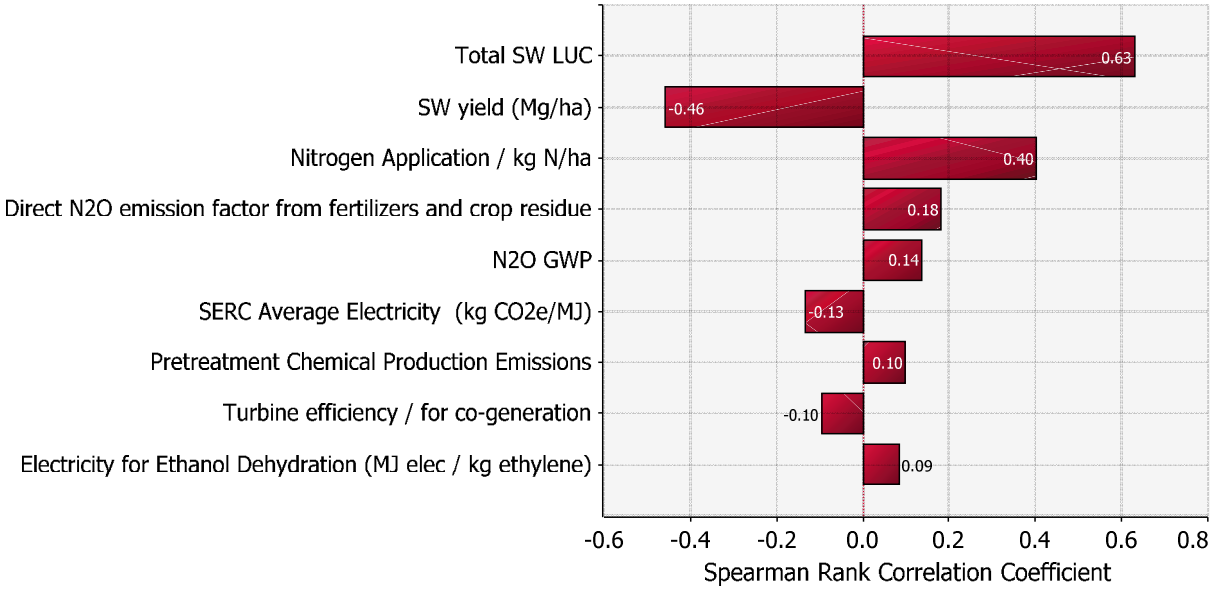


**Figure S-13. Spearman rank correlation coefficient for top contributors to uncertainty in the life cycle GHG emissions for switchgrass ethylene (near-term yield, using fermentation residues for steam and electricity, and including a system expansion credit for surplus electricity)**

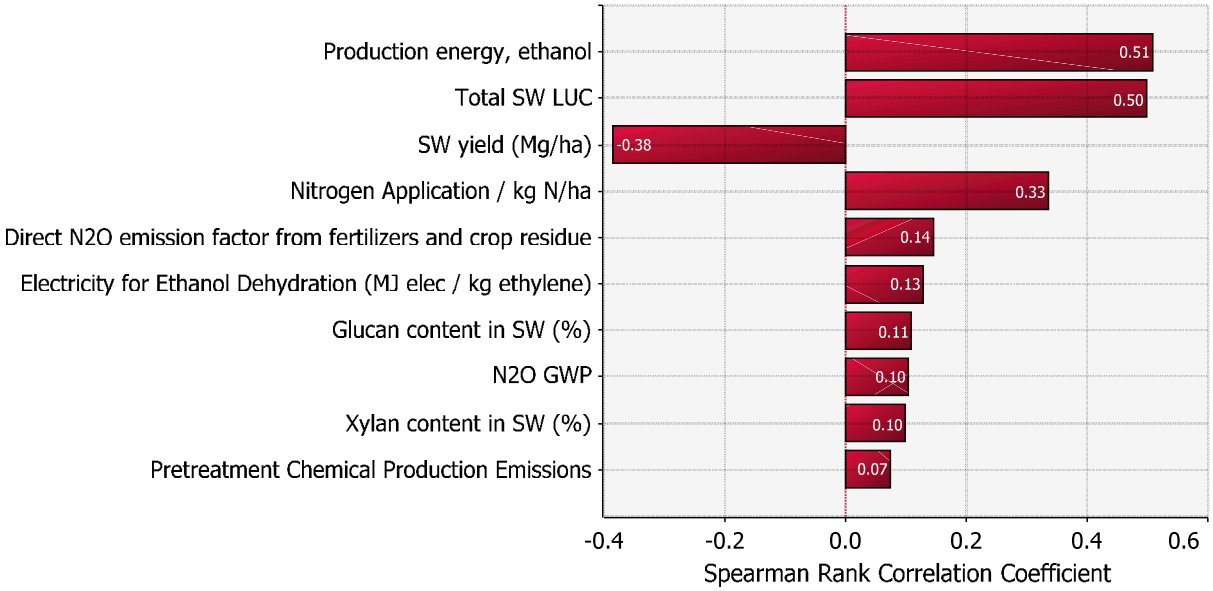


**Figure S-14. Spearman rank correlation coefficient for top contributors to uncertainty in the life cycle GHG emissions for switchgrass ethylene (mid-term yield, using fermentation residues for steam and electricity, and including a system expansion credit for surplus electricity)**

## S.3 References


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