

Fuel, Feedstock, or Neither? – Evaluating Tradeoffs in the use of Biomass for Greenhouse Gas Mitigation

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Abstract

Biomass is the world's largest renewable energy source, accounting for approximately 10% of global primary energy supply, and 5% of energy consumed in the United States. Prominent national programs like the U.S. Renewable Fuel Standard incentivize increased use of biomass, primarily as a transportation fuel. There has been comparatively little government support for using biomass as a renewable feedstock for the chemical sector. Such asymmetry in incentives can lead to sub-optimal outcomes in the allocation of biomass toward different uses.

Greenhouse gas reduction is among the most cited benefits of bioenergy and bio-based products, however, there is increasing controversy about whether increased use of biomass can actually contribute to greenhouse gas emission targets. If biomass is to play a role in current and future greenhouse gas mitigation efforts its use should be guided by efficient use of natural and economic resources. This thesis addresses these questions through a series of case studies, designed to highlight important tradeoffs in the use of biomass for greenhouse gas mitigation. Should biomass be used as a fuel, a chemical feedstock, or neither?

The first case study in this thesis focuses on the 'fuel vs feedstock' question, examining the greenhouse gas implications of expanding the scope of the U.S. Renewable Fuel Standard to include credits for bioethylene, an important organic chemical readily produced from bioethanol. Results suggest that an expanded policy that includes bioethylene as an approved use for ethanol would provide added flexibility without compromising greenhouse gas targets – a clear win scenario.

Having established that bioethylene based plastics can achieve similar greenhouse gas reductions to bioethanol used as fuel, this thesis expands the analysis by considering how the greenhouse gas emissions from a wider range of bio-based plastics compare to each of the main commodity thermoplastics produced in the U.S. The analysis demonstrates that there are large uncertainties involved in the life cycle greenhouse gas emissions from bio-based plastics, and that only a subset of pathways are likely to be preferable to conventional plastics. The following chapter then builds on the existing model to compare the greenhouse gas mitigation potential of bio-

based plastics to the potential for reducing emissions by adopting low carbon energy for plastics production. That chapter concludes that switching to renewable energy across the supply chain for conventional plastics energy cuts greenhouse gas emissions by 50-75%, achieving a greater reduction, with less uncertainty and lower cost, than switching to corn-based biopolymers – the most likely near-term biopolymer option. In the long run, producing bio-based plastics from advanced feedstocks (e.g. switchgrass) and/or with renewable energy likely offers greater emission reductions.

Finally, this thesis returns to the dominant form of policy surrounding biomass use: biofuel mandates. That study takes a consequential approach to the ‘fuel or neither’ question. Specifically, this work examines how petroleum refineries are likely to adjust their production in response to biofuel policies, and what this implies for the success of these policies. The research demonstrates that biofuel policies induce a shift toward greater diesel production at the expense of both gasoline and non-combustion petroleum products. This has the potential to result in an increase in greenhouse gas emissions, even before accounting for the emissions from producing the biofuels themselves.

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List of Abbreviations

ALCA	Attributional Life Cycle Assessment
AR5	IPCC 5 th Assessment Report
CAFE	Corporate Average Fuel Economy
CHP	Combined Heat and Power
CLCA	Consequential Life Cycle Assessment
CPP	Clean Power Plan
EIA	U.S. Energy Information Administration
EISA	U.S. Energy Independence and Security Act of 2007
EPA	U.S. Environmental Protection Agency
GHG	Greenhouse Gas
GPPS	General Purpose Polystyrene
GREET	Greenhouse Gas Regulated Emissions and Energy Use in Transportation (Argonne National Laboratory)
GWI	Global warming intensity
HDPE	High Density Polyethylene
HHV	Higher Heating Value
HIPS	High Impact Polystyrene
IDC	Indirect Demand Change (see also IOUC, IFUE)
IEA	International Energy Agency
IFUE	Indirect Fuel Use Effect (see also IDC, IOUC)
ILUC	Indirect Land Use Change
IOUC	Indirect Output Use Change (see also IDC, IFUE)
IPCC	Intergovernmental Panel on Climate Change
ISO	International Organization for Standardization
LCA	Life Cycle Assessment
LCFS	Low Carbon Fuel Standard
LDPE	Low Density Polyethylene
LHV	Lower Heating Value
LLDPE	Linear Low Density Polyethylene

LFG	Landfill Gas
LPG	Liquefied Petroleum Gases
LRG	Liquefied Refinery Gases
LUC	Land Use Change
OPGEE	The Oil Production and Greenhouse Gas Emissions Estimator (Stanford University)
PADD	Petroleum Administration Defense District
PE	Polyethylene
PET	Polyethylene Terephthalate
PHA	Polyhydroxyalkanoate
PHB	Polyhydroxybutyrate
PLA	Polylactic Acid
PP	Polypropylene
PRELIM	The Petroleum Refinery Life Cycle Inventory Model (University of Calgary)
PS	Polystyrene
PVC	Polyvinyl Chloride
RIN	Renewable Identification Number
RFS/RFS2	The U.S. Renewable Fuel Standard
RNG	Renewable Natural Gas
USDA	U.S. Department of Agriculture
U.S.	United States

Chapter 1. Introduction and Background

1.1. Motivation

Biomass (plant matter and organic waste) is the world's largest renewable energy source, accounting for approximately 10% of global primary energy supply, and 5% of energy consumed in both the United States alone, and across all developed countries.^{1,2} To date, national policies for increased use of biomass have focused primarily on road transportation, with 64 countries having implemented some form of biofuel mandate.³ The largest such program is the United States (U.S.) Renewable Fuel Standard (RFS2),⁴ which continues to incentivize large-scale production of biofuels, primarily ethanol. In contrast, government action to encourage the substitution of fossil-based materials with renewable, bio-based alternatives has been limited to smaller programs like the U.S. "BioPreferred" federal government procurement program.⁵ Such asymmetry in incentives may lead to sub-optimal outcomes in the allocation of biomass toward different uses.

Bulk chemical production is responsible for about 5-6% of U.S. greenhouse gas (GHG) emissions⁶ and U.S. energy consumption (including feedstock energy).⁷ As the fastest growing industrial user of energy,⁸ the chemical industry is a potentially rich target for fossil-fuel to renewable energy and/or feedstock substitution. In particular, plastics account for the largest share of organic chemical production.⁹ The technical substitution potential of bioplastics for fossil plastics has been estimated at a promising 90%.¹⁰ Despite limited policy incentives, private investment into bio-based plastics is already taking place.¹¹⁻¹³ This observation gives rise to the dual question: should there be greater incentives for producing bio-based plastics; alternatively, are existing private efforts misguided?

Although greenhouse gas reduction is among the most cited benefits of bioenergy and bio-based products there is increasing controversy about whether increased use of biomass can actually contribute to greenhouse gas emission targets.¹⁴ If biomass is to play a role in current and future greenhouse gas mitigation efforts, studies have shown that biomass resources are likely to be constrained by supply potential in the long run.¹⁵ Even in the short run, however, the use of

biomass for GHG mitigation should be guided by efficient use of natural and economic resources. This thesis addresses these questions through a series of case studies, designed to highlight important tradeoffs in the use of biomass for GHG mitigation. Should biomass be used as a fuel, a chemical feedstock, or neither?

1.2. Dissertation Overview and Research Questions

The remainder of this chapter provides additional background on greenhouse gas mitigation, life cycle assessment, uses of biomass, fossil and bio-based plastics and the global petroleum sector. Following the introduction (Chapter 1), the dissertation is divided into four research chapters and a concluding chapter, followed by appendices and references. The main chapters and the research questions they explore are outlined below:

Chapter 2: Changing the Renewable Fuel Standard to a Renewable Material Standard:

Bioethylene Case Study. This chapter focuses on the ‘fuel vs feedstock’ question, examining the greenhouse gas implications of expanding the scope of the U.S. Renewable Fuel Standard (RFS2) to include credits for bioethylene, an important organic chemical readily produced from bioethanol. Key research questions include:

- What are the life cycle GHG emissions from corn, switchgrass and sugarcane ethanol, and how uncertain are these numbers?
- What are the life cycle GHG emissions from conventional low density polyethylene (LDPE), produced in the U.S.?
- What are the life cycle GHG emissions from corn, switchgrass and sugarcane LDPE, and how uncertain are these numbers?
- Can ethanol used for bio-LDPE production meet the GHG reduction targets for ethanol set by RFS2? With what degree of confidence?
- Does bio-LDPE achieve similar (or better) GHG benefits to bioethanol used for fuel? With what degree of confidence?
- What are appropriate policy recommendations for RFS2 in light of the above results?

Chapter 3: *Uncertainty in the Life Cycle Greenhouse Gas Emissions from U.S. Production of Three Bio-based Polymer Families.* Having established in Chapter 2 that bioethylene based plastic can achieve similar GHG reductions to bioethanol used as fuel, Chapter 3 expands the analysis by considering how the GHG emissions from a wider range of bio-based plastics compare to each of the main commodity thermoplastics produced in the U.S. This chapter is primarily a ‘feedstock or neither’ investigation, and sets the stage for further analysis outlined in Chapter 4. Specific research questions for Chapter 3 include:

- What are the cradle-to-gate GHG emissions from producing each of the major commodity thermoplastics (polyethylene terephthalate (PET), polystyrene (PS), polyvinyl chloride (PVC), polypropylene (PP), high density polyethylene (HDPE) and low density polyethylene (LDPE)) in the U.S.? How uncertain are these numbers?
- What are the cradle-to-gate GHG emissions from producing polylactic acid (PLA), polyhydroxybutyrate (PHB), and bioethylene-based plastics in the U.S., using either corn grain or switchgrass as a feedstock? How uncertain are these numbers, and how do modeled emissions differ depending on the data source for fermentation and recovery (for PHB and PLA), and treatment of co-products.
- What are the expected end of life emissions from each of the fossil-based and bio-based polymers listed above?
- Accounting for uncertainty, how do GHG emissions from each of the modeled bio-based plastics compare to emissions from each of the modeled fossil-based plastics?

Chapter 4: *Greenhouse Gas Mitigation for U.S. Plastics Production: Energy First, Feedstocks Later.* This chapter uses the baseline models developed in Chapter 3 to explore alternate ways of reducing GHG emissions in the plastics industry. Specifically, the chapter compares the GHG mitigation potential of feedstock substitution (biopolymer production) to energy substitution (switching from fossil fuels to renewable energy). This chapter contains elements of each of the main tradeoffs explored in this thesis: fuel, feedstock or neither? Specific research questions include:

Chapter 1

- What GHG emission reductions are possible if fossil-plastics are produced using renewable energy (e.g. wind power and renewable natural gas) in place of conventional fuels?
- In the U.S. plastics industry, how do the GHG savings from energy substitution (i.e. using renewable energy in place of conventional energy) compare to the GHG savings achieved by feedstock substitution (i.e. replacing fossil-plastics with PLA, PHB or bioethylene based bio-plastics, produced from either corn or switchgrass, and using either conventional or renewable energy)?
- How might other factors such as cost and market size influence the choice between feedstock substitution and energy substitution?

Chapter 5: Biofuels and Indirect Output Use Change: the Role of Refineries. Finally, Chapter 5 returns focus to the dominant form of policy surrounding biomass use: biofuel mandates. This chapter takes a consequential approach to the ‘fuel or neither’ question. Specifically, this work examines how petroleum refineries are likely to adjust their production in response to biofuel policies (or other policies aimed at reducing the use of liquid fossil fuels), and what this implies for the success of these policies. Research questions include:

- Over the long run, what flexibility does the petroleum industry have to choose its product slate (i.e. the mix of finished petroleum products it produces)?
- How responsive is the crude oil refining sector to relative shifts in price among its major products?
- How is the petroleum industry likely to respond to shifts in demand for individual products, such as reduced demand for gasoline brought about by policies like RFS2?
- How does the existence of refiner flexibility affect the balance of GHG emissions and petroleum consumption that result from different policies aimed at reducing consumption of petroleum fuels?
- What recommendations does this analysis suggest for policies aimed at reducing petroleum use, and GHG emissions through the use of biofuels?

1.3. Climate Change and Greenhouse Gas Mitigation

It has been nearly two centuries since scientists first identified the importance of heat-trapping atmospheric gases in determining a planet's surface temperature.¹⁶ Although it did not gain significant traction until the latter part of the 20th century, the claim that human activity could alter the global climate had surfaced as early as 1896.¹⁷⁻¹⁹ There is now widespread acceptance within the scientific community that rising levels of anthropogenic greenhouse gas emissions are changing the climate in ways that could be catastrophic: from rising sea levels, to extreme weather events, to irreversible changes across both global and local ecosystems.²⁰ As a result, combating climate change is increasingly recognized as a top global priority: the World Economic Forum lists failure of climate change mitigation and adaptation as its single top global risk, in terms of impact, for 2016;²¹ the United Nations Environment Program lists Climate Change as one of its top priorities,²² as do the U.S. Environmental Protection Agency²³ and many other organizations.

In the recent Paris Agreement,²⁴ countries around the world agreed to “holding the increase in the global average temperature to well below 2°C above pre-industrial levels and pursuing efforts to limit the temperature increase to 1.5°C above pre-industrial levels.” As part of this effort, the United States has adopted a goal to reduce GHG emissions by 26-28% below 2005 levels by 2025, and to aim for an 80% GHG emission reduction by 2050.²⁵ In 2012, the U.S. was responsible for nearly 15% of global GHG emissions,²⁶ making its policies particularly important in the fight against climate change. There is thus a pressing need for research to quantify the change in GHG emissions that result from public and private interventions within the U.S., and to use these analyses to set GHG mitigation priorities.

U.S. GHG emissions come from a wide range of sources, with electricity production being responsible for 30% of national emissions, transportation accounting for 26%, industrial sources for 21%, commercial and residential sources for 12%, and agriculture for 9%.²⁷ Given the diversity of emissions sources, both domestic and international, no single mitigation activity will be sufficient to meet GHG reduction targets.^{28,29} Mitigation strategies tend to fall into one of three categories: efficiency and conservation, decarbonization of electricity and fuels, and increasing carbon sinks.²⁹ They range from large sector or economy wide measures, such as the

decarbonization of electricity generation (e.g. fuel switching toward solar, wind, nuclear and other low carbon electricity sources), to relatively small actions targeting individual industries, such as the decarbonization of plastics production discussed in Chapters 3 and 4. In the absence of a single coordinated national/international climate strategy, smaller targeted actions will have to collectively play an important role in meeting GHG mitigation targets.

Having repeatedly failed to pass legislation implementing national carbon pricing,³⁰ the U.S. is left with a patchwork of federal and state policies, together with voluntary private initiatives. At the federal level, flagship programs include the Clean Power Plan (CPP), Corporate Average Fuel Economy (CAFE) standards and the Renewable Fuel Standard (RFS2). The CPP – should it survive the ongoing court challenge – promises to reduce CO₂ emissions from the power sector by 32% below 2005 levels by 2030 through a combination of efficiency and fuel switching measures.³¹ CAFE standards target GHG emissions in the transportation sector indirectly, by requiring new vehicle sales in the U.S. to meet increasingly stringent minimum fuel economy requirements.³² RFS2 currently mandates the use of over 18 billion gallons of biofuel in the transportation sector, equivalent to approximately 10% of domestic gasoline consumption.³³ The standard, discussed in greater detail below, requires that these biofuels have lower life cycle GHG emissions than their fossil counterparts. RFS2 is also subject to ongoing court battles and legislative challenges.³⁴⁻³⁹ In addition to these sector-wide policies, the federal government also engages in a number of more targeted measures, ranging from the control of methane emissions from landfills⁴⁰ or oil and gas operations⁴¹ to appliance efficiency standards⁴² and building codes⁴³, to tax credits for investment into energy efficiency,⁴⁴ renewable energy generation,⁴⁵ and electric vehicle purchase,⁴⁶ among others.

Beyond federal measures, numerous state and local initiatives contribute to U.S. climate action. The U.S. National Climate Assessment⁴⁷ discusses a representative selection of these policies. Some notable initiatives include the Northeast's Regional Greenhouse Gas Initiative,⁴⁸ California's cap and trade system⁴⁹ and low carbon fuel standard (LCFS),⁵⁰ a variety of state-level renewable portfolio standards,⁵¹ and city-level climate action plans.⁵² Of these, only the LCFS includes a specific role for biofuels.

Despite the wide range of actions discussed above, many observers argue that the United States will need additional action to meet its stated greenhouse gas emission targets (e.g. refs^{53,54}). Increasingly, corporations are taking private measures to reduce their greenhouse gas emissions,⁵⁵ and could play an important role in meeting climate goals.⁵⁶ Over 80% of the world's 500 largest companies had targets for reducing GHG emissions or energy use in the 2014-2015 financial year.⁵⁷ Notably (for this dissertation), the list of companies with GHG reduction targets includes some of the world's largest consumers of plastics, such as Coca Cola, Procter & Gamble, and Heinz.^{58,59} These companies, among others, have been actively involved in promoting the use of biomass for energy,⁶⁰⁻⁶² and as a feedstock for bio-based plastics.⁶³ Thus, the case studies presented in this dissertation should be of interest to governments and private organizations alike.

1.4. Life Cycle Assessment

1.4.1. Overview

Tracing its origins to Coca Cola's 1969 "Resource and Environmental Profile Analysis," life cycle assessment (LCA) is the predominant tool for measuring the environmental impact of a product, process or policy.^{64,65} After two decades of ad-hoc methods and diverging approaches, the 1990s marked a "decade of standardization",⁶⁵ with the Society of Environmental Toxicology and Chemistry (SETAC) playing a leading role in the development of what would thereafter be known as LCA. The decade of standardization culminated in the adoption of LCA guidelines through the International Organization for Standardization (ISO). Most recently updated in 2006, ISO 14040 and 14044 together lay out the principles and framework underlying LCA, as well as minimum methodological requirements for conducting an LCA study.^{66,67}

In brief, LCA quantifies the environmental flows associated with a given product or process over its life cycle ('cradle to grave' or 'cradle to cradle') – from resource extraction, through manufacture, use and disposal. Models can be divided into bottom-up (process-based) LCA, top-down (input/output-based) LCA, or hybrid models that include elements of both. Increasingly, LCA has been used as a key tool to support legislative and regulatory actions, especially within the realm of biofuels and bio-based products. The U.S. government's Biopreferred procurement

program⁵ initially required companies to report on the life cycle environmental impact of their bio-based products, and continues to encourage companies to make such data available on a voluntary basis.⁶⁸ More recently, both California's LCFS and the federal government's RFS2 explicitly require regulators to use LCA to quantify the life cycle GHG emissions of biofuels covered under the respective mandates.

While the ISO guidelines discussed above set minimum LCA standards, there remains substantial researcher discretion when it comes to defining the product system and boundary, choosing which flows to quantify, what impact metrics to use, how to allocate emissions between products in joint-production systems, how to interpret LCA results, and so on. Although LCA studies can include a wide range of environmental impact categories (e.g. see EPA's TRACI tool for a typical subset⁶⁹), the recent policy push to combat climate change has encouraged many researchers to focus primarily on life cycle GHG emissions.

GHG emissions are characteristically globally mixed and long-lived. In contrast, environmental flows affecting air and water quality or local ecosystems require greater spatial resolution and local context. As a result, LCA has traditionally been limited in its treatment of non-GHG impacts. Development of spatially, and temporally resolved impact metrics that cover a broader range of environmental and social concerns are at the forefront of LCA research⁶⁵ and are potentially important directions for future research. Meanwhile, this dissertation focuses on providing answers to policy questions surrounding GHG emissions, forwarding the development and use of other advanced LCA techniques involving the treatment of uncertainty and consequential, market-based dynamics, discussed below.

1.4.2. Uncertainty in LCA

To enable appropriate use of LCA results, it is critical for LCA practitioners to convey the confidence with which those results are known. Thus, while most LCA studies continue to produce deterministic estimates, the research community has shown growing awareness of the need to account for the uncertainty and variability inherent to LCA models. Multiple authors have reviewed typologies of uncertainty and variability, along with methods for addressing these complications in LCA.⁷⁰⁻⁷² Source of uncertainty are many, and can generally be classified as

one of parameter uncertainty, scenario uncertainty or model uncertainty.⁷³ Parameter uncertainty is the most frequent type of uncertainty addressed in LCA, and relates primarily to errors in input data. Scenario uncertainty relates to normative modeling choices, such as the definition of the system under study, allocation procedures employed, choice of characterization factors, and so on. Finally, model uncertainty relates to the general structure of the LCA model and its relationship (or lack thereof) to real world outcomes. Uncertainty and variability differ in that the former generally refers to lack of information (i.e. epistemic uncertainty), while the latter refers to inherent randomness or heterogeneity of the system (i.e. aleatory uncertainty). Though conceptually different, uncertainty and variability are frequently addressed jointly under various approaches that include scenario analysis, ranges and bounding analysis, sensitivity analysis, analytical uncertainty propagation, and Monte Carlo simulation, among others.

Although methods for quantifying uncertainty in LCA have been well studied, methods to account for this uncertainty in the decision making process remain in their infancy. A notable exception is the ‘risk of policy failure’ framework developed by Mullins *et al.* (2011),⁷⁴ which regulators can use to set emission reduction targets in function of an acceptable probability that the adopted product or policy will fall short of these targets. This dissertation further develops that framework, and discusses several additional approaches to using uncertain LCA results for decision making.

1.4.3. Attributional and Consequential LCA

One of the most fundamental challenges faced by the LCA community is whether traditional LCA sufficiently captures real-world dynamics to be of use for policy making. In a poignant rebuke, Plevin *et al.* (2014)⁷⁵ argue that “static, context independent and average,” *attributional* life cycle assessment (ALCA) should not be used to inform climate policy; instead, the authors call for practitioners to make greater use of “dynamic, context specific and marginal” *consequential* life cycle assessment (CLCA). The formal distinction between ALCA and CLCA was introduced at a 2001 workshop.⁷⁶ In brief, while ALCA accounts for environmental flows in a static environment, CLCA attempts to answer how such flows will change in response to new decisions or activities. Though there is ongoing disagreement on the exact definition and

appropriate uses for CLCA vs ALCA,^{75,77} various authors have identified features that tend to distinguish CLCA from ALCA.⁷⁷⁻⁸⁰ These include:

- Use of marginal, rather than average data
- Use of economic models to account for market mediated effects of increased production or consumption
- Inclusion of other indirect effects, such as on research and development or efficiency of production.
- Use of system expansion to avoid emission allocation (though this is largely a misconception, as system expansion is still within the providence of ALCA)

Plevin *et al.* (2014)⁷⁵ argue that, by overlooking potentially important system-wide interactions, ALCA “fails to answer the policy questions that have motivated its application.” The authors imply that, with the exception of normative decisions about equitable allocation of impacts, costs or benefits, all LCA should be consequential in nature. This argument is echoed to varying degrees in previous work, such as Weidema (2003),⁸⁰ Ekvall *et al.* (2005),⁸¹ and Tillman (2000).⁸² In response, Suh and Yang (2014)⁸³ argue that the ideal CLCA model, sought by Plevin *et al.* (2014),⁷⁵ does not exist. Their response is reminiscent of the aphorism attributed to George Box: “all models are wrong, but some are useful.” The question then becomes one of whether a given LCA model captures sufficient information about the system under study to be useful. To that end, Suh and Yang argue – correctly, in the view of this author – that there is no strict dichotomy between ALCA and CLCA; rather that the approaches exist on a spectrum of models capturing varying degrees of complication and system dynamics. Yang (2016)⁸⁴ subsequently showed how CLCA can be viewed simply as an extension of ALCA. In other words, ALCA is an “important and indispensable part of the overall consequential modeling.”⁸⁴ This is the view adopted in the present thesis: ALCA is the starting point on top of which consequential modeling is layered. Thus, while the models presented in chapters 2-4 nominally employ attributional life cycle frameworks, they nonetheless include elements associated with CLCA, such as emissions from indirect land use change⁸⁵ and avoidance of allocation through system expansion. Additional market interactions not captured by these models are a limitation, but do not invalidate the insights these models provide. Chapter 5 then delves directly into consequential modeling for biofuel policies.

The remainder of Chapter 1 is devoted to providing background information on the specific systems studied in this dissertation.

1.5. Biomass

1.5.1. Overview

In 2013, bioenergy accounted for approximately 10% (60 EJ) of global primary energy supply.¹ Though this figure is currently dominated by traditional biomass use for cooking and heating in developing countries, more advanced uses have been growing steadily.⁸⁶ In 2012, over a quarter of bioenergy supply was used for modern heating in buildings, and process heat within the pulp and paper industry. Biomass was also the primary energy source for 1.5% of world electricity production in 2012 and 4% of road transport fuel in 2014.⁸⁶ In the United States, biomass accounts for 5% of primary energy consumption, most of which is either biofuel for road transport (46%) or wood products (43%) largely used in paper mills and for residential energy needs.⁸⁷

Motivated by energy security, rural development and GHG mitigation, the United States government has expressed a clear interest in laying the foundations for a national bioeconomy that includes biofuels, biopower, bioproducts and renewable chemicals.⁸⁸⁻⁹⁰ The U.S. is not alone in that vision, with many other groups touting the benefits from increased use of biomass. Countries around the world have adopted biofuel mandates,³ the European Commission has adopted an official Bioeconomy Strategy⁹¹ and the International Energy Agency (IEA) has produced reports that echo the energy security, rural development and GHG mitigation rationale of the U.S. government.^{92,93} Recently, a group of 137 researchers from 24 different countries declared (somewhat hyperbolically) that “there is broad consensus that modern bioenergy will be necessary to achieve a low-carbon future.”⁹⁴

Use of biomass falls somewhere between the fuel switching and carbon sink approaches to GHG mitigation. Like fossil fuels, the energy in biomass is stored primarily as carbon-carbon and carbon-hydrogen chemical bonds. As a result, combustion of biomass releases similar quantities

of CO₂ per unit energy to combustion of fossil fuels.⁹⁵ Thus, while a transition away from fossil fuels toward bioenergy literally involves fuel switching, claims of reduced GHG emissions rely on arguments about changes to the carbon cycle elsewhere in the system. For energy crops that are part of short-term carbon cycles, LCA studies typically assign a credit for the CO₂ that is removed from the atmosphere during plant growth.^{96,97} Thus, CO₂ emissions from biomass combustion are treated as carbon neutral, and long-lived bio-based products are treated as carbon-negative. In this approach, a separate term for emissions from land use change captures the release of carbon from longer-lived biomass (e.g. due to deforestation).⁹⁸ Although this method has been challenged in recent years,^{99,100} it remains standard and – in the view of both this author and others¹⁰¹ – reasonable. Wiloso *et al.* (2016)⁹⁸ and Downie *et al.* (2014)¹⁰² provide further discussion on methods for biogenic carbon accounting. Additional complications to biogenic emissions accounting arise due to differences in timing between carbon release and re-uptake – either due to one-time land use change, or regular crop rotations. With the exception of slow growing biomass (e.g. trees)¹⁰³ or temporary carbon storage in long-lived products,¹⁰⁴ however, timing of GHG emissions is generally not an important factor in the assessment of bioenergy systems.^{105,106}

A key challenge in the assessment of using biomass for GHG mitigation is the sheer number of possible product pathways. A broad range of different feedstocks can be transformed using a wide variety of conversion technologies to produce a large number of different end products. Feedstocks can generally be divided into dedicated energy crops like corn, soybeans, sugarcane, perennial grasses, and wood (among others), or waste sources like landfill gas, agricultural residue and the biogenic components of municipal waste. These feedstocks can be transformed into a variety of solid, liquid or gaseous products that can be used for anything from generation of heat and electricity, to transportation fuels, to chemical feedstocks. Feasible conversion pathways will depend on the available feedstock components, which can include sugar, starch, cellulose, lignin and oil, among others. Conversion from feedstocks to final products can involve either physical transformations (e.g. pelletizing biomass for direct combustion) or more complex transformations that rely on direct chemical processing (e.g., transesterification to produce biodiesel), biochemical conversion (i.e., fermentation, anaerobic digestion, etc.), thermochemical routes (i.e., pyrolysis, gasification), or direct photobiological conversion in the case of algae.¹⁰⁷

Biomass conversion technologies are frequently combined into multi-product systems, known as biorefineries.¹⁰⁸ Garcia and You illustrate the scale of the problem in their 2015 paper, which optimizes an enormous biofuel and bioproduct conversion network that contains 200 technologies and 142 different materials and compounds.¹⁰⁹ Their results suggest that the best biomass conversion networks in terms of cost and GHG emissions will use a mix of feedstocks and technologies to produce a variety of products. The remaining two subsections provide additional background on the primary uses for biomass considered in this thesis: biofuels and bio-based chemicals.

1.5.2. Biofuels and the U.S. Renewable Fuel Standard

Historically, transportation has relied on liquid transportation fuels, owing to their high energy density, quick refill times and ease of use within internal combustion engines. While electric light duty vehicles have made great progress over the last few years,¹¹⁰ they continue to suffer from limited range,¹¹¹ lack of charging infrastructure¹¹⁰ and high environmental impact in regions with low penetration of renewable electricity.¹¹² Further, the prospects of electrification for heavy duty vehicles and aviation are less promising.^{93,113-115} As a result, some authors have concluded that biofuels will likely be required to meet medium-term targets for the reduction of GHG emissions from transportation.^{93,111,115,116} The IEA projects that by 2050, biofuels could provide 27% of all transport fuels.⁹³ For many countries, biofuels are also a way to support rural communities, and increase energy security by decreasing their dependence on petroleum imports.⁹³

It is, thus, not surprising that 64 countries have adopted biofuel mandates.³ These mandates generally require minimum volumes or percentages of renewable fuels to be included in gasoline and diesel blends, respectively. Emission standards are an alternate model, pioneered by California's LCFS,⁵⁰ that set a target average carbon intensity reduction across all transportation fuels; parties meet the standard by trading credits generated from a wide range of alternative fuels, often including biofuels, electricity, natural gas and hydrogen. By far, the most ambitious biofuel mandate is the U.S. Renewable Fuel Standard (RFS2), described in greater detail below. Owing to RFS2 the U.S. is easily the world's largest biofuel producer, responsible for nearly 50% of global biofuel supply in 2012.¹¹⁷ The U.S. is particularly dominant in the world ethanol

market, producing nearly 15 billion gallons/year, representing 60% of global production in 2015.¹¹⁸ Brazil is a distant second, with 30% of global production (7 billion gallons/year). The U.S. is also the world's largest producer of biodiesel, at 15% (1 billion gallons/year) of the global total in 2012.¹¹⁷ The remainder of this sub-section is devoted to describing RFS2, a major focus of Chapters 2 and 5.

The U.S. created its first Renewable Fuel Standard (RFS) under the Energy Policy Act of 2005.¹¹⁹ The standard was subsequently expanded in 2007, under the Energy Independence and Security Act (EISA).⁴ The new standard (RFS2), administered by the U.S. Environmental Protection Agency (EPA), requires refiners, blenders and importers of transportation fuels to meet increased minimum annual biofuel production targets in each of three categories: cellulosic, advanced (anything other than corn ethanol), and renewable (no restrictions). Targets increase annually as shown in Figure 1.1. By 2022 RFS2 requires an annual total of 36 billion gallons of renewable fuel, including at least 15 billion gallons of cellulosic, and an additional 5 billion gallons of advanced biofuel. To qualify under RFS2, renewable fuels from facilities constructed after 2007 must achieve at least a 20% reduction in life cycle greenhouse gas (GHG) emissions relative to baseline (either gasoline or diesel). Steeper reduction targets of 50% and 60% (compared to baseline) are required to qualify as an advanced biofuel or cellulosic biofuel, respectively. Obligated parties can either market biofuels directly, or can purchase tradeable renewable identification number (RIN) certificates from other participants that have exceeded their obligations. Mandated production volumes and GHG reduction targets may be reduced by EPA waiver under certain circumstances.⁴

Nearly a decade after it was established, RFS2 is facing two seemingly opposite stumbling blocks: weak supply (of cellulosic biofuel), and weak demand. Although the standard initially called for no less than 4.25 billion gallons per year of cellulosic biofuel in 2016, existing and proposed cellulosic capacity barely exceeds 100 million gallons per year in 2016.¹²⁰ Meanwhile, on the demand-side, the ethanol "blend wall" limits the amount of biofuel that can be consumed by the existing vehicle fleet. Thus far, biofuel targets have been met predominantly by blending increasing quantities of bio-ethanol into conventional gasoline. This practice has reached its limit at 10% ethanol (E10) blends, the upper bound for which the warranty is valid on most cars.¹²¹

Although EPA has issued a partial waiver for use of a 15% ethanol blend (E15) in vehicles from model year 2001 and newer, the Congressional Research Services concludes the “limitation to newer models, coupled with infrastructure issues, are likely to limit rapid expansion of blending rates.”¹²¹ Lack of infrastructure further impedes use of ethanol at higher blends, such as E85.¹²² Taken together, these factors have induced the EPA to issue waivers, reducing target biofuel volumes every year since 2014 (inclusive).³³

The ‘implemented mandate’ line in Figure 1.1 shows the divergence between congressionally mandated production volumes and the standard actually implemented/proposed by the EPA. The present rollback is particularly unfortunate, as it occurs just as the more advanced and cellulosic biofuels were meant to start ramping up. EISA and RFS2 are thought to forward a number of key goals, most prominently including energy security, rural development and greenhouse gas (GHG) mitigation.¹²³ On the latter goal there has been much controversy surrounding the net GHG balance of corn ethanol – the dominant feedstock to date. A number of studies have even suggested that corn ethanol could result in increased emissions relative to gasoline (e.g. refs^{74,124,125}). The use of food crops for fuel production has also given rise to concerns about exacerbating global hunger.^{126,127} In contrast, cellulosic biofuels are generally reported to have a more favorable GHG balance,¹²⁸⁻¹³¹ and less impact on global food prices.¹²⁷ Even so, the entire biofuel endeavor remains controversial.^{14,126}

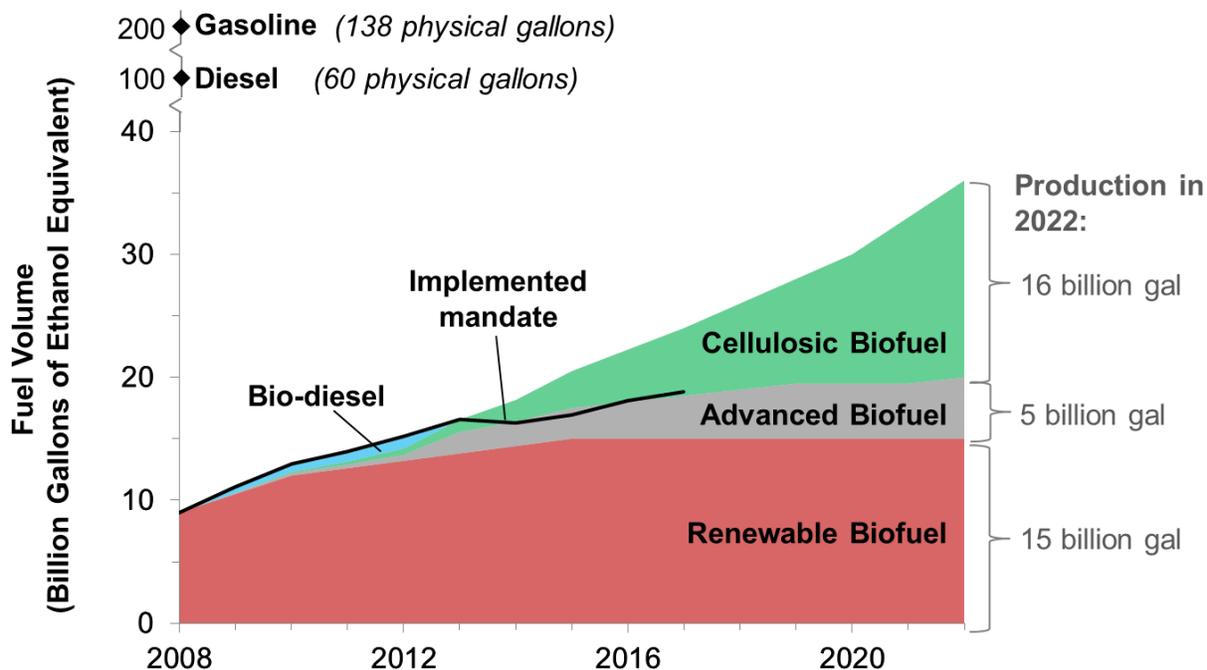


Figure 1.1. Renewable biofuel targets established under the Energy Independence and Security Act of 2007. ‘Renewable biofuel’ refers to any renewable source, ‘advanced biofuel’ refers to any renewable source other than corn starch and ‘cellulosic biofuel’ refers to fuel derived from cellulose, hemicelluloses or lignin. Reference gasoline and diesel production volumes are shown for 2008. The black line shows actual implemented mandates through 2016 and the proposed mandate for 2017. Figure is adapted from Mullins (2012).¹²⁹

1.5.3. Conventional and Bio-based Chemicals

In 2005, the global chemical industry was responsible for approximately 3.3Gt CO₂e, equivalent to 7% of world GHG emissions at the time.¹³² In the U.S., chemical production is responsible for about 5-6% of domestic GHG emissions⁶ and energy consumption (including feedstock energy).⁷ This amounts to 18% of U.S. industrial GHG emissions, second only to oil and gas production.⁶ Globally, the chemical sector is the fastest growing industrial user of energy,⁸ with projected GHG emissions reaching 6.5 GtCO₂e by 2030 under business as usual.¹³² Though its current contribution to global GHG emissions is small relative to transportation, the high value of products in the chemical sector make it a potentially attractive area for increased use of biomass.¹³³⁻¹³⁶ Moreover, while there exist numerous sources of renewable energy, biomass remains the only large-scale source for renewable organic chemicals. Indeed, both the International Council of Chemical Associations (ICCA) and the IEA identified greater use of renewable (bio-based) feedstocks as a potentially critical area for breakthrough innovations to

reduce the industry's GHG emissions.^{132,137} Chemicals produced from biomass have the potential to be carbon negative over their life cycles, a feature which may be critical in meeting long-term climate targets.¹³⁸

This thesis focuses specifically on plastics production, a major component of the chemical industry. Over the last six decades, global plastics production has grown from a nascent enterprise to a 300 million tonne (Mt) /year global industry in 2013.¹³⁹ North American plastic production accounts for approximately 20% of global production, and is expected to exhibit strong growth for the immediate future.^{140,141} In the U.S., a subset of plastics known as 'commodity thermoplastic' polymers (discussed in chapters 3 and 4) account for approximately 70% of plastics production.^{142,143} Applying previously reported emissions factors suggests these plastics are responsible for approximately 70 million tonnes of CO₂e emission per year¹⁴⁴ and nearly 3 quadrillion Btu of primary energy use.¹⁴⁵ This corresponds to slightly greater than 1% of total U.S. GHG emissions¹⁴⁶ and nearly 3% of total U.S. energy consumption.¹⁴⁷ In response, there has been a growing interest in switching to bio-based plastics as a form of greenhouse gas (GHG) mitigation. After fuels, bio-based polymers offer one of the largest potential markets (by volume) for bioproducts,¹³⁵ and have been suggested as a potential "linchpin category" in the operation of biorefineries.¹³⁴

In 2013, bio-based plastics accounted for less than 1% (1.6 million tonnes (Mt)) of global thermoplastics production.¹⁴⁸ Nonetheless, bio-based production is expected to grow rapidly, reaching nearly 7 Mt by 2018.¹⁴⁸ Four families of polymer are expected to figure prominently in future bio-plastics markets,^{10,149-151} and have been the focus of a number of studies in the existing life cycle assessment (LCA) literature:¹⁵²⁻¹⁵⁴ polylactic acid (PLA), polyhydroxyalkanoates (PHA), thermoplastic starch (TPS), and bioethylene based plastics. Three of these (PLA, PHA and bioethylene) are the focus of Chapters 2- 4.

1.6. The Petroleum Sector

Worldwide, crude oil represents the single largest source of primary energy, amounting to 31% of all primary energy production in 2013.¹ It is used primarily for transportation (64%), for a

range of non-energy products (16%), in industry (8.4%), and for a mix of other applications.¹ Petroleum products are responsible for just over 33% of global combustion CO₂ emissions.¹ In the U.S., petroleum represents 36% of primary energy consumption⁸⁷ and over a third of all GHG emissions.¹⁵⁵

Figure 1.2. shows a snapshot of the U.S. petroleum and liquid fuel sector for the year 2015. While crude oil is the dominant feedstock, natural gas liquids (NGLs) and ethanol make sizeable contributions. Domestic production slightly surpasses imports; though a majority of products are consumed domestically, exports represent a non-trivial share of final product disposition. Final petroleum products result from crude oil refining; the process also involves limited inputs of other products including oxygenates, unfinished oils, NGLs and hydrogen. The figure also highlights the critical role of blenders in producing gasoline, a role which has increased substantially over the last decade due to rising ethanol blending requirements imposed by RFS2. Gasoline and distillates are by far the dominant finished products, though the industry also produces a large range of other products that include jet fuel, liquefied petroleum gases (used primarily as chemical feedstocks and for space heating), petroleum coke, still gas, residual fuel oil, asphalt, lubricants and more. The following section provides a more in depth description of petroleum refining, a major focus of Chapter 5.

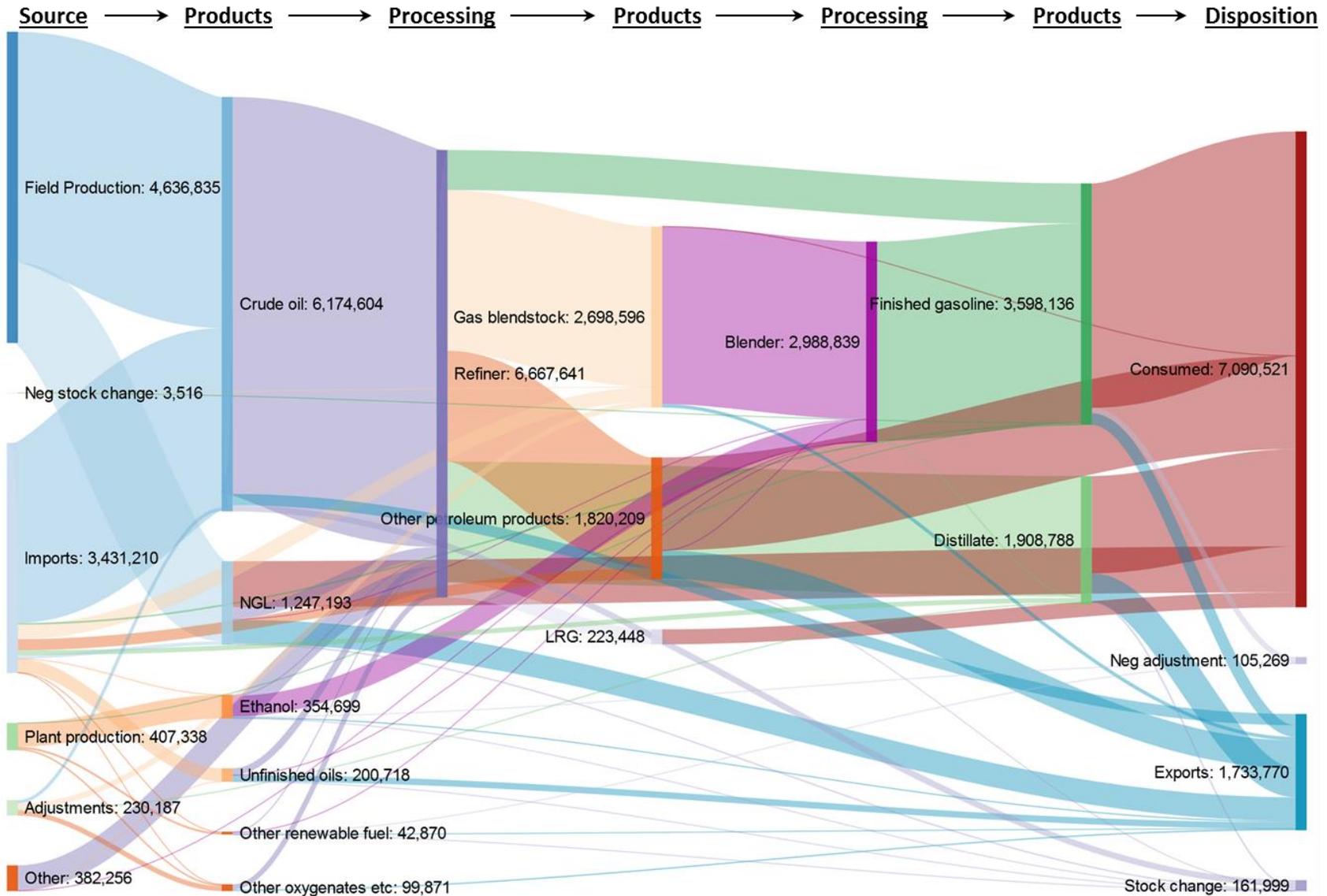


Figure 1.2. Sankey diagram of the U.S. petroleum industry for the year 2015. Generated from EIA data,¹⁵⁶ using sankeyMATIC software.¹⁵⁷ All units are in thousand barrels per year (Mbbbl/year); significant figures are as reported by EIA. NGL = natural gas liquids; LRG = liquefied refinery gases; the abbreviation ‘Neg’ precedes negative stock changes or adjustments. Volume gained during crude oil refining is included in the category ‘other.’

1.6.1. *Petroleum Refining*

Crude oil refineries are among the world's largest and most complex chemical operations. As of January 1st, 2016, there were 634 refineries around the world, with a combined processing capacity of nearly 90 million barrels of crude oil per calendar day.¹⁵⁸ With over double the installed capacity of any other country, the United States represented approximately 20% of the global base capacity (atmospheric distillation). U.S. refineries also tend to be more complex than the global average, representing 30-40% of the global installed capacity for downstream processing like vacuum distillation, catalytic cracking, thermal processing (e.g. coking), catalytic reforming, and so on.

Figure 1.3. shows a simplified block diagram of a representative refinery. Actual unit processes and overall plant structure will differ by refinery. A description of major refining processes follows, based on refs.¹⁵⁹⁻¹⁶¹

Desalting and Dewatering is not shown explicitly in Figure 1.3., but is a necessary step before refining can begin. Its purpose is to remove dirt, water and salt. The main technique is gravity separation of gas, crude oil and brine/dirt. The process may be aided by heating to 90-150 °C under pressure (50-250 psi), water washing, passing through sand/gravel, addition of de-emulsifiers, or application of an electrostatic field.

Atmospheric Distillation is the most fundamental step in oil refining. It involves fractional distillation of components which boil at less than 350°C under atmospheric pressure. A number of characteristic cuts are taken, including gas (C1-C4 components boiling at ambient temperature), light naphtha (C5-C6, boiling at 30-90°C), heavy naphtha (C6-C12 boiling at 90-200°C), kerosene (C10-C16, boiling at 140-320°C), middle distillate (C16-C20, boiling at 150-345 °C), atmospheric gas oil and finally atmospheric residuum. The purpose of this step is to separate out the components of crude oil without inducing any chemical transformations.

The atmospheric residuum is then fed to a **vacuum distillation** unit which can further separate out products under low pressure (1-2 psi) at no more than 350°C. The main cuts resulting from this phase are light vacuum gas oil (boiling at 340-470°C under ambient pressure) and heavy

vacuum gas oil (boiling at 470-560°C under ambient pressure), as well as lubricating oil (boiling >400°C) and vacuum residuum (boiling > 600°C). Once again, the purpose of this step is to separate out the components of crude oil without inducing any chemical transformations.

The heaviest components left over from vacuum distillation can be sent through **deasphalting and solvent extraction** processes. Under mild conditions, light paraffin solvents (C3-C5) are used to extract the relatively lighter components for further processing, leaving behind the heaviest component, asphalt (generally used for road paving). The purpose of this step is separation of components.

The **gas plant** is the final separation unit, producing liquefied petroleum gases, refinery fuel gas and petrochemical feedstocks. It may involve a number of steps including an amine absorber to strip acid gases and cryogenic separation of components.

Visbreaking (not shown in Figure 1.3.) is a form of mild thermal cracking. Inputs typically include heavy residua, either from the atmospheric or vacuum distillation unit or other processes. The primary purpose is to reduce the viscosity of the non-volatile inputs to produce products that can be used as part of a fuel oil blend, or as waxes with lower pouring temperatures. Typical conditions include high pressure (50-300 psi) and moderate temperatures (455-510°C).

Coking: Similar to visbreaking, the coking process involves thermal decomposition of the heavy residua (typically from vacuum distillation) into lighter products (including gas, naphtha, fuel oil, gas oil) as well as solid coke. Several different coking procedures are possible. In delayed coking, the raw materials are heated in a fractionator, with outlet temperature ranging from 480-515°C, and continue reacting in a coking drum held at around 415-450°C and moderate pressures of 15-90 psi. Other mechanical setups (with similar reaction conditions) include fluid coking and flexicoking.

Catalytic Cracking: Having progressively replaced thermal cracking since the 1940's, catalytic cracking takes heavy products like atmospheric gas oil and converts them to lighter feedstocks like kerosene and naphtha, which will typically be used for jet fuel and gasoline. The process

uses a solid acid catalyst like a mix of silica and alumina or an aluminosilicate zeolite and produces fuel with higher octane rating than the obsolete thermal cracking methods. Although the process is different from one termed thermal cracking, temperatures on the order of 480-540°C are still required, along with mild pressure (25-40 psi).

Hydrocracking: Visbreaking, coking and catalytic cracking all have the primary purpose to break down heavy components into more valuable lighter ones. Hydrocracking is the last process focused on decomposition. It is a catalytic process that differs from those above in that it is conducted in the presence of hydrogen. While the products from catalytic cracking are used predominantly for gasoline, a substantial proportion of hydrocracking products will also end up as diesel fuel. The inputs include heavy components like vacuum gas oil, which are heated (300°C-370°C) under high pressures (1000-2500 psi) in the presence of a metal catalyst (e.g. nickel, molybdenum, tungsten or palladium on silica-alumina support) and hydrogen. The presence of hydrogen reduces the likelihood of coking reactions and also reduces the yield of light ends like methane, ethane and propane relative to catalytic cracking.

Hydrotreatment is another hydroprocessing step, so named as it involves a reaction which occurs in the presence of hydrogen. It differs from the processes above in that it does not attempt to make any fundamental changes to the hydrocarbons, but rather is used for removal of impurities. The main goal is to remove nitrogen and sulfur atoms from the feedstocks. Just about any material flow in the refinery can (and will) be passed through a hydrotreater. Metal catalysts such as nickel, palladium, platinum, cobalt or iron can be used, along with temperatures of around 300-345°C and hydrogen pressures of 500-1000 psi. As mentioned above, there are no major changes to the underlying feedstock, so outputs are essentially just a cleaner version of the inputs. Certain olefins may also be hydrogenated, which avoids the formation of gum which would reduce gasoline stability.

Catalytic Reforming is part of a set of reactions that improve product quality without reducing the weight of its components. The main goal of catalytic reforming is to increase the octane rating of inputs (naphthas – either straight run or from a hydrocracker) for use as gasoline. The feedstock is heated to 510-595°C under pressures ranging from 400-1000 psi. One of the main

transformations at work is dehydrogenation, and so H₂ (for hydroprocessing) is also a valuable product from this phase.

Isomerization is used to increase the branching of compounds for later use in gasoline. Inputs include butane, pentane and hexane. The reaction may involve a metal catalyst with temperatures of 370-480°C and pressures of 300-750 psi, or aluminum chloride and hydrogen chloride catalyst at lower temperatures. The products can be used in a further alkylation step, or possibly directly for gasoline blending.

Alkylation takes lighter feedstocks and converts them to heavier products to be used as gasoline. Specifically, isoparaffins, like isobutane, are reacted with olefins, like propylene, butylenes or pentenes, to higher branched mid-molecular weight (~C7-C9) compounds with high octane ratings (and thus high value as a gasoline additive). The raw material generally comes from separations occurring at the gas plant. Alkylation is often acid catalyzed; in that case, the reaction takes place at low temperatures (1-40°C) and pressures (14-140 psi) in the presence of an acid catalyst like H₂SO₄ or HF.

Polymerization, properly termed oligomerization (not shown in Figure 1.3.), is a process that creates dimers, trimers or tetramers from olefin gases (e.g. propylene or butylenes), resulting in C4-C12 compounds for use in gasoline. The reaction can be conducted thermally, heating simple alkanes like propane and butane to high temperatures (510-595°C) for prolonged periods. Similarly, olefins can be polymerized directly using acid catalysts at 150-220°C and 150-1200 psi.

Methane Steam Reforming (not shown in Figure 1.3.), is used to produce hydrogen required for hydroprocessing, and is often integrated into (though conceptually separate from) the oil refinery. It usually involves the reaction of methane with water at high temperatures (700-1100°C) with a metal catalyst. The net reaction is $\text{CH}_4 + \text{H}_2\text{O} \rightarrow \text{CO} + 3\text{H}_2$.

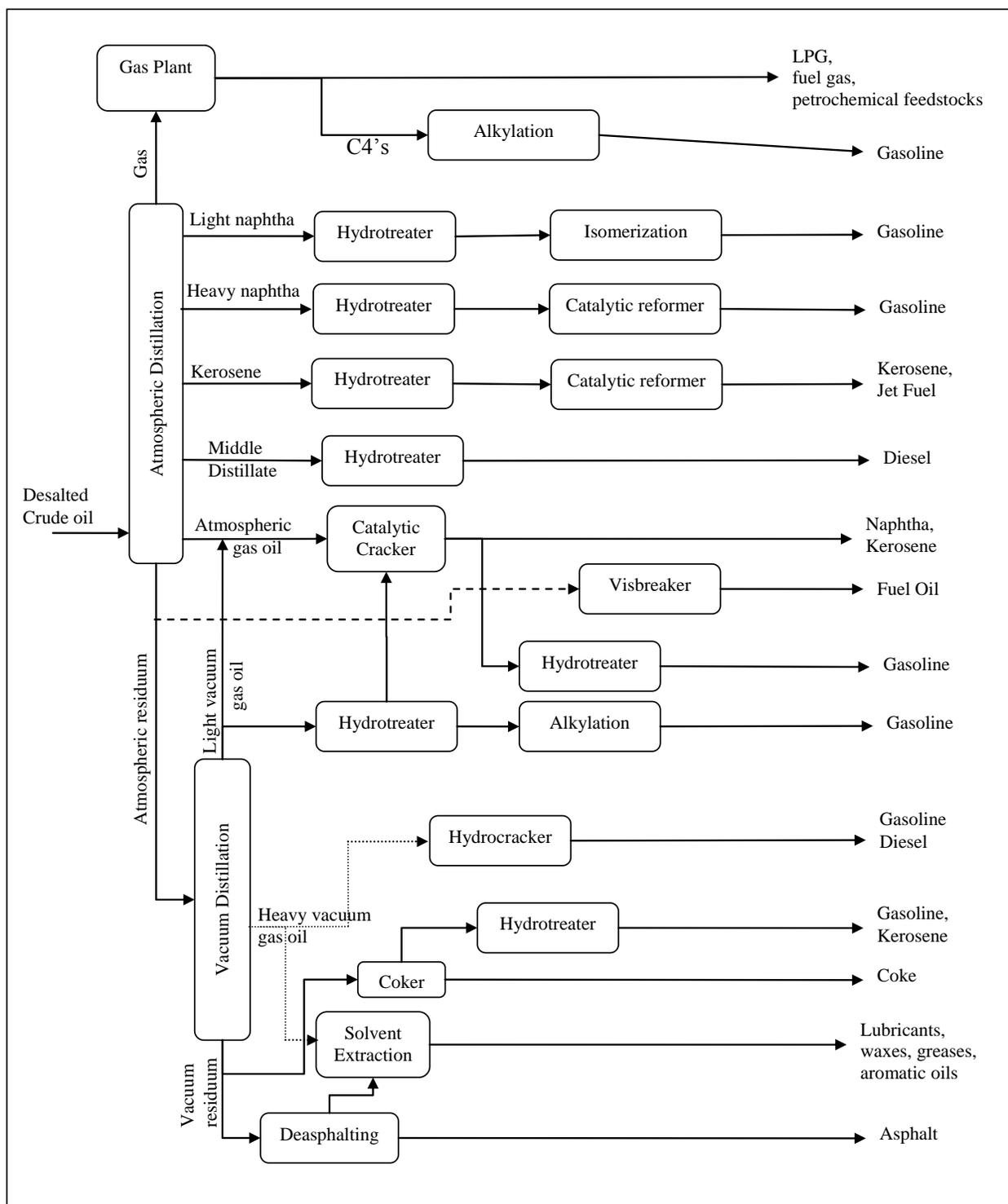


Figure 1.3. Simplified block diagram of a representative modern crude oil refinery, based on refs¹⁵⁹⁻¹⁶¹

A typical refinery product slate will include a wide range of products, such as still gas (refinery fuel), liquefied petroleum gases/liquefied refinery gasses (LPG/LRG), gasoline, distillate fuel oil (the parent category for diesel fuel), jet fuel, kerosene, residual fuel oil, waxes, lubricants, aromatic oils, petroleum coke, petrochemical feedstocks, and asphalt. Three main factors that determine the relative yields of petroleum products include: properties of the input crude oil, the configuration of the refinery, and the operation of the refinery.

As shown in Figure 1.4., crude oil characteristics are most commonly measured along two dimensions: density, and sulfur content.¹⁶² To predict processing requirements and product yields, however, far more information is needed about the composition of a given crude such as its distillation curve (quantity of oil within each characteristic cut), carbon residue content and hydrogen content.¹⁶³ Thus, for example, oils with a greater naphtha content will be able to produce more gasoline; oils with a greater kerosene content will produce more jet fuel; oils with a greater distillate content will produce more diesel; oils with a greater gas oil and residuum content will produce more residual fuel oils, lubricants, asphalts, and so on. As a result, overall density (i.e. API gravity) may only be weakly predictive of overall product slate.

Refineries will typically be configured to process a specific type of crude oil; plant managers can maintain target input feedstock properties by blending together mixes of crude oils from various sources. Nevertheless, refineries do have some flexibility regarding the specific blends processed and can thus influence the resulting product slate.¹⁶⁴ Generally, refineries with more downstream processing capacity (everything after atmospheric distillation) can process a wider range of input crudes, and produce a greater proportion of high value products like gasoline, jet fuel and diesel. Refineries can also adjust their configurations (and product slates) by adding new process units. Even for a fixed input blend and refinery configuration, refineries are able to make small changes to their product slates through internal operational adjustments. This can be accomplished by shifting the exact temperature of cut points in the atmospheric distillation process, or by controlling how much of a given cut is fed into each downstream operation.¹⁶⁴ Thus, refineries have some flexibility to respond to changes in relative prices for petroleum products by changing the type of crude oil processed, by installing (or removing) downstream processing capacity, or

by changing their internal operations. Finally, industry-wide, shifts in product slate can occur as more profitable refineries ramp up production (increase their utilization rate), while less profitable refineries ramp down.

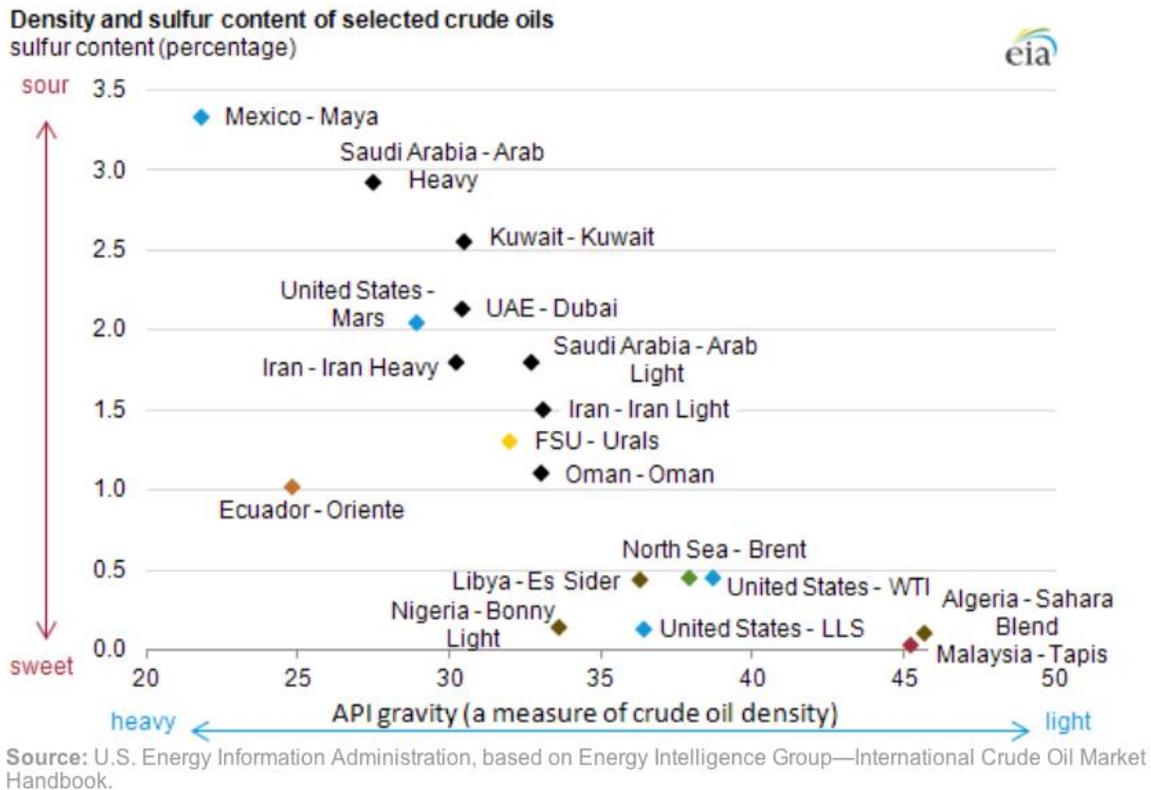


Figure 1.4. Key characteristics (sulfur content and API gravity, a measure of density) of common crude oils. Reproduced from ref.¹⁶²

1.7. Tradeoffs in the Use of Biomass for Greenhouse Gas Mitigation

Long term recommendations regarding different uses of biomass must consider a wide range of social, economic and environmental metrics. Meanwhile, as one of the key drivers behind the development of bio-based products, this thesis focuses on using biomass for GHG mitigation. There is already a growing literature surrounding the best use of biomass for meeting climate targets. The previously mentioned study by Garcia and You (2015)¹⁰⁹ is among the most extensive biofuel and bioproduct networks considered in a single study. Their model suggests that woody biomass and thermochemical conversion routes are often preferred over other feedstocks and pathways with respect to cost and GHG emissions; however, the model did not

explicitly consider emissions from displaced fossil products, and so results may not generalize well. Other authors (e.g. ref¹⁶⁵) have likewise considered the GHG emissions from a range of biomass pathways, but without direct reference to displaced fossil products. In another study, Monti (2012)¹⁶⁶ conducted a limited literature review, which showed that using switchgrass as a solid fuel (e.g., to produce bio-electricity) generally results in greater GHG mitigation than using switchgrass for liquid biofuels. Adler *et al.* (2007)¹⁶⁷ report a similar conclusion, that biomass gasification for electricity generation yields greater GHG benefits than converting biomass to ethanol or biodiesel. Bos *et al.* (2010)¹⁶⁸ compare various uses for different sugar/starch feedstocks, and conclude that producing PLA in place of PET results in the greatest GHG savings, followed by bioethanol replacing fossil ethanol, bio-LDPE replacing fossil LDPE and finally bioethanol replacing gasoline. Gustavsson and Le Truong (2016)¹⁶⁹ argue that using electric cars powered with bioenergy achieves greater and more immediate climate benefits than producing biofuels. Evans *et al.* (2015)¹⁷⁰ and Favero *et al.* (2015)¹⁷¹ both compare forest recovery/preservation to bioenergy options. Evans *et al.* conclude that the preferred option depends on both the local climate and yield of bioenergy crops; Favero *et al.* similarly argue that the two strategies can actually be complementary. This result is similar to an argument made by Slade *et al.* (2010)¹⁷² that, while it is important to set priorities for using biomass, there is no ‘one-size-fits-all’ best use.

Of particular interest to this thesis are a subset of studies that consider the energy vs. feedstock question with respect to biomass. Using a dynamic energy system simulation model, Daioglou *et al.* (2015)¹⁷³ conclude that biomass is more effective at GHG mitigation when used for electricity than for building services, industry or as a chemical feedstock. Morris (2016)¹⁷⁴ compares several recycle, bury or burn scenarios for wood waste and concludes that recycling wood into bio-based products has the lowest environmental impact across a range of metrics (including climate change). Kalt *et al.* (2016)¹⁷⁵ likewise conclude that higher GHG savings are achieved by using wood residue as material (for insulating boards) instead of for energy. Rass-Hansen *et al.* (2007),¹³³ Alvarenga and Dewulf (2013),¹⁷⁶ McKechnie *et al.* (2015)¹⁷⁷ and Kalt *et al.* (2016)¹⁷⁵ have all considered whether ethanol is best used for fuel or as a chemical feedstock. Rass-Hansen *et al.* provides only a general discussion, and Kalt *et al.* conclude that, subject to certain sensitivities, bioethylene is the preferred use for ethanol. Alvarenga and Dewulf, and McKechnie

et al. both conclude, in agreement with the present work (Chapter 2), that feedstock and fuel use of ethanol both achieve similar GHG savings.

Out of necessity, this thesis examines only a subset of the most important questions surrounding how, or whether to use biomass for GHG mitigation. Chapter 2 focuses on the most prominent biomass policy in the United States: RFS2. It asks whether the GHG mitigation goals of RFS2 could be well-served by expanding the RFS2 to include credits for other uses of ethanol. It is the first work to pose this question, and is among the first to quantify the GHG emissions from U.S. production of fossil-ethylene or bioethylene, compare bioethylene to bioethanol, or provide an in depth treatment of uncertainty. Likewise, Chapter 3 is among the first studies comprehensively to analyze uncertainty in the emissions from several of the most important bio-based plastics; Chapter 4 subsequently is the first work to compare the GHG mitigation potential of bio-based plastics to adopting low-carbon energy for plastics production. Finally, Chapter 5 returns to RFS2 and other similar biofuel policies. It is one of only a small number of papers to consider consequential market interactions in the evaluation of biofuel policies, and is the only such work to assess the GHG consequences that result from flexibility in petroleum refining.

Chapter 2. Changing the Renewable Fuel Standard to a Renewable Material Standard: Bioethylene Case Study

2.1. Abstract

The narrow scope of the U.S. renewable fuel standard (RFS2) is a missed opportunity to spur a wider range of biomass use. This is especially relevant as RFS2 targets are being missed due to demand-side limitations for ethanol consumption. This chapter examines the greenhouse gas (GHG) implications of a more flexible policy based on RFS2, which includes credits for chemical use of bio-ethanol (to produce bioethylene). A Monte Carlo simulation is employed to estimate the life cycle GHG emissions of conventional low-density polyethylene (LDPE), made from natural gas derived ethane (mean: 1.8 kg CO₂e/kg LDPE). The life cycle GHG emissions from bio-ethanol and bio-LDPE are examined for three biomass feedstocks: U.S. corn (mean: 97g CO₂e/MJ and 2.6kg CO₂e/kg LDPE), U.S. switchgrass (mean: -18g CO₂e/MJ and -2.9kg CO₂e/kg LDPE) and Brazilian sugarcane (mean: 33g CO₂e/MJ and -1.3kg CO₂e/kg LDPE); bio-product and fossil-product emissions are compared. Results suggest that neither corn product (bioethanol or bio-LDPE) can meet regulatory GHG targets, while switchgrass and sugarcane ethanol and bio-LDPE likely do. For U.S. production, bio-ethanol achieves slightly greater GHG reductions than bio-LDPE. For imported Brazilian products, bio-LDPE achieves greater GHG reductions than bio-ethanol. An expanded policy that includes bio-LDPE provides added flexibility without compromising GHG targets.

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<http://pubs.acs.org/articlesonrequest/AOR-PPRjXpeDcQ32ug9fgy8N>

2.2. Introduction

In 2007, the United States (U.S.) Energy Independence and Security Act (EISA) expanded the national Renewable Fuel Standard (RFS).⁴ The new standard (RFS2), administered by the U.S.

Environmental Protection Agency (EPA), requires refiners, blenders and importers of transportation fuels to meet increased minimum annual biofuel production targets in each of three categories: cellulosic, advanced (anything other than corn ethanol), and renewable (no restrictions). Targets increase annually as shown in Figure 1.1 on page 16. By 2022 RFS2 requires an annual total of 36 billion gallons of renewable fuel, including at least 15 billion gallons of cellulosic, and an additional 5 billion gallons of advanced biofuel. To qualify under RFS2, renewable fuels from facilities constructed after 2007 must achieve at least a 20% reduction in life cycle greenhouse gas (GHG) emissions relative to baseline (generally gasoline). Steeper reduction targets of 50% and 60% (compared to baseline) are required to qualify as an advanced biofuel or cellulosic biofuel, respectively. Mandated production volumes and GHG reduction targets may be reduced by EPA waiver under certain circumstances.⁴

Thus far, biofuel targets have been met predominantly by blending increasing quantities of bio-ethanol into conventional gasoline. This practice is approaching its limit at the 10% ethanol (E10) ‘blend wall’, the upper bound for which the warranty is valid on most cars.¹²¹ Although EPA has issued a partial waiver for use of a 15% ethanol blend (E15) in vehicles from model year 2001 and newer, the Congressional Research Services suggests the “limitation to newer models, coupled with infrastructure issues, are likely to limit rapid expansion of blending rates.”¹²¹ Lack of infrastructure further impedes use of ethanol at higher blends, such as E85,¹²² and so the EPA has begun reducing target biofuel production volumes starting in 2014.¹⁷⁸ The difficulties faced by RFS2 can be partially attributed to its limited scope of application (the transportation sector). This simultaneously limits the market for biofuels and places competing uses for bio-ethanol at a disadvantage in the marketplace. This chapter investigates the GHG emissions associated with an alternate use for bio-ethanol: to produce bio-based chemicals. The goal of this analysis is to inform on the potential impact from creating a new, more inclusive federal policy for use of bio-ethanol, modeled on RFS2. The main question addressed is whether bio-based chemicals (specifically bioethylene) from certain feedstocks could achieve similar GHG reductions to the targets laid out in RFS2. Regulatory hurdles and other potential impacts such as those highlighted by the food versus fuel debate (e.g. ref¹²⁶) are beyond the scope of this chapter but would need to be considered in the future in a broader assessment of the implications of such a policy.

Bulk chemical production is responsible for about 5-6% of both U.S. GHG emissions⁶ and U.S. energy consumption (including feedstock energy).⁷ Ethylene is one of the industry's most important chemicals and can be produced through the dehydration of ethanol.^{179,180} Current U.S. ethylene production is 24 million tonnes/year.⁹ Global production is about 5 times that,¹⁸¹ making ethylene the world's largest volume organic chemical. While transportation fuels represent a much larger proportion of U.S. energy use (28%) than bulk chemicals,¹⁸² the latter remains a sizeable market. For a point of comparison, the full RFS2 mandate (36 billion gallons of ethanol or ethanol equivalent) represents only about 3% of U.S. energy needs. This chapter is focused on bioethylene as a first step toward assessing whether a more comprehensive Renewable Materials Standard (RMS) should be considered as a way to reduce GHG emissions from various sectors. Replacing yearly demand of U.S. fossil ethylene with bioethylene could elevate the demand for bio-ethanol by roughly the equivalent of current national U.S. ethanol production.¹⁸³ In 2014, EPA waiver reduced RFS2 requirements by approximately 3 billion gallons of ethanol;¹⁷⁸ this gap could have been bridged by converting 20% of U.S. ethylene production (5 million tonnes) to bioethylene.

Bioethylene is chemically and functionally indistinguishable from its conventional fossil-fuel counterpart. This distinguishes it from bio-ethanol fuel in that bioethylene need only compete on costs, while bio-ethanol faces a host of other demand-side constraints, such as energy differences per gallon and new infrastructure requirements. Small amounts of bioethylene are already in production, with Brazil having the highest capacity.¹⁸⁴ Nevertheless, bioethylene production remains minimal compared to fossil ethylene (<1% of global ethylene production).^{181,184}

At present, U.S. ethylene production is dominated by steam cracking of light hydrocarbons (65% from ethane, and 15 to 20% from propane) derived from natural gas. Cracking of heavy feedstocks (primarily naphtha) accounts for most of the remaining 15 to 20%.¹⁸⁵⁻¹⁸⁷ Availability of light feedstocks is expected to remain strong for decades,¹⁸⁸ suggesting that ethane cracking will continue to dominate U.S. production for the foreseeable future.

The policy change assessed in this chapter would result in a partial shift away from fuel-use of ethanol toward chemical use (for bioethylene). Evaluating the GHG impact of this move requires comparing the difference in GHG emissions between gasoline and bio-ethanol to the difference in emissions between fossil ethylene and bioethylene. Numerous studies have investigated life cycle emissions from production of biofuels (reviewed in refs^{97,189,190}). Fewer studies investigate the impacts from bioethylene products^{168,176,191-197} and just two of these explicitly considered competition between fuel and chemical use for biomass.^{168,176} Two studies were tailored to a U.S. context,^{195,197} and just one explicitly modeled the emissions from a natural gas derived ethane to ethylene pathway.¹⁹⁷ Only two studies^{191,193} considered emissions from indirect land use change (ILUC). The studies in refs^{168,176,191-197} generally report that bioethylene based products can achieve reductions in GHG emissions and non-renewable energy use, though potentially at the expense of other environmental impacts (e.g. acidification and eutrophication). Notable exceptions include one of the scenarios from Liptow and Tillman¹⁹¹ (the “attributional” model with “higher estimate” ILUC shows a 10% increase in GHG emissions from sugarcane polyethylene relative to production from crude oil), and Ghanta *et al.*¹⁹⁷ who find highest GHG emissions for corn ethanol to ethylene (0.67 kg CO₂e/kg ethylene), followed by naphtha (0.50 kg CO₂e/kg ethylene) and finally ethane (0.42 kg CO₂e/kg ethylene). Alvarenga *et al.*,¹⁷⁶ focus exclusively on Brazilian sugarcane and report similar GHG savings for bio-ethanol (1.77-1.85 kg CO₂e/kg ethanol, depending on the ethanol content (E20-E25) of displaced fuel) and bioethylene (1.60-1.87 kg CO₂e/kg ethanol, depending on ethylene yield from ethanol). Bos *et al.*¹⁶⁸ focus on production in either the Netherlands or Brazil and report slightly greater GHG savings from bioethylene than from bio-ethanol (by ~2-3 tonnes of CO₂e/ha, depending on the biomass feedstock). None of the above studies provided a complete treatment of uncertainty and variability for both fossil and bio-based pathways.

Using a life cycle assessment approach with Monte Carlo simulation, this chapter develops an estimate for the cradle-to-gate GHG emissions for polyethylene production (specifically low-density polyethylene (LDPE)). Although ethylene is used as a raw material for many products, the majority (~70%) is used to manufacture polyethylene.⁹ Baseline GHG emissions from fossil-based production (ethane to ethylene) are compared to the expected GHG emissions from bio-based ethylene production for three biomass pathways: U.S. switchgrass (a cellulosic feedstock),

Brazilian sugarcane (an ‘advanced’ feedstock), and U.S. corn starch. Finally, competing uses for ethanol (as fuel, or to produce bioethylene) are examined: the difference in GHG emissions between bioethylene and fossil ethylene is compared to the difference in GHG emissions between ethanol and gasoline. The comparisons drawn in this chapter refer to changes in GHG emissions accounting and may not correspond to actual emission changes for several reasons, as elaborated in the results and discussions section.

2.3. Methods

2.3.1. Pathways Overview

Eight pathways are modeled as shown in Figure 2.1. Four of these are fuels: gasoline, switchgrass ethanol, corn ethanol and sugarcane ethanol. The other four are LDPE: natural gas LDPE, switchgrass LDPE, corn LDPE and sugarcane LDPE. The various pathways produce different products so a consistent functional unit such as kg of product, would be misleading. To facilitate comparisons, the functional unit for each pathway is normalized to the same quantity of ethanol (1.74 kg), corresponding to 1kg of LDPE production or 46.9 MJ energy (lower heating value).

For each bio-based pathway, an accounting of the following steps is included: cultivation (including emissions from land-use change), feedstock transportation, and ethanol production via fermentation. The ethanol produced from each pathway is chemically identical and is differentiated only by location (U.S. or Brazil). Corn ethanol is co-produced with dried distiller grains with solubles (DDGS). Switchgrass and sugarcane ethanol are co-produced with unused feedstock components, which may be used to generate electricity. Three additional steps are modeled for fuel-use ethanol: transport to the U.S. (for Brazilian ethanol only), fuel distribution, and combustion. For chemical use (polyethylene production), additional modeled processes include transport of ethanol to the ethylene production facility, dehydration of ethanol to ethylene, polymerization of ethylene to LDPE, and transport to the U.S. (Brazilian LDPE only). These steps are modeled using regionally applicable parameters for Brazilian and U.S. pathways, respectively.

For ethanol fuel, the conventional alternative is gasoline, for which the distribution of GHG emissions are as modeled by Venkatesh *et al.*¹⁹⁸ The conventional pathway for LDPE production in the U.S. is via natural gas derived ethane. The life cycle analysis includes pre-production, wet natural gas extraction, processing, steam cracking and polymerization. A number of co-products are produced throughout the process as shown in Figure 2.1.

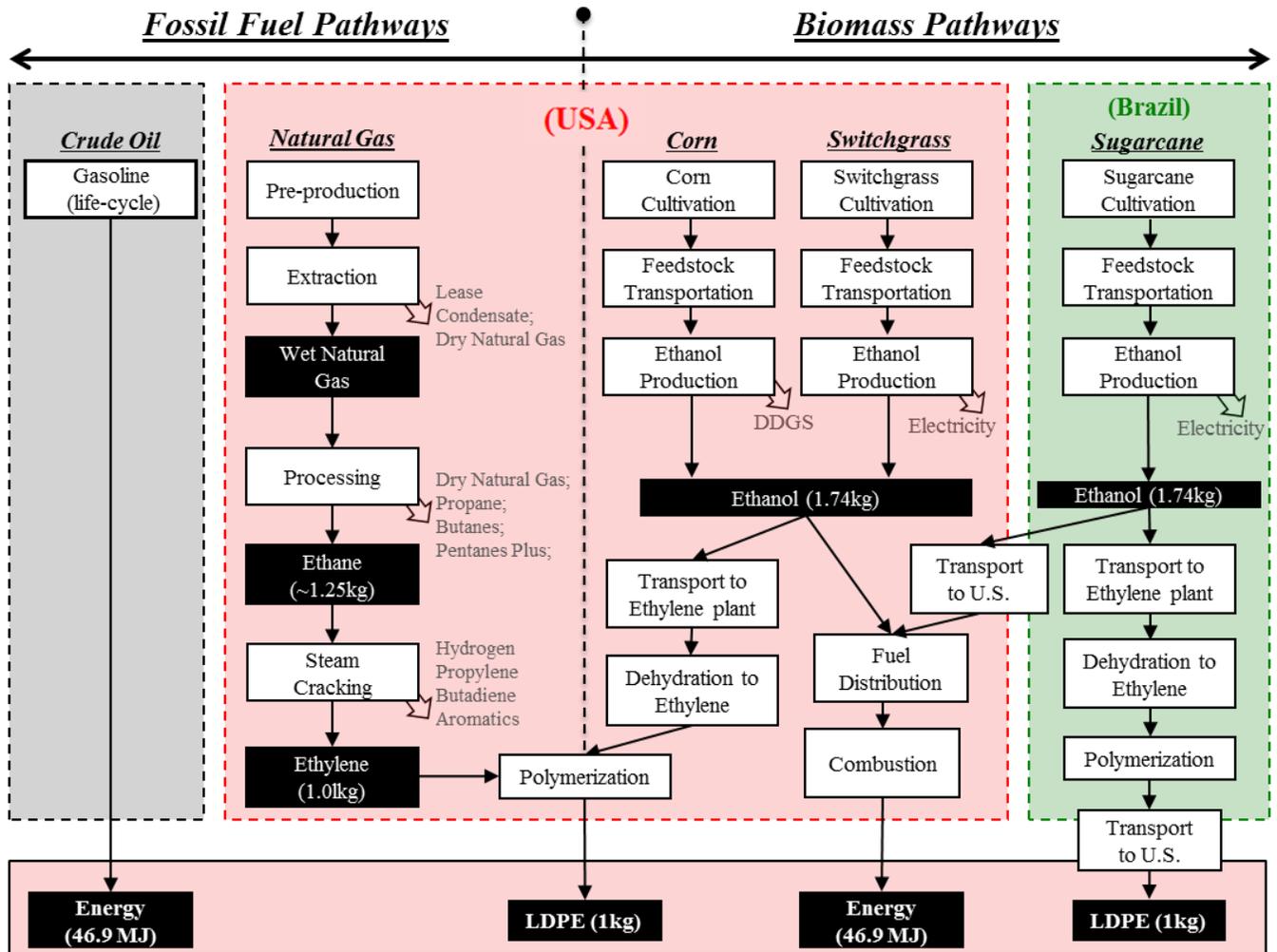


Figure 2.1. Pathways considered in the life cycle assessment. Five unique feedstocks (sugarcane, corn, switchgrass, natural gas, and crude oil) are considered. Target products (Energy and LDPE) are indicated at the bottom. The functional unit is 46.9 MJ of energy for fuel or 1kg of LDPE for chemical use. Key intermediate product flows are shown in black. Co-products are shown in grey text.

2.4. Model Overview and Selection of Distributions and Parameters

The models for switchgrass and corn ethanol production are adapted from Mullins *et al.*⁷⁴ The model for sugarcane ethanol is adapted from Liptow and Tillman¹⁹¹ and Seabra *et al.*¹⁹⁹ The former paper was selected as it is among the only papers directly to consider a bio-LDPE pathway for Brazilian sugarcane and is thoroughly documented in an earlier report.²⁰⁰ The study by Seabra *et al.*¹⁹⁹ is among the more recent studies for Brazilian sugarcane ethanol, was based heavily on primary survey data and directly provides parameters for inputs to Monte Carlo simulation. Parameters have been updated where new information is available, as detailed in the text below and in Appendix A. Upstream emissions from natural gas associated with the production of ethylene follow the modeling approach from Venkatesh *et al.*,²⁰¹ updated with more recent data, the inclusion of pre-production emissions, a more complete allocation of emissions to co-products, plant-level data for natural gas processing emissions, and the weighting of data prior to fitting each distribution.

When literature sources contain multiple estimates for a single parameter, simple distributions capturing this range are used. Where there is a clear best estimate or a clustering of central estimates, triangular distributions are employed. If only a range is available, then a uniform distribution is used. Where there are a large number of data points, Palisade's @RiskTM software is used to fit a continuous distribution.

For the natural gas ethylene pathway, estimates for the emissions from a given process are made separately for each U.S. state (34 in all as the remaining 16 do not produce natural gas), whenever data disaggregated by state are available. In the Monte Carlo analysis, these estimates are the inputs to a discrete distribution with weights being proportional to each state's share of current national ethane production.

2.4.1. Allocation

Each of the pathways discussed above involves co-products. Where possible, these are treated by system expansion, as follows. Switchgrass and sugarcane ethanol are credited for surplus electricity production with displaced GHG emissions from U.S. and Brazilian average electricity

production emissions factors, respectively. Corn ethanol is credited for DDGS with displaced emissions from other animal feeds as modeled by Argonne National Laboratory's GREET model.²⁰² Natural gas LDPE is credited for hydrogen production (from ethane steam cracking) with displaced emissions from producing hydrogen via methane steam reforming, the dominant method for hydrogen production in the U.S.²⁰³

Emissions from natural gas LDPE production are allocated to remaining products on a mass basis. Though arbitrary, this is a common convention for assigning emissions, and allows for a consistent basis of comparison between pathways. Pre-production and extraction emissions are allocated to all products produced prior to steam cracking (dry natural gas lease condensate, propane, butane, isobutane, pentanes plus and ethane). Processing emissions and steam cracking emissions were allocated to products at the point of exit from the processing plant (processed dry natural gas, propane, butane, isobutane, pentanes plus and ethane) and cracker (propylene, butadiene, aromatics and ethylene), respectively. Appendix A, section A.1.1 provides additional details.

In the estimate for emissions from gasoline, Venkatesh *et al.*²⁰¹ performed allocation of emissions to oil refinery products on the basis of both mass and energy.

2.4.2. Global Warming Potential

Results for this study are reported for the 100-year global warming potential (GWP), using equivalence factors (in kg CO₂e) as reported by the Intergovernmental Panel on Climate Change (IPCC) 5th assessment report (AR5).²⁰⁴ Equivalence factors are assumed to be normally distributed with uncertainty ranges as presented in the AR5 supplementary material.²⁰⁵ Mean global warming potentials for CH₄ and N₂O are 36 and 298, respectively. Certain sources used as inputs to this chapter report only total GWP (not disaggregated by gas) and could not be adjusted to reflect the latest equivalence factors; further details can be found in appendix section A.1.2.

2.4.3. Fuels and Electricity

For life cycle emissions from coal and from petroleum derived fuels (diesel, residual fuel oil and gasoline), distributions from Venkatesh *et al.*^{198,206} are used. For emissions from natural gas used as a fuel, an approximate distribution of emissions is fitted to the parameters provided in Venkatesh *et al.*²⁰¹ Emissions from processes taking place in Brazil are modeled using a distribution for average Brazilian grid emissions.^{200,202,207} Processes taking place in the U.S. employ a distribution for average emissions by North American Electric Reliability Corporation (NERC) region:²⁰⁸ MRO for corn ethanol production, the combined SPP, TRE and SERC region for switchgrass ethanol production, and the combined SERC and TRE region for both dehydration of ethanol to ethylene and ethylene polymerization. See appendix A, section A.1.3 for further explanation.

2.4.4. Natural Gas Pre-production

Before a natural gas well becomes operational, various development stages must be concluded, such as the construction of a staging area (the well pad) and well drilling, both of which require energy inputs. In addition, for unconventional wells (e.g., in shale formations), the hydraulic fracturing procedure requires the production of specialty chemicals and the management of large quantities of produced water. These pre-production emissions are modeled using distributions developed in a recent review paper by Weber and Clavin.²⁰⁹ Emissions from well completions and workovers are described in Appendix A. See section A.1.4 for more details.

2.4.5. Natural Gas Extraction (Production)

Emissions from natural gas production arise through the combustion of ‘lease fuel’ used to power the extraction process, through intentional venting and flaring of natural gas, and through unintentional leaks or fugitive emissions. The U.S. Energy Information Administration (EIA) reports total lease fuel consumed (by volume) in each state.²¹⁰ Lease fuel is assumed to be composed entirely of CH₄ and CO₂ and to be combusted with 100% efficiency. Emissions are then allocated to the relevant products (and normalized by the total mass of each product) by state.

EIA reports natural gas vented and flared in each state.²¹¹ As for lease fuel, vented/flared gas is assumed to be all CH₄ and CO₂ and, following Venkatesh *et al.*,²⁰¹ it is assumed that all such gas is flared. Emissions are then allocated and normalized across products by state. Finally, the annual EPA Greenhouse Gas Inventory provides data on other CH₄ emissions from the natural gas production phase²¹² by National Energy Modeling System (NEMS) region.²¹³ The emissions in each NEMS region are fit to a triangular distribution, assuming the relative uncertainty on production emissions within each region is on the same order as for the entire natural gas system (-19% to +30%) as reported by EPA.²¹⁴ Emissions from each NEMS region are allocated to each of its constituent U.S. states in proportion to their total natural gas production. See appendix section A.1.5 for details.

2.4.6. Natural Gas Processing

Natural gas processing involves the separation of whole gas from the wellhead into different hydrocarbon products including dry natural gas, ethane, propane, *n*-butane, isobutane and pentanes plus as well as the removal of non-hydrocarbon gases such as N₂, CO₂, and sulfur containing compounds. Emissions in the stage result from fuel used to power the process, intentional release of scrubbed CO₂ and fugitive emissions of natural gas. Processing emissions were modeled using 2011 data from actual processing facilities as reported to the EPA Greenhouse Gas Reporting Program.²¹⁵ To the extent possible, each facility was matched with the corresponding processing plant in the EIA processing capacity database, which gives average daily plant flow from mid-2011 to mid-2012.²¹⁶ In all, 222 plants were matched, accounting for 80% of EIA reported daily plant flows. The total GHG emissions from each processing plant (recalculated to reflect the AR5 GWP values) are then normalized by its annual plant flow. These emissions are weighted by the plant flow and fit to a continuous distribution. Emissions are then allocated to the relevant products (and normalized by the total mass of each product) on a national basis. See appendix section A.1.6 for more details.

2.4.7. Steam Cracking

The conversion of ethane to ethylene is an energy intensive process known as steam cracking. In this process, saturated hydrocarbons like ethane are heated to high temperatures (≥ 750 °C) in the

presence of steam, resulting in a mix of products that is usually optimized for olefins like ethylene. Valuable co-products result from this process and include ethylene, propylene, butadiene, aromatics (e.g., benzene) and hydrogen. Specific energy requirements for the production of a tonne of ethylene via steam cracking of ethane are estimated by a number of sources,²¹⁷⁻²¹⁹ as are volumes for co-products²¹⁷⁻²²¹ and direct CH₄ emissions.²²² It is assumed that produced methane, C4 components (i.e., butanes) and C5/C6 (i.e., pentanes, hexanes) components are used as fuel to power the steam cracking process, and that any residual energy needs are provided by natural gas. Ethylene, propylene, butadiene and aromatics (treated as benzene) are all treated as products, and subject to mass allocation. Hydrogen is treated by system expansion, as discussed above. See appendix section A.1.7 for more details.

2.4.8. Land Use Change (LUC)

All bio-based pathways considered in this study 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 method to account for their impact, LUC emissions are potentially critical to the GHG impact of bio-based products. The U.S. EPA provides estimates for LUC emissions specifically designed to account for the impact of RFS2;¹²⁸ these estimates assume a 30-year time horizon and are used for the base-case model in this study. Though arbitrary, a 30-year amortization period is common in the treatment of LUC emissions. Point estimates for domestic LUC emissions from U.S. corn and switchgrass ethanol production (both are negative, representing carbon sequestration) are combined with triangular distributions fit to EPA's 95% confidence intervals for international land use change emissions from each feedstock. The confidence intervals provided by EPA ignore uncertainty in their economic model of land-use change. In addition, EPA's results rely on 2022 as the year of analysis, which creates inconsistencies with other assumptions (based on current technologies) made in this analysis. Furthermore, there is a large range of estimates for LUC emissions in the literature,^{85,223,224} which is not fully captured by the distribution employed here. Nevertheless, the EPA analysis provides a common set of assumptions for the three feedstocks under study. Sensitivity to LUC emissions is further examined in section 2.5.3.

2.4.9. Cultivation of Biomass Feedstock

Remaining emissions from agriculture include use of fossil fuels for farming equipment, emissions from agrochemical production, N₂O emissions from volatilized nitrogen fertilizer and CO₂ from calcium carbonate fertilizer. For sugarcane, there are also emissions of CH₄ and N₂O from field burning during harvest. Emissions of CO₂ from field burning are excluded because the carbon source is biogenic,⁹⁶ and so the carbon was only recently removed from the atmosphere. For corn and switchgrass pathways, application of synthetic nitrogen fertilizer and crop residue is modeled as in Mullins *et al.*;⁷⁴ quantities of other agrochemicals and emissions from fossil fuel use are calculated from the data provided by GREET,²⁰² using default input parameters. For sugarcane cultivation, distributions for diesel consumption (in L/ha), cane productivity (in t/ha), the quantity of trash burned and quantities of applied fertilizers and pesticides are taken from Seabra *et al.*¹⁹⁹; the emissions factor for straw burning is taken from GREET.²⁰² The emission factor for N₂O from applied fertilizer is modeled stochastically using the uncertainty range provided by the IPCC,²²⁵ although there is some evidence this may underestimate potential N₂O emissions.²²⁶ For all pathways, emissions for the production of agrochemicals are taken from GREET,²⁰² using separate estimates for U.S. (corn and switchgrass) and Brazilian (sugarcane) production.

2.4.10. Ethanol Production

Production of ethanol from sugarcane can be entirely powered by the combustion of bagasse, the dried residue left over after extracting juice from the sugarcane. CO₂ emissions from bagasse burning are annual biogenic emissions, and are thus disregarded. Yield of ethanol from sugarcane and quantity of surplus electricity generated by bagasse combustion are modeled as in Seabra *et al.*¹⁹⁹ See appendix section A.1.8 for more details.

Total heat and electricity required for corn and switchgrass ethanol production, their respective feedstock chemical composition, and yields from the hydrolysis and fermentation processes are as modeled in Mullins *et al.*⁷⁴ In the case of switchgrass, it is assumed that all non-fermentable and unreacted components are combusted in a 68% efficient boiler (higher heating value basis) to produce heat. Any surplus heat is used to drive an 80% efficient turbine, which generates electricity for the process and potentially surplus electricity for sale to the grid. Any heat

shortfall in either process is provided by natural gas, while any electricity shortfall is made up by grid electricity.

2.4.11. Ethanol Dehydration

For all bio-based pathways, ethanol to ethylene conversion follows the fuel and electricity inputs outlined in a 1981 article¹⁸⁰ using the commercial Syndol catalyst, which still represents the dominant technology in use today.¹⁷⁹ Generic uncertainty factors were applied following the method proposed by Geisler *et al.*²²⁷ Although the data used here is over 30 years old, it is in close agreement with modeling based on a recent patent¹⁹¹ and results from actual plant data.¹⁹⁴ See appendix section A.1.9 for more details.

2.4.12. Polymerization

The last step in the production of LDPE plastic from ethylene is polymerization of individual ethylene molecules to make the final polymer. This process requires both heat (fuel) and electricity. For U.S. pathways, polymerization is modeled using average U.S. industry data.¹⁴⁵ Brazilian polymerization is assumed to follow European parameters, uniformly distributed between the values reported by Liptow and Tillman²⁰⁰ and PlasticsEurope.²²⁸ Electricity emissions are calculated using Brazil-specific emissions factors. See appendix section A.1.10 for more details.

2.4.13. Transportation

At several stages throughout the pathways considered, intermediates must be moved from one location to another. For switchgrass and corn, emissions for feedstock transportation to the ethanol production facility are taken from GREET.²⁰² For U.S. LDPE production, it is assumed that ethanol is transported by single unit truck using fuel requirements from NREL.²²⁹ For corn ethanol, the transportation distance is assumed to range from 1,000 to 1,800 km, the approximate distance from the U.S. Midwest, where most ethanol biorefineries are located,²³⁰ to the gulf coast states, where most ethylene production and infrastructure is located.²³¹ Switchgrass production is expected to occur primarily in the southeast,¹²⁸ resulting in shorter distances (modeled as 0 to 1,500 km with a mode of 1,000 km). For sugarcane, the diesel required for feedstock

transportation to the ethanol production facility and subsequent transport of ethanol to the ethylene plant is modeled as in Liptow and Tillman.¹⁹¹ Transport of the final product (ethanol or LDPE) from Brazil to the U.S. is modeled as a residual fuel oil tanker (fuel requirements from NREL²³²) shipping from Paranagua, Brazil to Houston, Texas.²³³ Fuel distribution for ethanol within the U.S is modeled as in GREET.²⁰²

2.4.14. Use Phase and End of Life

The final stage for both ethanol fuel and gasoline is combustion. For ethanol, all emissions in this phase are biogenic and so are not included in the accounting of GHG emissions. For gasoline, these emissions are already accounted for in the distribution from Venkatesh *et al.*¹⁹⁸

For LDPE, use phase and end of life (EOL) are not explicitly modeled as all pathways have converged at the point of production of U.S. LDPE or arrival of Brazilian LDPE to the U.S. While alternative EOL strategies may impact on the life cycle emissions for LDPE, they will not affect the comparison between fossil-based and bio-based production. For the bio-based LDPE pathways, carbon taken up during plant growth is now locked away in a non-biodegradable product. The carbon content of polyethylene accounts for 12/14 of the total mass and is treated as a credit for the amount of CO₂ this carbon would otherwise represent: 3.1 kg CO₂ / kg LDPE. More explicit treatment of end of life would not appreciably change the life cycle emissions for LDPE consumed domestically. In the United States, approximately 85% of plastics are landfilled;²³⁴ the EPA estimates emissions of approximately 0.04 kg CO₂e/kg LDPE landfilled²³⁵ – roughly 2% of fossil LDPE life cycle GHG emissions. Key parameters for all pathways are given in appendix section A.1.11.

2.5. Results and Discussion

2.5.1. Main Results and Discussion

The results presented below must be interpreted with caution. Parameters used in this study are taken as the closest approximation of present operating conditions. However, data is drawn from multiple sources, which could produce inconsistencies. Further, with the exception of land-use change accounting, this study follows an attributional life cycle assessment (ALCA) approach,

which is a form of environmental accounting. It does not predict the actual changes in emissions that would result from increased production of bio-based products, for which the use of average electric grid emissions and the implicit assumption of 1:1 displacement of fossil products would be inappropriate. The ALCA approach, however, is indicative of the emissions that may be attributed to each pathway (taken in isolation from market forces), and as such provides a consistent basis to establish how pathways perform relative to EISA targets.

Simulated life cycle GHG emissions for each of the 8 pathways considered are shown in Figure 2.2 (see appendix section A.2.1 for numerical results). To allow comparison between pathways, results are normalized to the amount of ethanol needed to produce 1 kg LDPE, which is 46.9 MJ of ethanol for fuel pathways; fossil-based pathways are likewise scaled to 1kg LDPE and 46.9 MJ gasoline, respectively. Fuel use of ethanol has higher modeled emissions when compared to LDPE from the same feedstock. This is due primarily to combustion of the produced ethanol as a fuel.

When comparing across bio-based pathways, the lowest modeled emissions are for the cellulosic feedstock (switchgrass), followed by the ‘advanced’ feedstock (sugarcane), and finally corn starch. For both sugarcane and switchgrass, both LDPE and ethanol fuel will result in decreased modeled emissions relative to their fossil fuel counterparts, with probability approaching 1. On the other hand, corn products result in higher modeled emissions with a high degree of confidence (~90% chance for LDPE and ~70% chance for ethanol). There is substantial probability that switchgrass and sugarcane LDPE pathways result in negative emissions (net carbon sequestration). This suggests that no amount of improvement to the fossil LDPE pathway (e.g. via recycling) would lead to the fossil route being preferred. Switchgrass ethanol for fuel may also result in negative modeled emissions if displacement of grid emissions by surplus electricity generation occurs. This is not the case for sugarcane ethanol, as less surplus electricity is produced, plus displaced Brazilian electricity has a relatively low carbon intensity.

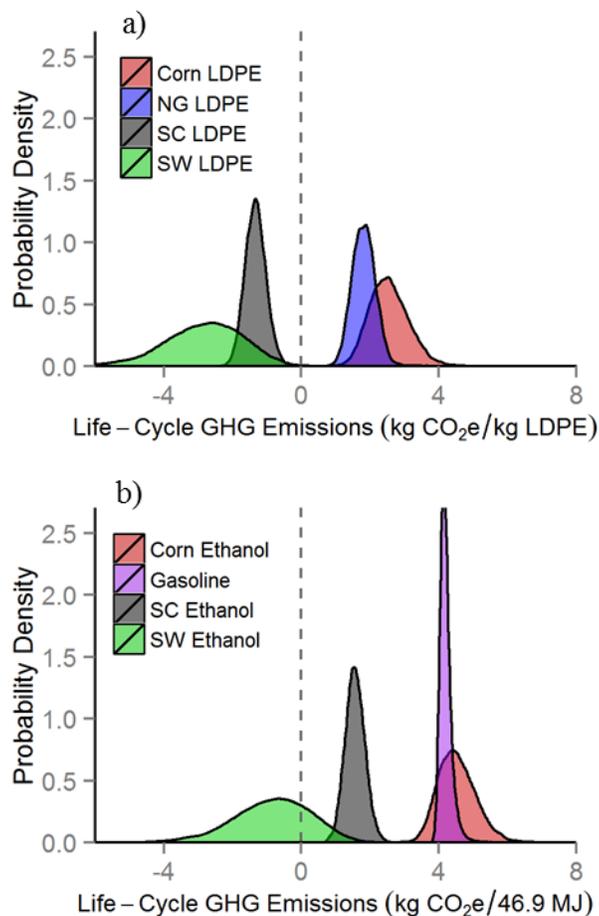


Figure 2.2. Modeled life cycle GHG emissions from all pathways. a) Simulated GHG emissions from production of LDPE from corn, natural gas (NG), sugarcane (SC) or switchgrass (SW). b) Simulated GHG emissions for the production and combustion of 46.9 MJ of fuel, using corn ethanol, gasoline, sugarcane (SC) ethanol or switchgrass (SW) ethanol. The functional units (1 kg LDPE or 46.9 MJ) represent equivalent quantities of ethanol.

Following the ‘risk of policy failure’ framework developed by Mullins *et al.*,⁷⁴ Figure 2.3 shows the modeled probability (proportion of model runs) of achieving a given GHG reduction target from pursuing any of the considered pathways. Each curve on the figure is produced by taking the difference in life cycle emissions between the labeled bio-based product (ethanol or LDPE) and the corresponding conventional fossil counterpart (gasoline or LDPE). This gives net GHG savings for each pathway. Consistent with EISA ethanol targets, net GHG savings are expressed as a percent of life cycle emissions from gasoline. Higher values on the x-axis represent more aggressive GHG reduction targets; higher values on the y-axis represent higher confidence that a

given GHG reduction target can be achieved. A more conventional cumulative distribution function is presented in appendix section A.2.2, with numerical results presented in Table A.15 (section A.2.1). Further, appendix section A.2.3 discusses which inputs contribute most to uncertainty in the net GHG emissions for each pathway.

Figure 2.3 shows that corn pathways achieve the ‘renewable biofuel’ 20% reduction target in very few model runs, which is in agreement with results previously presented by Mullins *et al.*⁷⁴ Both sugarcane pathways can meet the ‘advanced biofuel’ 50% reduction target. Both switchgrass pathways achieve the ‘cellulosic biofuel’ 60% reduction target with probability approaching 1 – a slightly more optimistic result than presented by Mullins *et al.*,⁷⁴ due to higher estimates of feedstock energy and GHG intensity of displaced electricity employed here.

Feedstock choice (corn, sugarcane or switchgrass) has a larger impact on modeled GHG savings than how the ethanol is used (for fuel or LDPE). For U.S. production (corn and switchgrass), fuel use of the ethanol stochastically dominates (greater GHG savings) chemical use, while the reverse is true for Brazilian production (sugarcane). The difference stems first from the lower emissions of Brazilian electricity used in ethanol dehydration and ethylene polymerization and second from the reduced weight of shipping LDPE relative to ethanol when transporting the end-products to the U.S.

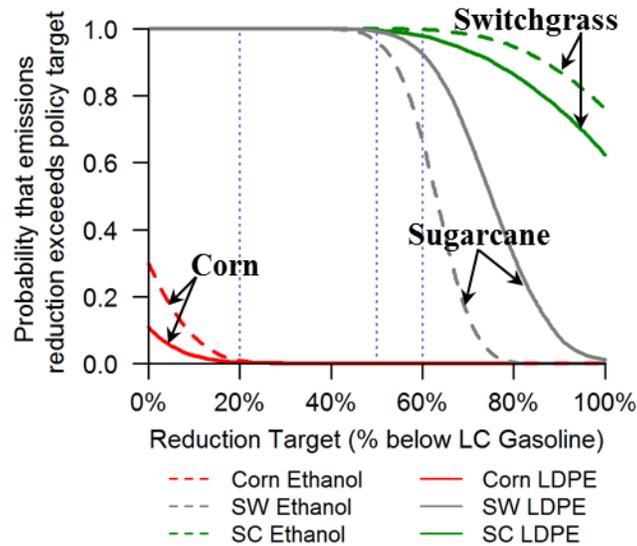


Figure 2.3. Probability (proportion of model runs) that modeled GHG emissions from each bio-based pathway are below those of the fossil fuel counterpart (at 0%), or below some policy target. Policy targets are given as a percent reduction relative to simulated gasoline life cycle (LC) emissions. EISA targets (20% for corn biofuel, 50% for advanced biofuels and 60% for cellulosic biofuels) are shown with vertical blue lines. SC = sugarcane; SW = switchgrass.

Finally, Figure 2.4. presents the GHG savings (if any) that bio-LDPE can achieve above and beyond the modeled GHG savings from bio-ethanol fuel. Results are expressed as a percent of gasoline life cycle emissions. U.S. production of bio-LDPE would require a relaxation of expected emission reductions compared with bio-ethanol fuel (e.g., by 17% of gasoline emissions for an 80% confidence level). Brazilian production would allow for additional GHG savings (e.g., by 5% of gasoline emissions for an 80% confidence level). Numerical results (in kg CO₂e/functional unit) are available in Table A.16. A major advantage of this presentation is that it is independent of the emissions from ethanol production (ethanol emissions are subtracted out when taking the difference between net emissions from bio-ethanol and bio-LDPE) and can be readily applied to new feedstocks or other studies on cradle-to-gate ethanol emissions. An alternative way to frame this discussion would be to establish a GHG equivalence factor between bio-LDPE and bio-ethanol fuel for policy achievement purposes – that is, for every unit of ethanol diverted from fuel use, how much ethanol must go toward bio-LDPE to achieve the same GHG reduction. This idea is explored in the following section (section 2.5.2). Figures 2.3 and 2.4 implicitly assume that bio-based products replace their conventional fossil counterparts on a 1:1

basis. Though 1:1 replacement is accurate in physical terms, the resulting changes in market prices make 1:1 replacement unlikely across the entire market. This is discussed further in the sensitivity analysis. Alternate versions of Figures 2.3 and 2.4, which also incorporate indirect market effects, are available in appendix section A.2.5.

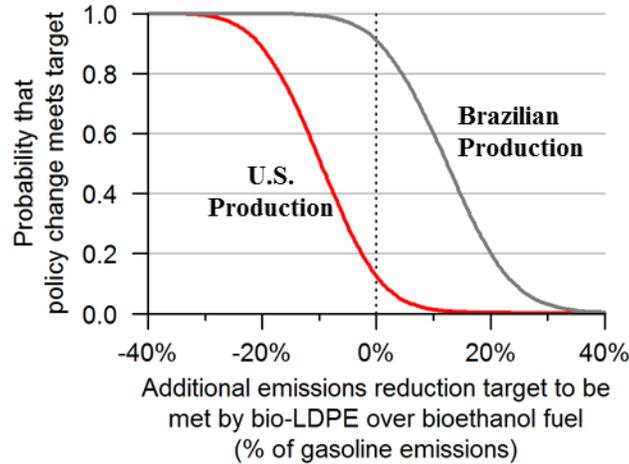


Figure 2.4. Probability (proportion of model runs) that GHG reductions from fossil LDPE replacement are superior to those from gasoline replacement (at 0% on the x-axis) or in excess of some policy target. Positive values indicate that more stringent reductions can be met through LDPE replacement. Negative values represent needed relaxation in the target emissions reductions (as a % of gasoline emissions).

2.5.2. Bio-LDPE GHG Equivalence Factor

The discussion above introduces the possibility of establishing a bio-LDPE to bio-ethanol GHG equivalence factor. To do so, policy makers could first choose an acceptable level of confidence (y-axis in Figure 2.3), as suggested by Mullins *et al.*,⁷⁴ and legislate the corresponding percentage target for ethanol fuel (x-axis in Figure 2.3). A separate target for bioethylene products would then be set by scaling bioethylene requirements to achieve the same GHG reduction and confidence level (proportion of model runs). The required scaling for switchgrass and sugarcane is shown in Figure 2.5 a) for different confidence thresholds. For example, sugarcane ethanol and switchgrass ethanol can meet EISA GHG reduction targets with confidence levels of 99% and 96% respectively. Figure 2.5 a) shows that bio-LDPE can achieve the same GHG reduction and confidence level if 10% *less* ethanol is used for sugarcane bio-LDPE (corresponding to a 90% equivalence factor), and 20% *more* ethanol is used for

switchgrass bio-LDPE (corresponding to a 120% equivalence factor). Alternatively, results may be reported using a direct simulation of the ratio of GHG emissions savings from bio-LDPE to bio-ethanol fuel, as shown in Figure 2.5 b). As an example, consider a desired probability of 0.8 that bio-LDPE achieves at least the same emission reduction as bio-ethanol fuel (y-axis of Figure 2.5 b)). To achieve this level of confidence, approximately 0.9 kg sugarcane ethanol must be used for bio-LDPE for each kg of sugarcane ethanol used for fuel (90% equivalence factor). For switchgrass, approximately 1.2 kg ethanol must be used for LDPE to achieve the same GHG reduction as using 1 kg ethanol for fuel (120% equivalence factor).

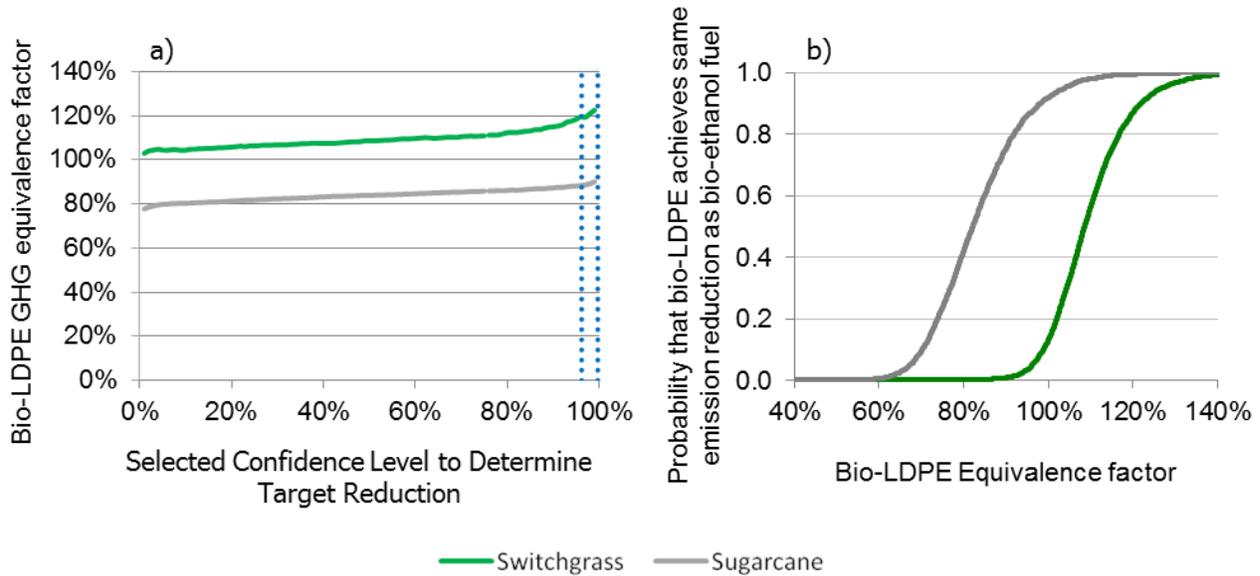


Figure 2.5. Bio-LDPE ethanol use equivalence factor for achieving the same GHG emission reduction targets as bio-ethanol fuel. a) relative quantity of ethanol used in bio-LDPE (y-axis) to achieve the same reduction target as bio-ethanol fuel for a reduction target set by fixed level of confidence (x-axis) as applied to main text Figure 2.3. The vertical dotted lines at 99% and 96% show respectively the degree of confidence with which sugarcane ethanol and switchgrass ethanol can achieve EISA targets (50% reduction for sugarcane and 60% reduction for switchgrass). b) probability that bio-LDPE will achieve the same reduction in emissions as bio-ethanol fuel (y-axis) in function of the quantity of ethanol used for bio-LDPE (x-axis) relative to a unit amount of ethanol used for fuel.

2.5.3. Sensitivity to Emissions from Land Use Change

Emissions from land use change are highly uncertain and subject to much controversy. These emissions may also respond to increased demand for agricultural products, in a non-linear way

that is not captured in the present model. In Figure 2.6 to Figure 2.8, land use change is treated parametrically for each of the bio-based pathways considered. Excluding land use change (i.e. 0 g CO₂e / MJ) leads to a high probability (>0.8) that corn ethanol and LDPE achieve some emission reduction (i.e. “break-even”) relative to gasoline and fossil LDPE, respectively (Figure 2.6). It is still only with limited probability (0.6 for ethanol and 0.3 for LDPE) that either corn-based bio-product achieves the 20% emission reduction required by EISA. For switchgrass and sugarcane, high values of LUC may prevent those pathways from achieving EISA targets but are unlikely to result in a net increase in emissions relative to fossil products (Figure 2.7 and Figure 2.8).

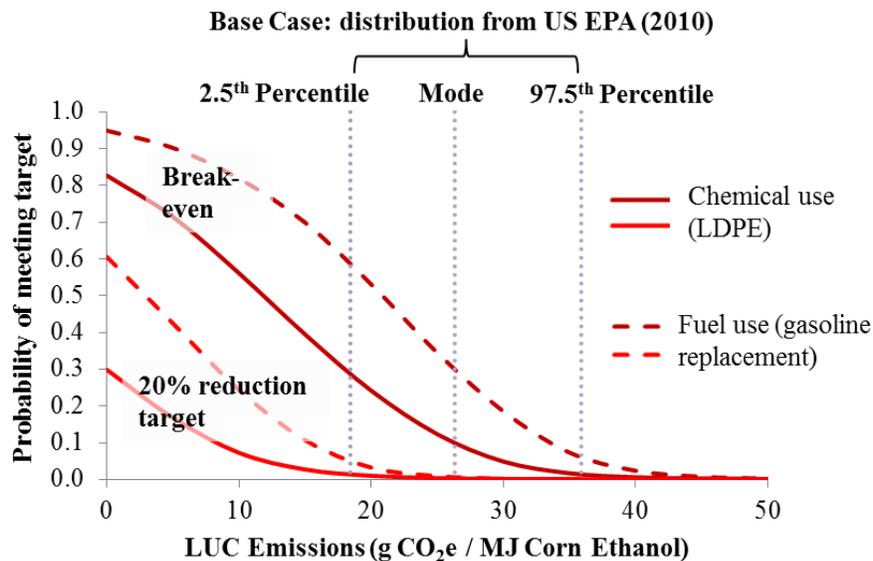


Figure 2.6. Probability (proportion of model runs) that GHG emissions from corn ethanol and corn LDPE are below gasoline and fossil LDPE respectively (“break-even”), or below the RFS2 renewable biofuel reduction target (20% reduction compared to gasoline) as a function of LUC emissions. The figure also shows base case LUC emissions based on ref.¹²⁸

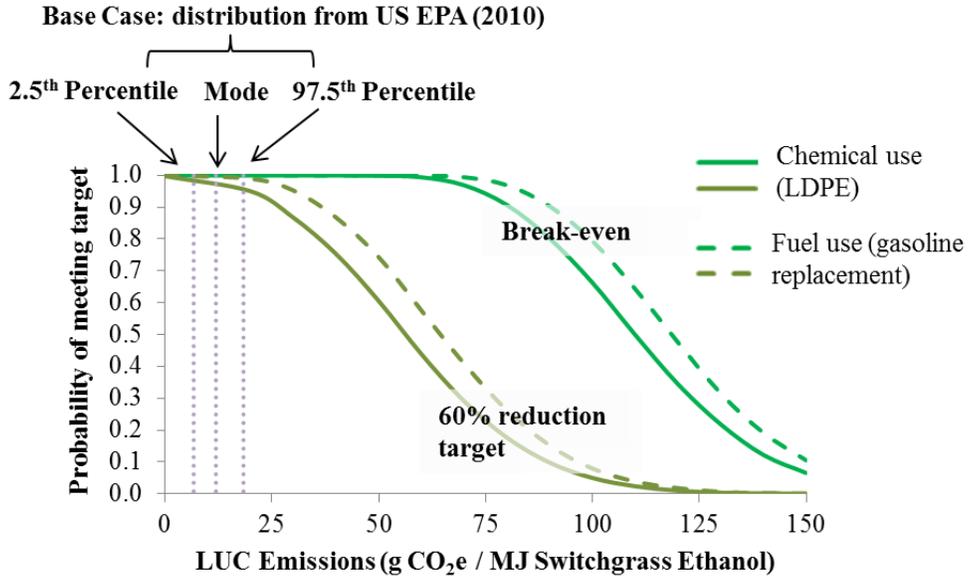


Figure 2.7. Probability (proportion of model runs) that GHG emissions from switchgrass ethanol and switchgrass LDPE are below gasoline and fossil LDPE respectively (“break-even”), or below the RFS2 cellulosic biofuel reduction target (60% reduction compared to gasoline) as a function of LUC emissions. The figure also shows base case LUC emissions based on ref.¹²⁸

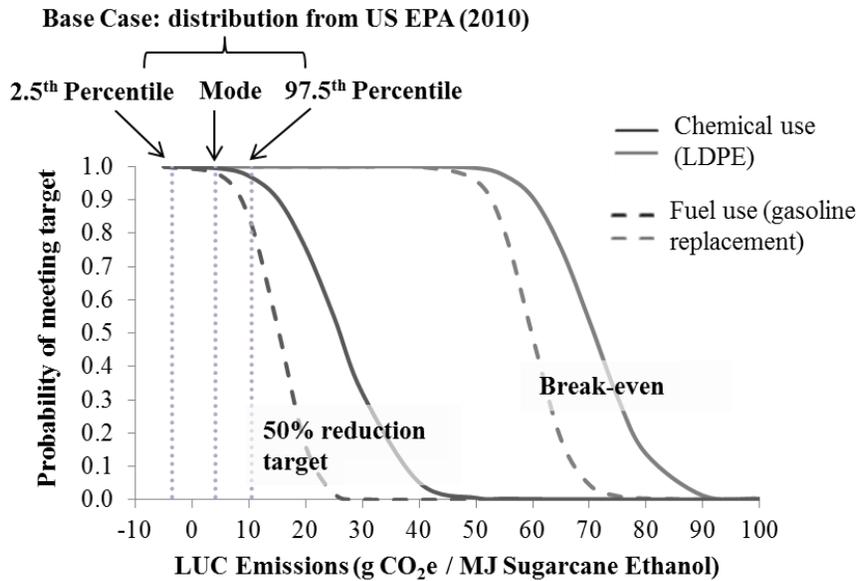


Figure 2.8. Probability (proportion of model runs) that GHG emissions from switchgrass ethanol and sugarcane LDPE are below gasoline and fossil LDPE respectively (“break-even”), or below the RFS2 advanced biofuel reduction target (50% reduction compared to gasoline) as a function of LUC emissions. The figure also shows base case LUC emissions based on ref.¹²⁸

2.5.4. Additional Sensitivity Analyses

Appendix sections A.2.4 to A.2.6 present sensitivity to the treatment of displaced electricity, to the use of marginal electricity, to the choice of feedstock for displaced fossil LDPE, to the assumption of 1:1 displacement of fossil products, and to select other assumptions. Noteworthy findings are described here. Without credit for displaced electricity, switchgrass LDPE is less likely to meet EISA's cellulosic biofuel targets (50% probability), although substantial GHG savings are still achieved. The choice of feedstock for displaced fossil LDPE, credit for displaced electricity for switchgrass ethanol or for sugarcane pathways, and the use of average rather than marginal electricity emissions factors affect net emissions for each pathway, but without overturning conclusions regarding the ability to meet EISA GHG targets. Finally, while market effects, such as the indirect fuel use effect,²³⁶ may significantly affect the GHG savings from biofuel pathways, bio-LDPE pathways are far less vulnerable to similar market-induced indirect demand increases for fossil LDPE (due to the relatively low emissions from fossil LDPE). Alternate end of life scenarios (e.g. incineration) for LDPE could overturn this result. Further discussion of this effect, which I term indirect demand change (IDC) is available in appendix section A.2.5.

2.5.5. Cost Considerations

Production costs for bio-ethanol and bioethylene have been estimated by the International Renewable Energy Agency.¹⁸⁴ Ranges for the cost of production of fossil ethylene and gasoline were estimated from recent historical data and official sources.²³⁷⁻²⁴¹ Details are available in appendix section A.2.7. Bioethylene (from any source) is substantially more expensive to produce than ethane-derived ethylene. In contrast, ethanol, particularly from sugarcane, may already be competitive with gasoline. Implicit carbon prices were calculated by simulating cost data along with GHG emissions.

While bio-ethanol appears to be a reasonable GHG mitigation strategy (leading to implicit carbon prices of -200 to 0 \$/tonne CO₂e for sugarcane and 0 to 100 \$/tonne CO₂e for switchgrass), bioethylene can only be justified at current production costs (corresponding to implicit carbon prices of 150 to 350 \$/tonne CO₂e for sugarcane and 200 to 500 \$/tonne CO₂e for switchgrass) if substantial co-benefits are expected. Fuel use of ethanol is more cost effective

than production of bioethylene in part because ethane-based ethylene is currently very inexpensive to produce (mean: 0.44 \$/kg ethylene). As a result, gasoline is over twice as costly to produce as fossil ethylene per functional unit (1.01 kg ethylene or 46.9 MJ gasoline). Additionally, bioethylene is more expensive to produce than bio-ethanol, since it requires strictly greater processing. This additional cost amounts to approximately 0.6 \$/functional unit. The low cost of fossil ethylene compared to gasoline, and high cost of bioethylene compared to fossil ethylene contribute nearly equally to the higher cost-effectiveness of bioethanol fuel over bioethylene. Nevertheless, *private* investment into bioethylene is already taking place.^{11,12} Adopting a more flexible standard in place of RFS2 will likely decrease the overall cost of compliance, particularly as market prices change and new production technologies evolve. Further details and results are available in section A.2.7.

2.5.6. Concluding Thoughts: The Way Forward

The relative desirability of the pathways studied here depends both on market conditions and the goals of the policy effort. The preamble to EISA makes clear that its goals include both energy security and independence as well as the promotion of ‘clean’ renewable fuels.⁴ Currently, U.S. ethane production is almost entirely used for the production of ethylene. Ethane displaced from ethylene production may be included (to a limited extent) in existing natural gas streams, or used as fuel for upstream fossil fuel production, displacing methane and thereby increasing the availability of natural gas. It should be noted, however, that the U.S. is already expected to become a net *exporter* of natural gas by 2020.¹⁸⁸ In contrast, the EIA reference scenario assumes continued reliance on *imports* for liquid fossil fuels through 2040.¹⁸⁸ Thus, from the standpoint of energy independence, there is less to be gained by incentivizing bioethylene production and focus should remain on fuel use of ethanol with an emphasis on domestic production.

If the policy goal is simply to encourage production of biofuels (e.g., for rural development, to achieve learning by doing cost savings, etc.), then any expansion of bio-based production should be viewed favorably, and so incentives for bioethylene production would be beneficial. In light of existing constraints on biofuel consumption discussed at the outset of this chapter, continued expansion of bio-ethanol production may need to rely on new pathways like bioethylene.

The focus of this analysis, however, is the impact of strategies for biomass use on GHG emissions. From a global warming perspective, the choice of feedstock is significantly more important than whether it is used for fuel or ethylene production. This suggests that in an environment of constrained demand for ethanol fuel, promoting bioethylene would be a promising alternative. Indeed, between the imported Brazilian products, bio-based LDPE is actually the preferred route (as modeled) for GHG mitigation. Under the specific scenario of U.S. production with supply-side constraints (as is currently the case for cellulosic biofuel), and no demand-side limitations, then fuel-use for ethanol should be given priority. If GHG equivalence factors are employed as discussed above, then there is no need for policy makers to choose between bio-LDPE and bio-ethanol fuel. More work is still needed, however, to quantify other (non-GHG) environmental and social impacts (e.g., changes in air and water quality, food security, etc.) of such a move.

The expanded policy analyzed in this chapter constitutes a partial departure from the energy security emphasis of EISA, and the transportation fuels focus of RFS2. Nevertheless, increasing incentives for bio-based chemicals would open new opportunities to conserve fossil fuels, to reduce GHG emissions and to bolster the ethanol industry by shifting toward higher value products. Further work is needed to establish the details of a new standard and its economic, social and sustainability implications. One possibility would be to allow manufacturers of bioethylene to sell credits into the existing renewable identification number market for biofuels. A carefully revised policy has the potential to provide added flexibility to obligated parties while having no adverse impact on GHG emission targets.

Chapter 3. Uncertainty in the Life Cycle Greenhouse Gas Emissions from U.S. Production of Three Bio-based Polymer Families

3.1. Abstract

Interest in bio-based products has been motivated, in part, by the claim that these products have lower life cycle greenhouse gas (GHG) emissions than their fossil counterparts. This study investigates GHG emissions from U.S. production of three important bio-based polymer families: polylactic acid (PLA), polyhydroxybutyrate (PHB) and bioethylene-based plastics. The model incorporates uncertainty into the life cycle emission estimates using Monte Carlo simulation. Results present a range of scenarios for feedstock choice (corn or switchgrass), treatment of co-products, data sources, end of life assumptions, and displaced fossil polymer. Switchgrass pathways generally have lower emissions than corn pathways, and can even generate negative cradle-to-gate emissions if unfermented residues are used to co-produce energy. PHB (from either feedstock) is unlikely to have lower emissions than fossil polymers once end of life emissions are included. PLA generally has the lowest emissions when compared to high emission fossil polymers, such as polystyrene (mean GHG savings up to 1.4 kg CO₂e/kg corn PLA and 2.9 kg CO₂e/kg switchgrass PLA). In contrast, bioethylene is likely to achieve the greater emission reduction for ethylene intensive polymers, like polyethylene (mean GHG savings up to 0.60 kg CO₂e/kg corn polyethylene and 3.4 kg CO₂e/kg switchgrass polyethylene).

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Posen, I. D.; Jaramillo, P.; Griffin, W. M., Uncertainty in the Life Cycle Greenhouse Gas Emissions from U.S. Production of Three Bio-based Polymer Families. *Environ Sci Technol* **2016**, *50*, (6), 2846-2858.

<http://pubsdc3.acs.org/articlesonrequest/AOR-ZNgeGqkhUhFY476qhYii>

3.2. Introduction

Over the last decade, the United States government has expressed a clear interest in laying the foundations for a national bioeconomy.^{88,89} Increased reliance on renewable, rather than

depleting, resources appears to be an inherently desirable step in the transition to a more sustainable society. Although policies like the U.S. Renewable Fuel Standard¹²¹ emphasize the use of biomass for energy, recent publications have called for consideration of strategies that include a broader range of bio-based products.^{134,136,154,242} After fuels, bio-based polymers offer one of the largest potential markets (by volume) for bioproducts,¹³⁵ and have been suggested as a potential “linchpin category” in the operation of biorefineries.¹³⁴

In 2013, bio-based plastics accounted for less than 1% (1.6 million tonnes (Mt)) of global thermoplastics production.¹⁴⁸ Nonetheless, bio-based production is expected to grow rapidly, reaching nearly 7 Mt by 2018.¹⁴⁸ Four families of polymer are expected to figure prominently in future bio-plastics markets,^{10,149-151} and have been the focus of a number of studies in the existing life cycle assessment (LCA) literature:¹⁵²⁻¹⁵⁴ polylactic acid (PLA), polyhydroxyalkanoates (PHA), thermoplastic starch (TPS), and bioethylene based plastics. Most conventional plastics contain some ethylene. Though ethylene is predominantly fossil-derived, it can be made from renewable feedstocks via dehydration of bioethanol.^{179,180} Plastics made using bioethylene are chemically identical to their fossil derived counterparts. In contrast, bio-based polymers such as PHAs and PLA are chemically distinct from existing fossil-derived thermoplastics, but provide similar functionality. Both can replace a range of conventional fossil-based polymers, depending on the application. PHAs can frequently replace PE, PP, and PS,^{151,243-248} and may also substitute for PET and PVC in some applications.¹⁰ PLA most often substitutes for PS and PET,^{151,153,249-253} but can also replace PE, PP, and PVC in some applications.^{10,250,254} TPS, on the other hand, has relatively poor mechanical properties,²⁵⁵ and is used in specialized agricultural applications, as filler in plastic composites, or in single-use packaging.^{148,152,256} Thus, TPS does not usually compete directly with conventional polymers; this study focuses on PLA, PHA and bioethylene plastics.

A wide variety of benefits have been cited as drivers for the development of bio-based products.⁸⁸ Common motivations include rural economic development, energy security, and reduced impact on the environment. In terms of environmental performance, bio-based products tend to compare poorly to conventional products on impact categories such as eutrophication and stratospheric ozone depletion.²⁵⁷ Mixed results have been reported for other categories, including

acidification and tropospheric ozone formation.²⁵⁷ Thus, claims of environmental benefits for bio-products often rely on reduced greenhouse gas (GHG) emissions and non-renewable energy use.^{88,257,258} As a result, it is important to understand the degree of confidence with which bio-products can achieve GHG emissions reductions, and to define the drivers of uncertainty and variability in their life cycle emissions. This study builds on previous work that has quantified uncertainty in the life cycle GHG emissions for fossil fuels,^{198,201,206} ethanol biofuel,^{74,259} and bioethylene,¹⁵⁴ by considering additional cases for bioethylene and extending the analysis to include PLA and PHA.

Previous work on the environmental performance of PLA, PHA, and bioethylene plastics has focused on a cradle-to-gate (cradle to the production of the polymer pellet) comparison with petroleum-based polymers. Several recent papers reviewed these studies, and found that results are variable across studies, with life cycle emissions being strongly tied to modeling assumptions and feedstock choice.¹⁵²⁻¹⁵⁴ Many studies report lower GHG emissions and non-renewable energy use for bio-based polymers than for their fossil counterparts; however, few consider emissions from land use change (LUC) or from end of life.

Corn is currently the dominant feedstock for producing PLA,²⁶⁰ PHA,¹⁵³ and ethanol in the U.S.²³⁰ This study investigates the use of corn grain as the sugar source for bio-based polymer production. Studies often report lower environmental footprints from other crops.^{74,154,166} To account for possible improvements from crop-choice, this analysis includes the use of switchgrass as an illustrative 2nd generation (cellulosic) feedstock. This chapter compares emissions from each bio-based plastic to emissions from each of the highest volume conventional (fossil-based) thermoplastics: polyethylene (PE), which includes high density polyethylene (HDPE), low density polyethylene (LDPE), and linear low density polyethylene (LLDPE); polypropylene (PP); polyethylene terephthalate (PET); polyvinyl chloride (PVC); and polystyrene (PS), which includes high impact polystyrene (HIPS) and general purpose polystyrene (GPPS). Bioethylene pathways are possible for each of these commodity thermoplastics, with the exception of PP, which contains no ethylene. Results from this study are indicative of average U.S. conditions, and should help guide future, more context-specific work.

3.3. Methods

3.3.1. Study Overview

This study uses LCA to evaluate the GHG emissions associated with both corn-based and switchgrass-based PLA, PHA, and bioethylene based plastics. For PHA production, this study uses data that is either for generic PHA production or is specific to poly-3-hydroxybutyrate (PHB), a common representative of the PHA family. The baselines for this study are the eight fossil-based thermoplastics discussed above. This study is conducted primarily under an attributional LCA framework.

3.3.2. Fossil Polymer Model Overview

The model for the production of fossil polymers relies on data from a 2011 report for the American Chemistry Council (ACC), prepared by Franklin Associates.¹⁴⁵ The study provides cradle-to-gate inventories for each of the conventional plastics described in the introduction. Figure 3.1. presents a flow diagram of unit processes included in the model.

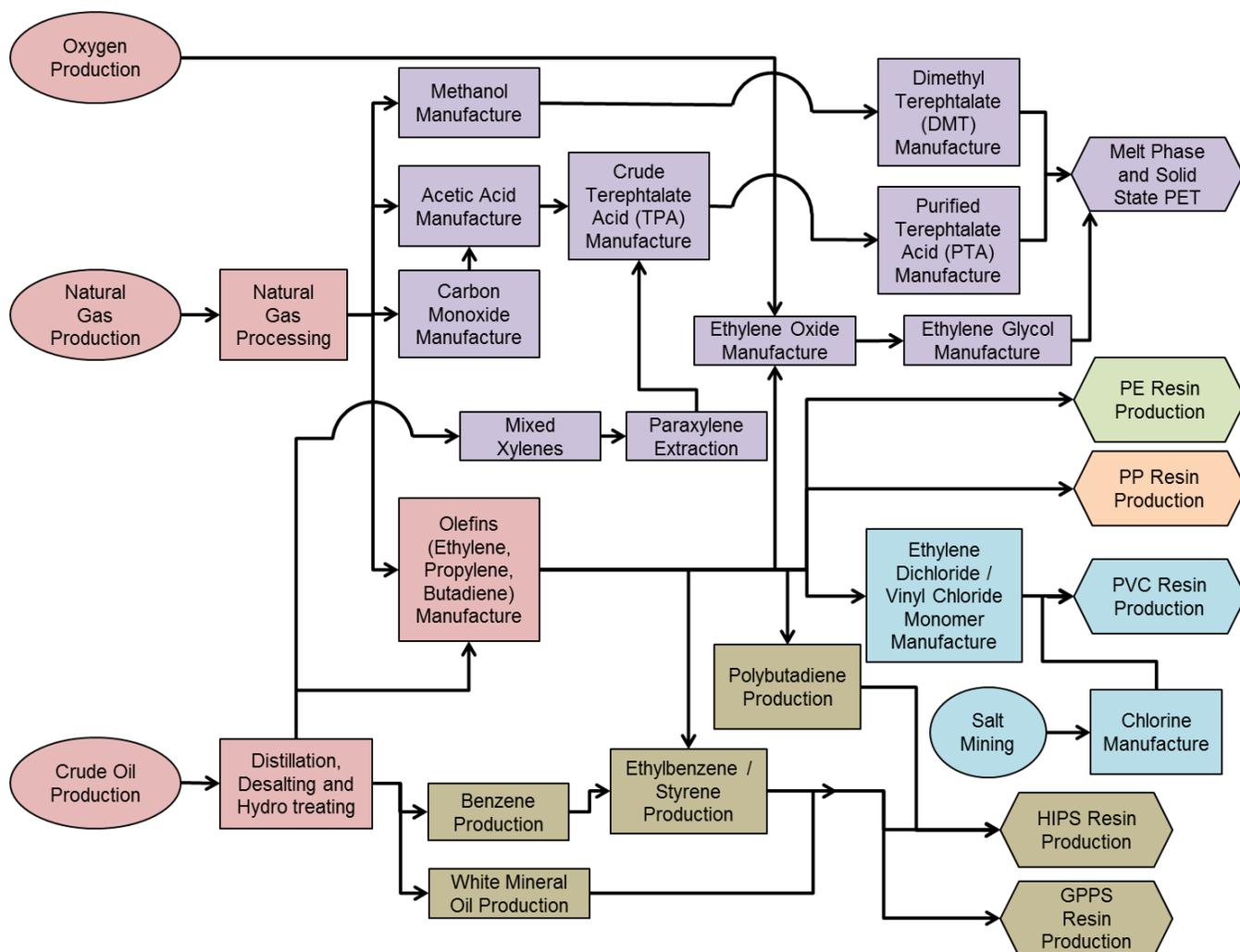


Figure 3.1. Manufacturing processes for selected thermoplastic polymers: polyethylene terephthalate (PET), polyethylene (PE), polypropylene (PP), polyvinyl chloride (PVC), high impact polystyrene (HIPS) and general purpose polystyrene (GPPS). Circles represent feedstocks, rectangles production/manufacturing, and hexagons the final manufacturing stage. Pink processes are common to multiple polymers, while other colors are unique to each polymer family. This figure is based, in part, on the flow diagrams by Franklin Associates (2011).¹⁴⁵

The ACC report relies on data from 17 manufacturers, with over 80 plants in North America.¹⁴⁵ It is the most up to date, publically available inventory for North American plastics production. Reported energy requirements and direct process emissions are industry averages for each unit process. This study accounts for uncertainty by linking the point estimates from the ACC report to the full distributions developed by Venkatesh *et al.* (2011)¹⁹⁸ for crude oil extraction and refining, as well as those reported in Posen *et al.* (2015) (Chapter 2)¹⁵⁴ for natural gas extraction

and processing, and for ethane and naphtha steam cracking (for the production of olefins and pygas). Further details are available in appendix section B.1.1.

3.3.3. *Bio-based Polymer Model Overview.*

Figure 3.2. shows a flow diagram for the production of bio-based polymers (PLA, PHB and bioethylene-based plastics) from either corn or switchgrass. All bio-based pathways include emissions from land-use change and agriculture (fuel use, agrochemical production, and N₂O field emissions) as well as feedstock transportation. Corn-based pathways for the production of PLA and PHB include emissions from wet milling, fermentation, polymerization (for PLA), and product recovery (PHB). Corn-based bioethylene polymer production includes emissions from ethanol production (dry milling and fermentation), dehydration to ethylene, and incorporation into conventional polymers (as per the fossil polymer model overview above). Switchgrass-based pathways include additional emissions from dilute acid pre-treatment and saccharification, along with fermentation and other steps further downstream that are in common with the corn-based pathways. The main emission sources quantified for biomass processing include electricity, on-site fuel (heat), and chemical/enzyme production. Based on Spatari *et al.* (2010),²⁶¹ the bioethylene scenarios include near-term and mid-term (higher) yield of sugars from pretreatment and yield of ethanol. For PLA and PHB, there are limited data available on yield from different sugar types, so this study models only a mid-term yield scenario, which assumes the same product yield (on a mass basis) as from corn glucose^{244,246,262,263} or sugarcane sucrose.^{247,251} This study does not include product manufacture and consumer use of the resins, as these steps will not differ much between conventional and bio-based plastics. In the cradle-to-gate analysis, all bio-based pathways receive a GHG credit for the amount of biogenic carbon stored in the polymer. This chapter also includes emissions from a range of end of life (EOL) scenarios. To simplify the presentation of a large number of scenarios, EOL results are reported separately from the cradle-to-gate model.

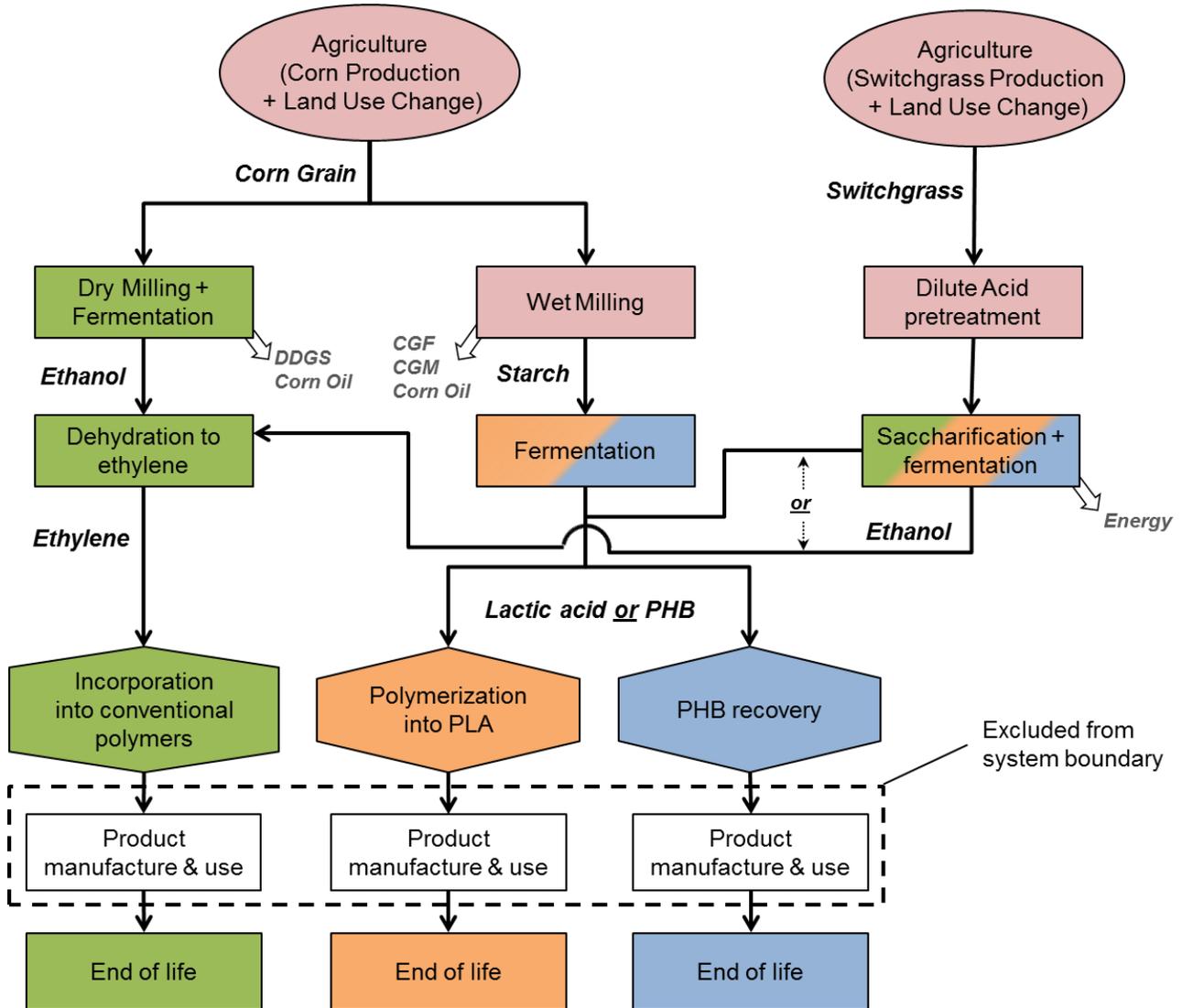


Figure 3.2. Bio-based polymer production processes. Black arrows indicate main reference flows, while white arrows indicate co-product production: dried distiller’s grains and solubles (DDGS), corn oil, corn gluten feed (CGF), corn gluten meal (CGM), and energy. Circles represent feedstocks, and hexagons are the final resin production stages, which represent the end of the cradle-to-gate model. All other stages are shown as rectangles. Pink processes are common to multiple polymers and white processes are excluded from the system boundary. Green processes are for producing bioethylene-based polymers, orange for polylactic acid (PLA), and blue for polyhydroxybutyrate (PHB). Boxes with multiple colors indicate equivalent, but separate processes for multiple polymer families.

3.3.4. *Uncertainty, Variability, and Scenarios*

This study uses Monte Carlo simulation to model uncertainty and variability for key parameters, as detailed in appendix section B.1. For PLA and PHB, fermentation and recovery processes are still under development, and so different data sources may represent fundamentally different technologies. Thus, this study treats energy requirements, material inputs, and product yields from different data sources as different scenarios or cases, as outlined in Table 3.1, which contains a summary of all data sources. For PLA production, 4 cases are based respectively on Groot and Boren (2010),²⁵¹ Vink *et al.* (2015),²⁶² and 2 hybrid cases based on both Vink *et al.* (2015)²⁶² and Sakai *et al.* (2003).²⁶⁴ For PHB production, 5 cases are based respectively on Harding *et al.* (2007),²⁴⁷ Akiyama *et al.* (2003) case 9,²⁶³ Akiyama *et al.* (2003) case 10,²⁶³ Kim and Dale (2008)²⁴⁴ and Gerngross (1999).²⁴⁶ These data sources were selected from reviewed literature as they are the only ones to provide sufficient information to estimate emissions from the plastic production (fermentation and polymerization/recovery) unit processes. Each data source provides information on the yield of either PLA or PHB, and, with the exception of Vink *et al.* (2015),²⁶² enough information to extrapolate electricity and on-site heat requirements, along with emissions from the production of process chemicals, as described in appendix sections B.1.7 and B.1.8. Rather than process inputs, Vink *et al.* (2015)²⁶² provide only total emissions for PLA fermentation and polymerization respectively. As a result, only Groot and Boren (2010)²⁵¹ (PLA case 1) provide sufficient detail to adapt for switchgrass PLA production. For switchgrass-based PHB pathways, there is no evident representative or bounding scenario; thus, the results section presents an additional case which combines the 5 cases into a single distribution as described in appendix section B.1.8.

3.3.5. *Impact Metrics*

The key impact metric employed in this chapter is the 100-year global warming potential (GWP), modeled using equivalence factors (in kg CO₂e) as reported by the Intergovernmental Panel on Climate Change (IPCC) fifth assessment report (AR5).²⁰⁴ As in several recent studies,^{154,265,266} this study assumes normally distributed equivalence factors, with uncertainty ranges based on the AR5 Supplementary material.²⁰⁵ Mean global warming potentials for CH₄ and N₂O are 36 and 298, respectively, as summarized in appendix B, Table B.13.

3.3.6. Treatment of Co-Products

Model decisions regarding the treatment of co-products are potentially important contributors to differences between LCA studies. As such, it is important to understand the degree to which co-product allocation methods drive results. For corn-based production pathways, this analysis includes four different scenarios for co-product allocation: mass allocation, energy allocation, no allocation (i.e. 100% of emissions to bio-based plastic), or avoiding allocation via system expansion. For system expansion scenarios, corn co-products displace soybean meal (dry milling pathway only), whole corn, urea, and soybean oil. Displacement factors and corresponding displaced emissions are based on GREET 2014,²⁶⁷ as described in appendix section B.1.5. For switchgrass-based pathways there are several scenarios to account for surplus biomass (lignin and unfermented sugars) as an internal energy source. These include disposal (no energy generated), steam generation, or steam and electricity generation in a combined heat and power (CHP) plant. The model assumes this energy is used first to power the pre-treatment and fermentation processes. Process heat requirements are always satisfied before generating electricity. If surplus energy generation is possible, scenarios include cases with and without emission credits for surplus steam and/or electricity (displacing natural gas and/or grid electricity, by system expansion). Otherwise, any additional energy required for the switchgrass-based pathways comes from conventional sources (grid electricity and natural gas fuel), with the exception of a switchgrass fuel scenario in which combustion of whole switchgrass provides additional energy. A final switchgrass scenario assumes all residues are sold as a co-product, and allocates emissions between the main product and the residues based on energy content. Further details are available in appendix section B.1.10.

For fossil fuel pathways, upstream emissions data comes from existing studies (see Table 3.1) that used either mass or energy allocation to account for co-products. As noted in Posen *et al.* (2015) (Chapter 2),¹⁵⁴ treatment of hydrogen produced during steam cracking (olefin production) has a greater influence on results than other allocation decisions. This analysis thus includes three scenarios for hydrogen co-product accounting: system expansion (displacing H₂ produced by methane steam reforming), energy recovery (combustion to power the steam cracking process), or mass allocation.

3.3.7. *End of Life (EOL)*

In the United States, over 85% of plastic waste is landfilled, with the remainder split between recycling (primarily HDPE and PET) and incineration with energy recovery.²³⁴ Certain bio-based plastics like PLA and PHB can also be composted at industrial facilities.²⁴⁹ This study includes scenarios to represent these four disposal options, for each plastic type, as applicable. The U.S. Environmental Protection Agency (EPA) Waste Reduction Model (WARM) provides the data for modeling most EOL pathways,²⁶⁸ but is supplemented with additional data for the composting scenarios²⁴⁴ and for emissions from landfilling PHB.^{269,270} Like fossil-based polymers, PLA has been shown to be inert under landfill conditions,²⁷¹ so emissions result only from transportation and use of landfill equipment.²⁶⁸ In contrast, PHAs are known to degrade to methane and CO₂, even under anaerobic conditions.²⁴⁹ The probability distribution used for emissions from landfilled PHB spans a range of average U.S. landfill conditions, based on key parameters reported in the literature.²⁶⁸⁻²⁷⁰ Additional details are available in appendix section B.1.11.

3.3.8. *Fuels and Electricity*

This study employs stochastic modeling for the life cycle GHG emissions of energy, based on the previously reported distributions for different fuel types.^{198,206,266} Distributions for the life cycle emissions from grid electricity span the range of available literature estimates at the level of individual North American Reliability Corporation (NERC) regions,^{267,272-275} where production of the feedstocks is most likely to take place: the region covered by the Midwest Reliability Organization (MRO) for corn-based processes,^{37,40} the south/southeast region spanned by the Southwest Power Pool (SPP), the Southeast Electric Reliability Council (SERC), and the Texas Regional Entity (TRE) reliability corporations for the switchgrass-based processes,¹²⁸ and TRE/SERC for conventional chemical and plastics production.²⁷⁶ Additional details are available in appendix B, section B.1.12.

Table 3.1 presents a summary of modeled production stages, data sources, treatment of uncertainty and treatment of co-products.

Table 3.1. Summary of key data sources. Details on the stochastic (probability) distributions employed are presented in appendix B, section B.1.

Production stage	Data source	Uncertainty	Co-product treatment
Petroleum feedstock (extraction and refining) or petroleum fuels (life cycle)	Venkatesh, <i>et al.</i> (2011) ¹⁹⁸	Stochastic distribution	Mixture of mass and energy allocation.
Natural gas feedstock (extraction, processing)	Posen, <i>et al.</i> (2015) (Chapter 2) ¹⁵⁴	Stochastic distribution	Mass allocation
Natural gas fuel (life cycle)	Tong, <i>et al.</i> (2015) ²⁶⁶	Stochastic distribution	Energy allocation
Coal fuel (life cycle)	Venkatesh, <i>et al.</i> (2012) ²⁰⁶	Stochastic distribution	
Electricity	Various ^{267,272-275,277}	Stochastic distribution	
Olefin production	Posen, <i>et al.</i> (2015) (Chapter 2) ¹⁵⁴	Stochastic distribution	Hydrogen: scenarios; other co-products: mass allocation
Conventional chemical and polymer production	Energy requirements from Franklin Associates (2011) ¹⁴⁵	Deterministic (together with stochastic emissions factors)	
Land-use change	Range from GREET 2014 CCLUB model ²⁶⁷	Stochastic distribution; uncertainty likely underestimated.	
Agriculture	Own analysis of data for corn ^{225,267,278,279} and switchgrass ^{225,267,280}	Stochastic distribution	
Wet milling (corn)	Various ^{244,262,263,267}	Stochastic distribution	Scenarios
Dry milling and ethanol production (corn)	Mean from Mueller and Kwik (2013); ²⁸¹ uncertainty based on Mueller (2010) ²⁸²	Stochastic distribution	Scenarios
Pre-treatment & saccharification (switchgrass)	MacLean and Spatari (2009), ²⁸³ Spatari <i>et al.</i> (2010), ²⁶¹ Laser <i>et al.</i> (2009) ²⁸⁴ and GREET 2014. ²⁶⁷	Stochastic distribution	Scenarios (treatment of fermentation residues)
PLA downstream (fermentation and polymerization)	Case 1: Groot and Boren 2010 ²⁵¹ Case 2: Vink, <i>et al.</i> (2015) ²⁶² Cases 3: Vink, <i>et al.</i> (2015) ²⁶² for fermentation + Sakai, <i>et al.</i> (2003) ²⁶⁴ for polymerization (energy from electricity) Cases 4: Vink, <i>et al.</i> (2015) ²⁶² for fermentation + Sakai, <i>et al.</i> (2003) ²⁶⁴ for polymerization (energy from heat)	Point estimates for energy requirements (case 1, cases 3-4 polymerization), with stochastic emissions factors as above. Point estimate for emissions (case 2, cases 3-4 fermentation)	
PHB downstream (fermentation and recovery)	Case 1: Harding, <i>et al.</i> (2007) ²⁴⁷ Cases 2 & 3 : Akiyama, <i>et al.</i> (2003) ²⁶³ cases 9 & 10 Case 4: Kim and Dale (2008) ²⁴⁴ Case 5: Gerngross (1999) ²⁴⁶	Point estimates for energy requirements (by case), plus a ‘full distribution’ case. Stochastic emissions factors as above.	
Switchgrass Ethanol	Energy inputs from Mullins <i>et al.</i> (2011) ⁷⁴ , yield from MacLean and Spatari (2010) ²⁶¹	Near term: stochastic distribution Mid-term: stochastic for energy inputs only; deterministic yields	
Ethanol dehydration to bioethylene	Kochar, <i>et al.</i> (1981), ¹⁸⁰ with uncertainty based on Geisler <i>et al.</i> (2005), ²²⁷ as modeled in Posen, <i>et al.</i> (2015) (Chapter 2) ¹⁵⁴	Arbitrary stochastic distribution.	
End of Life (EOL)	Based on EPA WARM, ²⁶⁸ with additional sources ^{244,269,270} for certain scenarios.	Partially stochastic	

3.4. Results and Discussion

3.4.1. Cradle-to-Gate GHG Emissions

Figures 3.3-3.6 show the modeled GHG emissions for each of the main pathways considered, including the different biopolymer cases defined in Table 3.1. Appendix B, sections B.2.1 and B.2.2 provide numerical results for these pathways; section B.2.3 includes a comparison between results in this chapter and the data sources on which the different PLA and PHB cases are based. The results include a range of alternate assumptions regarding allocation of co-products, alternate data sources (PHB and PLA), and product yields (switchgrass-based bioethylene). For increased clarity, Figure 3.3 excludes the results for HIPS and LLDPE, as emissions from these pathways are nearly identical to emissions from GPPS (hereafter, PS) and HDPE, respectively. Fossil polymer emissions differ based on polymer-type, with PS being responsible for roughly double the emissions of HDPE (Figure 3.3). The treatment of hydrogen co-product is important only for polyolefins (PE and PP), since a larger proportion of the raw material for these plastics is produced via the steam cracking process from which the hydrogen co-product results.

Figure 3.4 shows results for all PLA cases, and for the switchgrass PHB ‘full distribution’ case. These results are supplemented with Figure 3.5, which shows results for switchgrass PHB broken down by case number (data source). Figure 3.6 shows results for bioethylene. For a given feedstock, GHG emissions from PHB (Figure 3.4b,d and Figure 3.5) are generally higher than emissions from the production of PLA (Figure 3.4a,c) or bioethylene (Figure 3.6) (note differences in scale of the Y-axis across these figures). Switchgrass PHB scenarios with GHG emission credits for surplus energy generation are a potential (though highly uncertain) exception to this observation. Modeled emissions for PLA are largely consistent across the two industrial data sources^{251,262} (Figure 3.4a cases 1 and 2); mean emissions and confidence intervals are within 0.2 kg CO₂e/kg PLA for these cases. The final PLA data source (for polymerization only)²⁶⁴ is based on laboratory-scale experiments, and provides more extreme estimates (Figure 3.4a cases 3 and 4), with mean emissions ranging by about 1 kg CO₂e/kg PLA across these cases. Results for PHB differ greatly depending on the data source (Figure 3.4b for corn and Figure 3.5 for switchgrass), with mean emissions ranging between (2.7)-(6.9) kg CO₂e/kg corn PHB in the system expansion scenario and spanning a range of about 3 kg CO₂e/kg switchgrass PHB, within

a given scenario for treatment of fermentation residues. For corn PLA and PHB pathways, the choice of allocation method is a minor determinant of life cycle emissions (Figure 3.4a,b). GHG emissions from corn-based bioethylene are sensitive to allocation decisions, though mean emissions are generally lower than for fossil ethylene (Figure 3.6a). For all biopolymers, switchgrass-based pathways generally result in lower GHG emissions than corn-based pathways, due to lower agriculture emissions, and the possibility for energy co-production (Figure 3.4 c,d, Figure 3.5, and Figure 3.6b).

Scenarios for the treatment of fermentation residues are critical for biopolymer pathways with significant quantities of biomass residue: PHB, bioethylene near-term, and, to a lesser extent, bioethylene mid-term. Fermentation residue scenarios for switchgrass-based PLA are more similar to one another, as there is typically insufficient energy in the residue to generate much surplus steam or any surplus electricity. Treating switchgrass residues by energy allocation results in lower emissions and narrower confidence intervals, though it may be argued that this method masks uncertainty by transferring it to the residue product. The specific scenarios for the use of process residues provide more insight into actual net process emissions.

The effect of different yield scenarios for switchgrass ethanol (the precursor to bioethylene) depends on how residues are treated. The lower yielding “near-term” scenario has lower mean emissions than the “mid-term” scenario, provided that credits are applied for export of the surplus energy co-product(s). Spatari *et al.*²⁶¹ had already noted this counter-intuitive correlation between yield and emissions: biopolymers have lower emissions when more of the biomass is used for energy than for product. This raises important questions surrounding the best use of biomass.

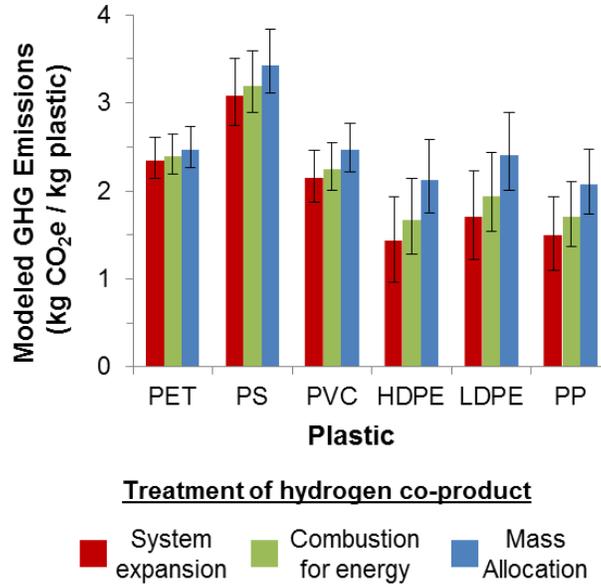


Figure 3.3. Cradle-to-gate greenhouse gas emissions for fossil polymers with hydrogen co-product treated by system expansion (displacing H₂ produced by methane steam reforming), combusted for energy, or subject to mass allocation. Error bars span 95% of simulations. Fossil polymers include polyethylene terephthalate (PET), polystyrene (PS), polyvinyl chloride (PVC), high density polyethylene (HDPE), low density polyethylene (LDPE) and polypropylene (PP).

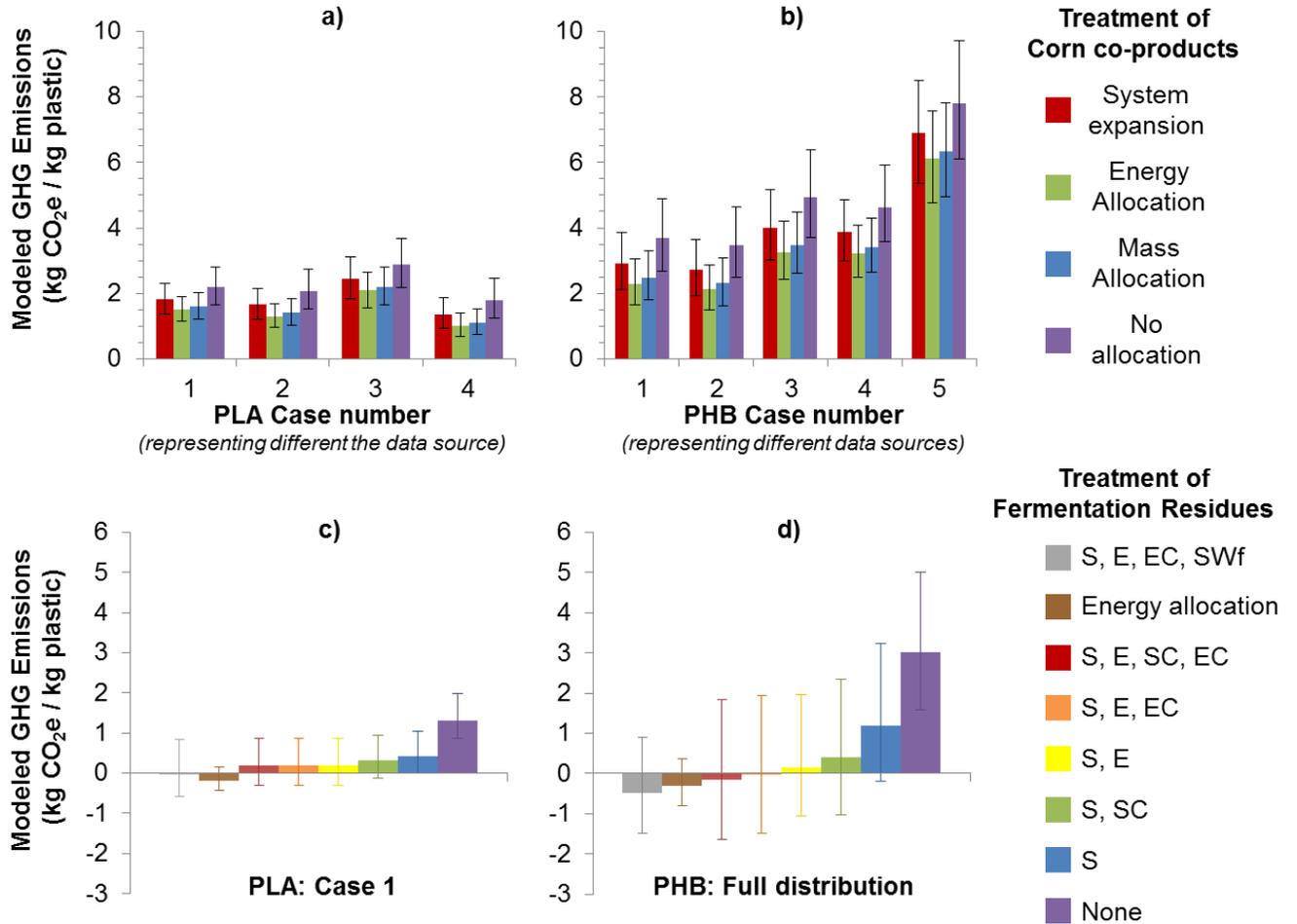


Figure 3.4. Cradle-to-gate greenhouse gas emissions for a) corn-based PLA (cases 1-4), b) corn-based PHB (cases 1-5), c) switchgrass-based PLA (case 1), d) switchgrass-based PHB (distribution spanning all cases). Error bars span 95% of simulations. Case numbers for panels a)-c) are defined in Table 3.1. The Legend for panels c) and d) 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 or PLA on the basis of energy content.

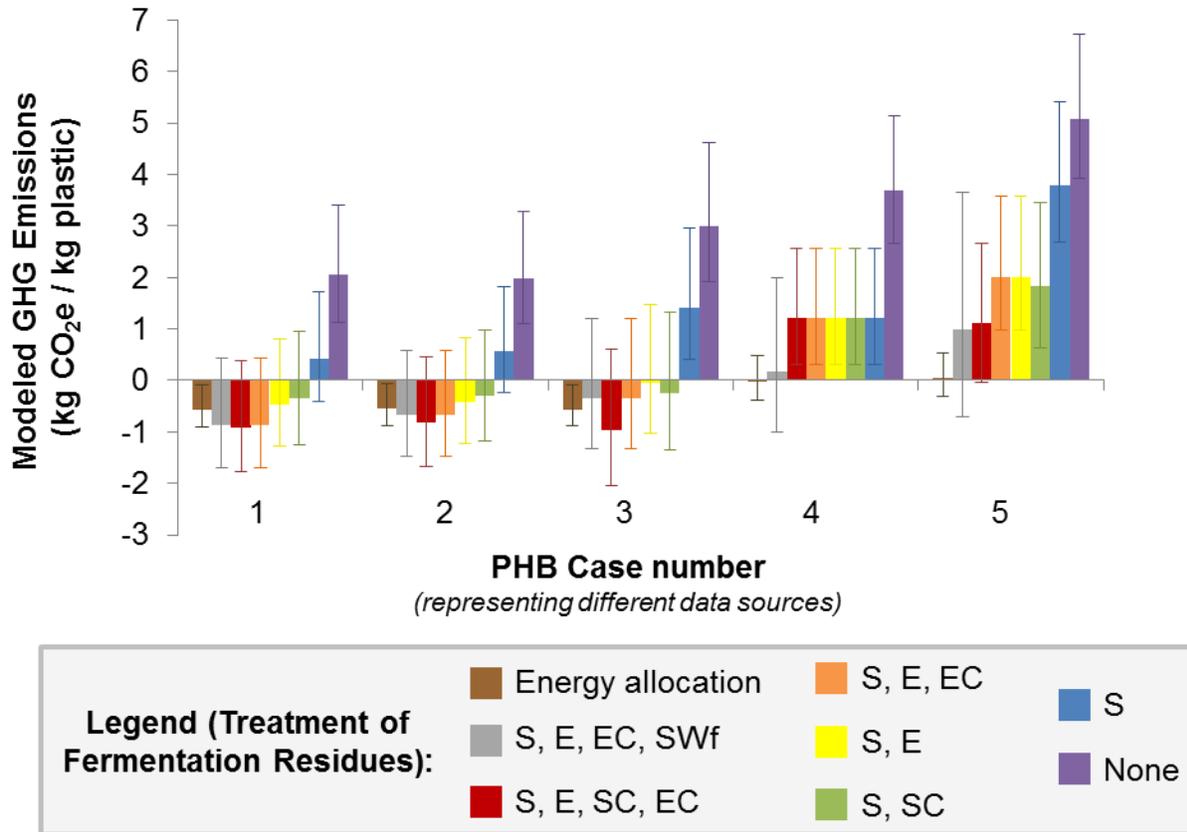


Figure 3.5. Cradle-to-gate greenhouse gas emissions for switchgrass-based PHB (cases 1-5). Error bars span 95% of simulations. Case numbers are defined in Table 3.1 The legend refers to assumptions about the use (or allocation) of unfermented residues: S = steam, E = electricity, C = emission credit 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.

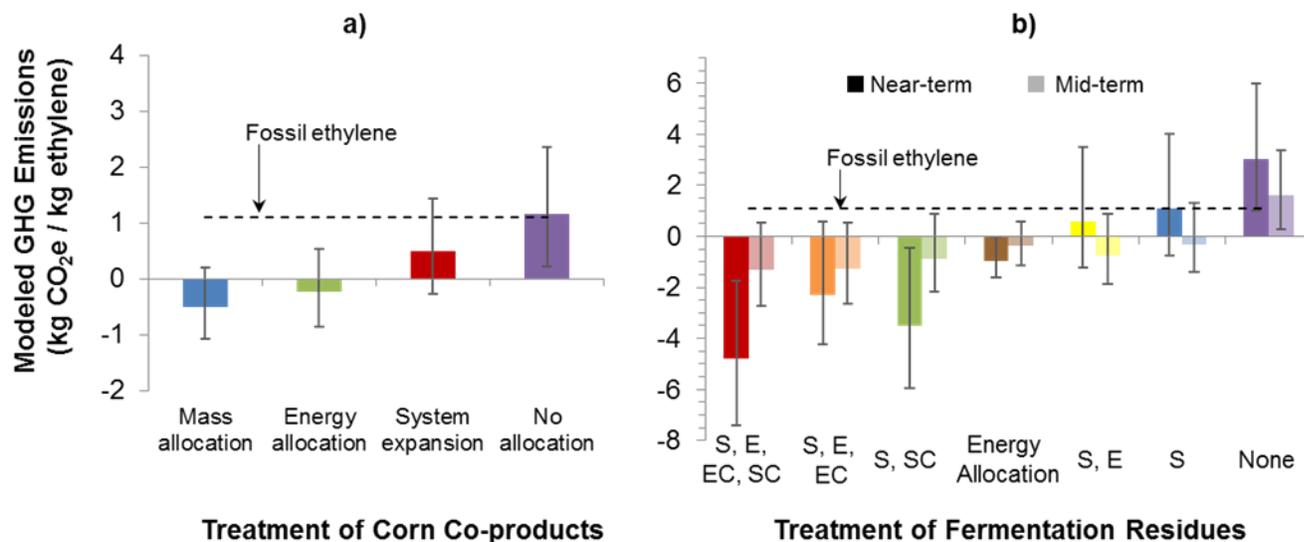


Figure 3.6. Cradle-to-gate greenhouse gas emissions for a) corn-based bioethylene and b) switchgrass-based bioethylene. Error bars span 95% of simulations. The results for corn-based production include different allocation scenarios. The results for Switchgrass-based production include different scenarios for the treatment of fermentation residues, for both near-term and mid-term yields. The horizontal lines represent the mean results for fossil ethylene, shown for reference. Legend for panel b) 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.

Appendix section B.2.4 presents an uncertainty importance analysis for select pathways. The uncertainty in factors relating to field N₂O emissions (especially the N₂O emission factor and GWP of N₂O), emissions from land use change, and emissions from grid electricity heavily influence the uncertainty of corn-based biopolymers. For corn PHB and PLA, gross emissions from the corn wet milling are an important source of uncertainty. For corn ethylene, energy used in ethanol production and in ethanol dehydration to ethylene also contribute substantially to modeled uncertainty. For switchgrass pathways, key uncertainties relate to field N₂O emissions (especially synthetic nitrogen application per unit area, and crop yield) and emissions from land use change. Upstream emissions are less important in higher yield pathways. Thus, for the mid-term bioethylene yield scenario, energy use for ethanol production also emerges as one of the more important contributors to uncertainty. Results from combining all data sources into a full distribution for emissions from PHB fermentation and recovery (e.g. Figure 3.4d) suggest that variability in process energy requirements may be the most important source of uncertainty in the

life cycle GHG estimates for this biopolymer. The adoption of a standardized production process could potentially reduce this uncertainty.

Uncertainty for PLA scenarios is generally lower than for other bio-based scenarios. This is largely due to the fact that PLA has a much higher yield per unit sugar (~0.7 kg PLA/kg sugar) than PHB (~0.3-0.4 kg PHB/kg sugar) or bioethylene (modeled yield ranging from 0.1-0.3 kg ethylene/kg sugar depending on the scenario). Thus, PLA requires less corn or switchgrass, which results in lower uncertainty from agriculture. Uncertainty in fossil polymer production and for switchgrass bioethylene pathways with mid-term ethanol yield is likely underestimated due to the use of certain deterministic parameters (see Table 3.1). Similarly, uncertainty for PLA cases 2-4 is likely underestimated because the report by Vink *et al.* (2015)²⁶², a key data source for these cases, does not include sufficient data to extrapolate energy requirements. It was thus not possible to apply stochastic emissions factors like those used for the other cases modeled in this chapter. Uncertainty for all bio-based pathways may likewise be underestimated due to the potential for an even wider range of emissions from land use change than is reported in the GREET CCLUB model,²⁶⁷ as discussed for example by Plevin *et al.*^{285,286}

Figure 3.7 presents the difference in emissions that result from switching from fossil-based polymers to select corn-based or switchgrass-based production pathways, on a cradle-to-gate basis. This figure shows results obtained by taking the difference between emissions from each fossil polymer and each bio-based polymer within each simulation run, while maintaining correlation between common inputs. Appendix B, sections B.2.5 and B.2.6 present numerical results corresponding to Figure 3.7, along with additional scenarios. All comparisons are for 1 kg of bio-based plastic replacing 1kg of fossil-based plastic and do not account for possible changes in market equilibrium. Appendix section B.2.7 explores sensitivity of the results to this assumption of 1:1 mass equivalence between plastics. Each fossil polymer likely has applications for which PLA and PHB will be unable to substitute; thus, these comparative results should be treated with caution.

Consistent with ISO 14044 LCA guidelines,⁶⁶ system expansion is the baseline method for handling co-products (where possible) and is the basis of the results in Figure 3.7. For corn PLA,

the study by Vink, *et al.* (2015)²⁶² is both the most recent and the best tailored to a U.S. context; thus, Figure 3.7 presents results based on PLA case 2. For corn PHB, results are unfavorable even in the lowest emission scenario (case 2) so Figure 3.7 focuses on this optimistic bounding case. The results for the bioethylene pathways (corn and switchgrass), assume that this bio-product replaces fossil-based ethylene used in the production of the final plastic resins (with the exception of PP, which contains no ethylene). Thus, differences among bioethylene pathways represent different quantities of ethylene incorporated into each polymer.

Switchgrass pathways illustrate the potential for future improvement, and so Figure 3.7 presents optimistic scenarios by assuming internal production of steam and electricity from non-fermented switchgrass, as well as a credit for surplus electricity, when available (cases labeled as S, E, EC in Figures 3.4-3.6). For PLA, only one data source (case 1)²⁵¹ provided enough data to adapt to a model for switchgrass-based production. For switchgrass PHB, Figure 3.7 presents results based on an aggregate (“full distribution”) scenario, with fermentation and recovery parameters modeled stochastically based on all 5 input cases. For switchgrass bioethylene plastics, the figure presents results for mid-term yields.

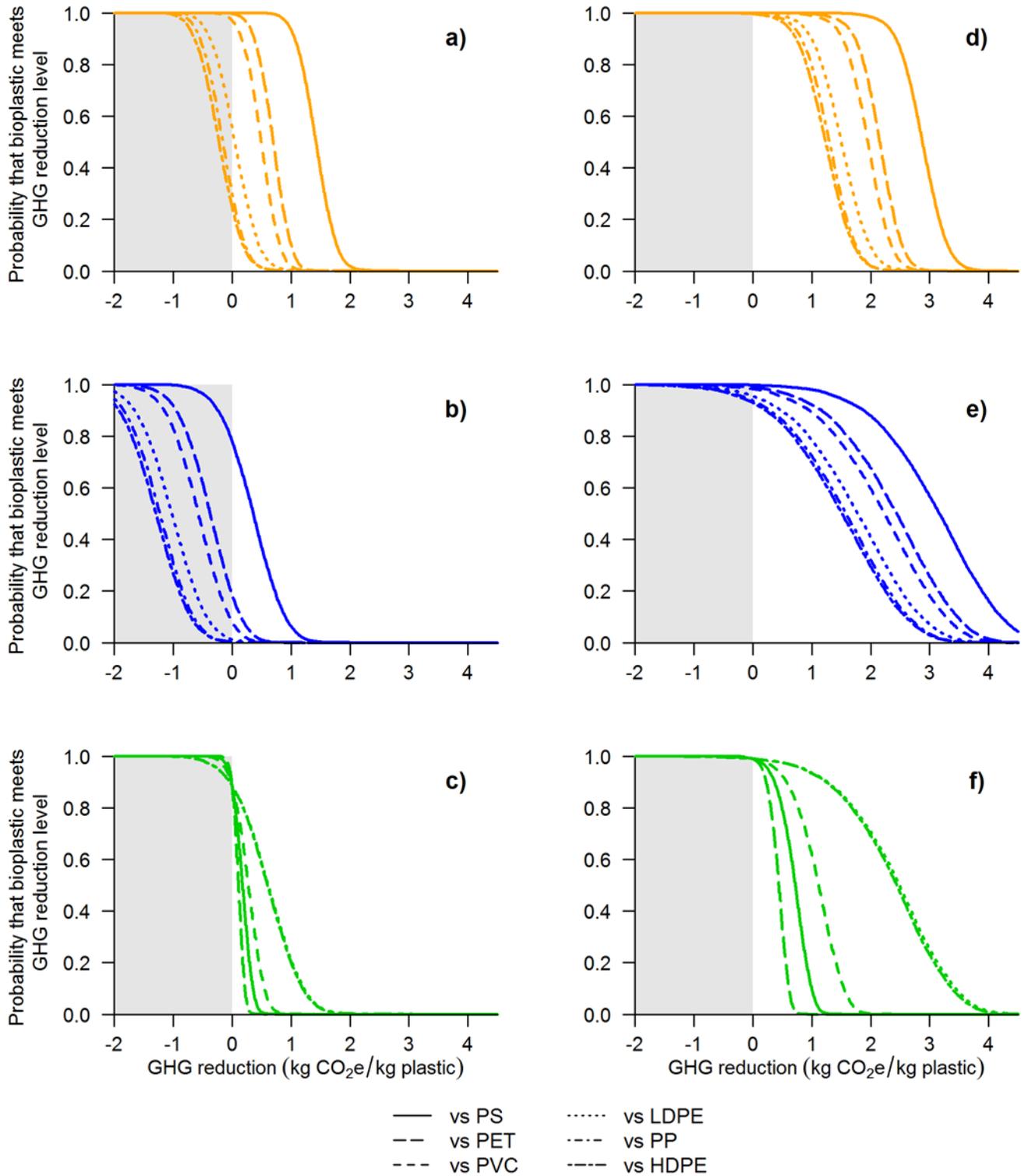


Figure 3.7. Difference in cradle-to-gate GHG emissions between bioplastics and fossil plastics. Positive numbers (white background) indicate the bioplastic has lower GHG emissions than the fossil plastic. Negative numbers (gray background) indicate the bioplastic has higher GHG emissions than the fossil plastic. The

panels represent a) Corn PLA (baseline: case 2, system expansion), b) Corn PHB (optimistic: case 2, system expansion), c) Corn ethylene plastics (baseline: system expansion) d) Switchgrass PLA (case 1), e) Switchgrass PHB (full distribution), f) Switchgrass bioethylene (mid-term). 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. The overlapping lines at the left side of panels a), d) and e) are for PP and HDPE. The overlapping lines at the right side of panels c) and f) are for LDPE and HDPE.

It is likely that corn PLA (Figure 3.7a) has lower emissions than the more energy intensive conventional polymers (mean GHG reductions of 23-46% compared to fossil PS, PET and PVC), but it compares poorly against polyolefins (mean GHG increases of 0-19% compared to fossil HDPE, LDPE, PP). As a reminder, PLA most often competes with PS and PET in the marketplace. In most model runs, corn PHB has higher emissions than conventional polymers, with a partial exception for PS (Figure 3.7b). Use of less optimistic data sources (especially cases 3-5) or inclusion of emissions from landfilling PHB (discussed below) would further increase the modeled emissions for PHB. As a reminder, PHB usually competes with PS and polyolefins. Finally, in most of the model runs, corn bioethylene has lower emissions than fossil ethylene (Figure 3.7c), however the total change on the final polymer life cycle is much smaller for PET, PS, and PVC, where ethylene is just one of several inputs (mean GHG reductions of 5-13%), than it is for HDPE and LDPE (mean GHG reductions of 35-41%). The corn bioethylene results presented here are more favorable (lower GHG emissions) than those reported by Posen *et al.* (2015) (Chapter 2)¹⁵⁴ due primarily to a lower estimate for LUC emissions employed here. As can be observed in Figures 3.4 and 3.6, system expansion is the least favorable way to account for corn co-products, and the most favorable method to account for hydrogen co-produced in the fossil polymer supply chain. Using other allocation methods would create more favorable results for corn-based polymers relative to conventional plastics, but violates the hierarchy of methods established by ISO standards.⁶⁶

For switchgrass-based scenarios, emissions from PLA (case 1, S, E, EC) and bioethylene polymers (shown for mid-term yield, S, E, EC) are lower than for all modeled fossil polymers, with a large degree of confidence (Figure 3.7 d,f). Switchgrass PHB, (full distribution, S, E, EC) likely has lower GHG emissions than any fossil polymer, but the magnitude of the potential

emission reduction is highly uncertain. Mean GHG emissions approach 0 for these PLA and PHB pathways, and so mean emission reductions approach 100% against any fossil polymer (90-95% for PLA and 110-120% for PHB). Use of a more pessimistic data source (e.g. PHB case 5), or inclusion of emissions from end of life (discussed below) substantially reduces the probability that PHB achieves any emission reductions relative to fossil polymers. Use of internal switchgrass energy is essential to achieving lower emissions than conventional fossil polymers for PHB and bioethylene pathways. Thus, energy recovery from unfermented residues should be a key goal in the design of switchgrass bioplastic production facilities.

3.4.2. End of Life (EOL)

The results in the previous section present cradle-to-gate emissions, without EOL. Table 3.2 presents additional emissions incurred for each plastic type due to a range of EOL scenarios. Bioethylene based polymers are identical to their fossil counterparts, so EOL scenarios do not affect the comparison between the two. Landfilling, the most common disposal mechanism, does not alter the comparison between PLA and fossil polymers, but substantially worsens the GHG emissions balance for PHB under average U.S. conditions, due to methane and carbon dioxide emissions released from anaerobic degradation of PHB. This conclusion holds qualitatively even when limited to landfills with LFG capture and energy recovery. Composting likewise worsens the emissions balance for PHB and PLA relative to landfilled fossil plastics, by re-releasing much of the stored carbon (primarily as CO₂) from the bioplastics. Only when compared to incinerated fossil polymers, can inclusion of EOL improve the results for biopolymers. This result depends on the assumption of low efficiency for energy recovery (17.8%),²⁶⁸ and would not hold under higher efficiency energy recovery scenarios (due to the higher energy density of conventional polymers). Compared to recycled plastics, biopolymers are even less likely to result in decreased GHG emissions.

Table 3.2. Mean GHG emissions due to end of life scenarios for each type of plastic (kg CO₂e/kg plastic). Plastics include high density polyethylene (HDPE), low density polyethylene (LDPE), polypropylene (PP), polyethylene terephthalate (PET), polystyrene (PS), polyvinyl chloride (PVC), polylactic acid (PLA) and polyhydroxybutyrate (PHB). Numbers in parentheses represent the 5th and 95th percentile of simulated values, where available. All values are in addition to cradle-to-gate emissions, which already include credits for stored carbon in PHB (2.05 kg CO₂/kg PHB), PLA (1.83 kg CO₂/kg PLA), or bioethylene (3.14 kg CO₂/kg ethylene), as applicable.

Plastic	Incineration (with energy recovery) ^a	Compost	Landfill	Recycling ^b
HDPE	1.7 (1.6,1.9)	-	0.04	-0.6 (-1.0,-0.3)
LDPE	1.7 (1.6,1.9)	-	0.04	-0.6 (-1.2,-0.5) ^c
PP	1.7 (1.6,1.9)	-	0.04	-0.5 (-0.9,-0.1) ^c
PET	1.6 (1.5,1.6)	-	0.04	-1.0 (-1.2,-0.9)
PS	2.1 (2.0,2.3)	-	0.04	-1.9 (-2.2,-1.5) ^c
PVC	0.9 (0.8,0.9)	-	0.04	-1.0 (-1.3,-0.7) ^c
Corn PLA ^d	1.3 (1.2,1.3)	1.7	0.04	-0.6 (-1.0,-0.2) ^c
Switchgrass PLA ^d	1.3 (1.2,1.3)	1.7	0.04	0.7 (0.2, 1.1) ^c
Corn PHB ^d	1.3 (1.2,1.4)	1.9	3.4 (2.2,4.8)	-1.6 (-2.2,-0.9) ^c
Switchgrass PHB ^d	1.3 (1.2,1.4)	1.9	3.4 (2.2,4.8)	0.8 (-0.6, 2.1)

- a) Incineration uncertainty range stems from grid emissions. Energy recovery efficiency is modeled deterministically at 17.8%.
- b) Recycling includes a credit for displaced virgin polymer. The uncertainty range is highly correlated to the emissions from virgin polymer production
- c) Approximate result, estimated from data on HDPE and PET.
- d) Differentiation between corn-based and switchgrass-based production only matters for recycling, which includes a credit for displaced virgin polymer. Virgin PLA and PHB scenarios are the same as those presented in Figure 3.7.

The following figures (Figure 3.9 and Figure 3.8) present the difference in cradle-to-grave GHG emissions between fossil-based and bio-based polymers; they are analogous to Figure 3.7 above, but with the addition of various EOL scenarios. Figure 3.8 shows the difference in cradle-to-grave GHG emissions between fossil-based and bio-based PLA. 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. Finally, composted switchgrass-based PLA likely has lower emissions than PS, PVC and PET, but is unlikely (probability < 0.4) to have lower emissions than polyolefin plastics (LDPE, HDPE or PP).

Figure 3.9 shows the difference in cradle-to-grave GHG emissions between fossil-based and bio-based PHB. 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). Even broken down by data source (results not shown), landfilled switchgrass PHB remains unlikely to have lower emissions than fossil plastics, for all but the most optimistic scenarios (e.g. cases 1 and 2, with surplus electricity credits, vs PS). When both PHB and fossil polymers are incinerated, however, switchgrass PHB results in lower GHG emissions than all fossil polymers, with probability approaching 1 (Figure 3.9, panel f)).

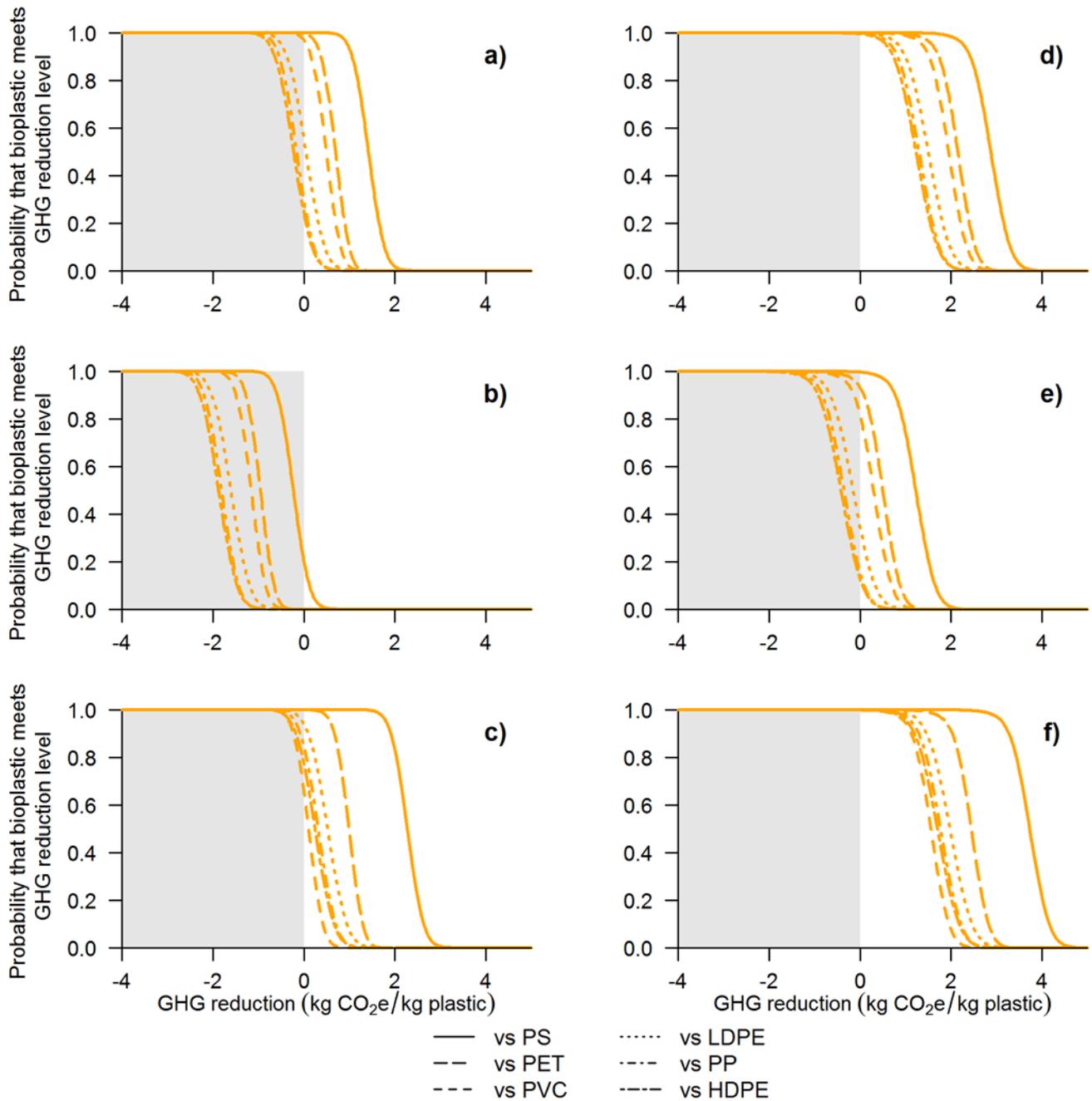


Figure 3.8. Difference in GHG emissions between PLA and fossil plastics. Positive numbers indicate PLA has lower GHG emissions than the fossil plastic. Negative numbers (gray background) indicate PLA has higher GHG emissions than the fossil plastic. Panels a), b) and c) represent corn PLA (baseline: 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.

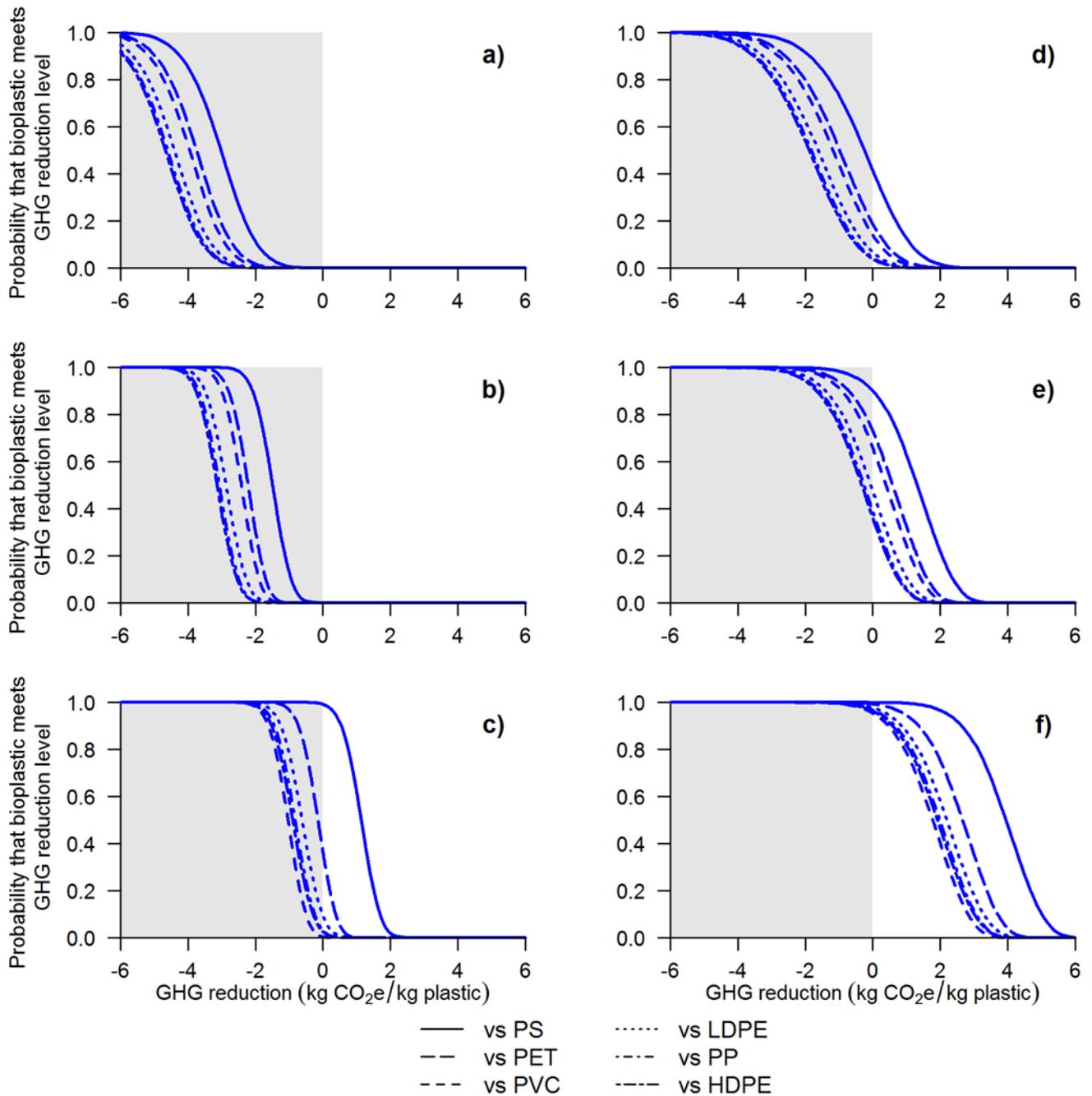


Figure 3.9. Difference in GHG emissions between PHB and fossil plastics. Positive numbers (white background) indicate the bioplastic has lower GHG emissions than the fossil plastic. Negative numbers (gray background) indicate the bioplastic has higher GHG emissions than the fossil plastic. Panels a), 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.

3.4.3. Sensitivity

Appendix sections B.2.5 and B.2.6 present a range of additional sensitivity scenarios for cradle-to-gate emissions from corn and switchgrass bio-based pathways, respectively. Excluding LUC emissions or assuming a lower N₂O emission factor for applied nitrogen improves the emissions balance for bio-base pathways, but in minor ways. In contrast, using higher values for LUC (e.g. the distribution from Plevin *et al.* (2015)²⁸⁵ for corn, or the Winrock scenario from the GREET CCLUB model²⁶⁷ for switchgrass) substantially increases emissions for PHB or bioethylene, and, to a lesser extent, PLA. Similarly, increasing the estimate of nitrogen in switchgrass crop residue,²²⁵ or excluding unfermented sugars from switchgrass residues used from internal energy recovery,²⁶⁷ substantially increase emissions from switchgrass pathways (especially PHB and bioethylene). Assuming a higher switchgrass yield,²⁵⁹ or a higher correlation between nitrogen application and yield, reduces the uncertainty in switchgrass pathways without substantially affecting mean results.

3.4.4. Some Limitations, Caveats and Additional Sensitivity Scenarios

Although the inclusion of uncertainty/variability is a major focus of this chapter, there are a number of important ways in which it does not capture the full possible range of emissions. As summarized in Table 3.1, some parameters include only point estimates (e.g. fossil polymer energy requirements), and others include distributions that likely underestimate uncertainty (e.g. LUC). Further, this study is conducted under a primarily attributional LCA framework, which does not account for marginal changes in emissions or changes in market equilibria. Thus, the ranges presented in this chapter should be interpreted as indicative rather than rigorous probabilities.

Additionally, this study uses values representative of average U.S. production, but does not account for all possible variations in local conditions such as electricity emissions or transportation distances. Further, this study examines only two crops (corn and switchgrass), representative of potential U.S. production; emissions would likely differ for other crops, like sugarcane, which is an important feedstock from existing bio-based plastic operations in other countries like Brazil and Thailand.^{184,251} The use of a waste feedstock instead of a dedicated crop system could likewise affect the GHG balance for bio-based plastics. This paper also excludes

emissions from product manufacture and use, which may affect the comparison between fossil plastics and PHB or PLA (but not bioethylene, which is chemically identical to fossil ethylene). In particular, the assumption that 1 kg of bioplastic can displace 1 kg of fossil plastic may not be valid for certain product systems; appendix section B.2.7 explores the sensitivity of model results to this assumption of 1:1 displacement. Additionally, appendix section B.2.8 considers the potential impact of omitted life cycle stages like product transportation and downstream processing energy.

Finally, this chapter considers only the GHG emissions arising from the life cycle of bio-based plastics. This is an important metric that has garnered much attention in recent years, and is often the basis for claims of environmental superiority among advocates of bio-based products. As mentioned in the introduction, however, bio-based products often compare poorly to conventional products on impact categories such as eutrophication and stratospheric ozone depletion.²⁵⁷ Studies specific to PLA and PHA likewise tend to indicate poor performance relative to fossil polymers on metrics like acidification and eutrophication¹⁵³ and ecotoxicity.¹⁵² Final recommendations will require a deeper investigation of other environmental metrics, together with an evaluation of broader economic and social implications of producing/using bio-based plastics.

3.4.5. Key Lessons

Substituting bioplastics for conventional fossil polymers can potentially result in a substantial decrease in GHG emissions. For switchgrass scenarios with energy recovery from unfermented residues, bioplastics can even result in net negative emissions (due to carbon sequestered in the plastic, and emissions credit from surplus electricity generation). The choice of baseline fossil polymers is an important modeling decision that is often overlooked. For ethylene-intensive polymers (i.e. PE) substituting bioethylene for fossil ethylene generally results in the greatest GHG reduction. Bioethylene offers an additional benefit in that it is chemically identical to fossil ethylene, so there is no change in the properties of the resulting bio-based resin. For other polymers (e.g. PS, PET, PVC, PP), PLA offers the greater potential GHG savings, assuming it can substitute functionally for these polymers on a 1:1 mass basis. This is an important assumption that is not appropriate for all plastic applications, and which merits additional

context-specific analysis by decision makers using the results of this study. Unsurprisingly, the greatest GHG reductions are possible when targeting the higher emission fossil polymers (PS, then PET and PVC). Fortunately, the fossil polymer with the highest GHG emissions (PS), is usually the most costly fossil resin,^{287,288} and would thus be the most economic to replace. PHB is generally the highest emission choice of the bio-based polymers considered, due to low yields, the potential for high process energy requirements (cases 3-5), and the likelihood of high end of life (EOL) emissions. EOL scenarios have a substantial effect on life cycle GHG emissions, particularly for plastics such as PHB, which are likely to degrade in landfills. To minimize GHG emissions, decision makers should consider the degradation characteristics of plastics and select EOL pathways that reduce this impact.

Switchgrass pathways generally result in lower emissions than corn-based pathways, although this result is partly attributed to the availability of switchgrass residues for energy generation. This chapter also demonstrates the importance of considering uncertainty in LCA. As Figure 3.7 demonstrates, potential GHG reductions from bioplastics can span a range of several kg CO₂e/kg plastic. These ranges are on the same order of magnitude as the mean emissions from conventional polymers.

Agricultural operations result in large and potentially irreducible emissions uncertainties – particularly with respect to N₂O emissions and land use change. As a result, emissions from bio-based products carry large uncertainties. Choosing higher yielding products (e.g. PLA instead of bioethylene or PHB) can help constrain this uncertainty by reducing the amount of agriculture required. Beyond this, companies considering switching to bio-based plastics should consider the range of expected emission reductions and develop strategies that account for this uncertainty. For example, companies could look for stochastic dominance among pathways, or set a given GHG reduction target and then select the pathway that maximizes the probability of achieving this target (e.g. as discussed in Mullins *et al.* (2011)⁷⁴). Alternatively companies could perform a constrained optimization – simultaneously maximizing mean GHG reductions, while ensuring a minimum probability that the new pathway is at least as good as the original production method. Regardless of the specific approach taken, ignoring uncertainty should no longer be an option.

Chapter 4. Greenhouse Gas Mitigation for U.S. Plastics Production: Energy First, Feedstocks Later

4.1. Abstract

Plastics production is responsible for 1% and 3% of U.S. greenhouse gas (GHG) emissions and primary energy use, respectively. Replacing conventional plastics with bio-based plastics (made from renewable feedstocks) is frequently proposed as a way to mitigate these impacts.

Comparatively little research has considered the potential for green energy to reduce emissions in this industry. This chapter compares two strategies for reducing greenhouse gas emissions from U.S. plastics production: using renewable energy or switching to renewable feedstocks. Renewable energy pathways assume all process energy comes from wind power and renewable natural gas derived from landfill gas. Renewable feedstock pathways assume that all commodity thermoplastics will be replaced with polylactic acid (PLA) and bioethylene-based plastics, made using either corn or switchgrass, and powered using either conventional or renewable energy. Switching to renewable energy cuts mean GHG emissions by 50-75%, achieving greater reductions, with less uncertainty and lower cost, than switching to corn-based biopolymers – the most likely near-term biopolymer option. In the long run, producing bio-based plastics from advanced feedstocks (e.g. switchgrass) and/or with renewable energy likely offers greater emission reductions.

4.2. Introduction

Over the last six decades, global plastics production has grown from a nascent enterprise to a 300 million tonne (Mt) /year global industry in 2013.¹³⁹ North American plastic production accounts for approximately 20% of that global total and is expected to exhibit strong growth for the immediate future.^{140,141} In the U.S., seven families of ‘commodity thermoplastic’ polymers account for approximately 70% of plastics production.^{142,143} These include polypropylene (PP), polystyrene (PS), polyvinyl chloride (PVC), polyethylene terephthalate (PET), and polyethylenes (PE). The latter family includes high-density polyethylene (HDPE), low-density polyethylene (LDPE), and linear low-density polyethylene (LLDPE). Applying previously reported emissions factors suggests these plastics are responsible for approximately 70 million tonnes of CO₂e

emission per year¹⁴⁴ and nearly 3 quadrillion Btu of primary energy use.¹⁴⁵ This corresponds to slightly greater than 1% of total U.S. GHG emissions¹⁴⁶ and nearly 3% of total U.S. energy consumption.¹⁴⁷ In response, there has been a growing interest, globally, in switching to bio-based plastics as a form of greenhouse gas (GHG) mitigation.^{10,11,134,136,242,289-296}

Three of the most important families of bio-based polymers include polylactic acid (PLA), polyhydroxybutyrate (PHB, a representative of the polyhydroxyalkanoate (PHA) family) and bioethylene based plastics (e.g. bio-PET, bio-PE, bio-PVC, etc.). Replacing fossil-ethylene with bioethylene is an example of *direct feedstock substitution* as this requires no change in the final product. In contrast, PHAs and PLA are chemically distinct from existing fossil-derived thermoplastics, but may perform the same functions. As discussed in Chapter 3, PHAs can frequently replace PE, PP, and PS,^{151,243-248} and may also substitute for PET and PVC in some applications.¹⁰ PLA most often substitutes for PS and PET,^{151,153,249-253} but can also replace PE, PP, and PVC in some applications.^{10,250,254} These are examples of *functional feedstock substitution*. Chapter 3 further demonstrated that some of these bio-based plastics have lower emissions than their fossil counterparts. It remains unclear, however, if adoption of such products is the best way to reduce GHG emissions in the plastics sector.

As an alternative or possibly complementary strategy, this chapter analyzes the potential role of renewable energy in reducing GHG emissions in the U.S. plastics sector. In particular, this chapter compares the GHG emissions resulting from two broad emission reduction strategies: 1) *feedstock substitution* – switching from fossil-based to bio-based plastics, or 2) *energy substitution* – switching from conventional (fossil) fuels to renewable energy sources in the production of conventional fossil-based plastics. Figure 4.1 shows a simplified schematic of these strategies.

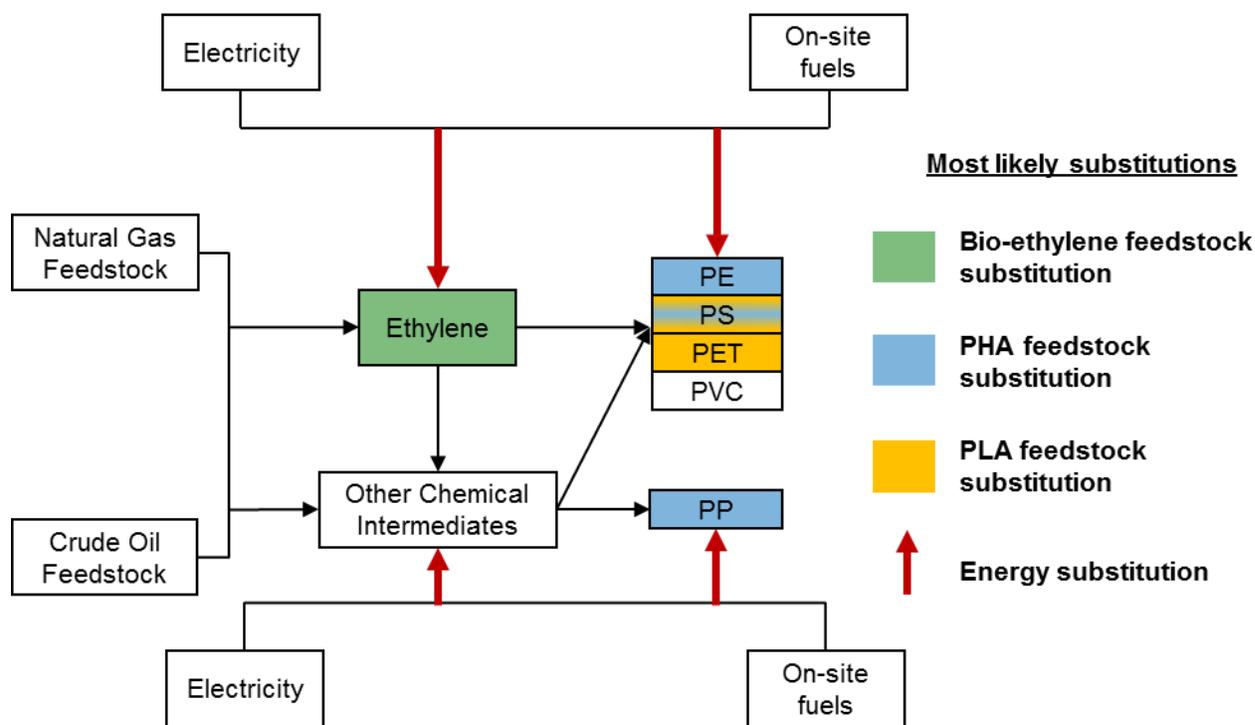


Figure 4.1. Schematic overview of the commodity thermoplastics industry. PE = polyethylene, PS = polystyrene, PET = polyethylene terephthalate, PVC = polyvinyl chloride, PP = polypropylene, PHA = polyhydroxyalkanoate, and PLA = polylactic acid. Shaded boxes indicate the most likely opportunities for feedstock substitution. Red arrows indicate potential opportunities for energy substitution.

All plastics require process related electricity and heat (on-site fuels) at various stages throughout their life-cycles. Substituting renewable energy sources (e.g. wind power, bio-gas, etc.) for grid electricity and direct fossil fuel combustion can reduce emissions without changing the fundamental processes employed to produce conventional plastics. A major advantage of either process energy substitution or direct feedstock substitution is that the product remains unchanged. Resin manufacturers may green their electricity use implicitly by purchasing renewable electricity certificates²⁹⁷ or explicitly through power purchase agreements and/or with on-site renewable electricity generation. Process heat requirements can be met with fuels such as renewable natural gas (RNG)²⁹⁸ or via electrification coupled with renewable electricity. Likewise, resin manufacturers can achieve direct feedstock substitution either by changing suppliers of specific input materials, or by on-site production of renewable bulk chemicals. In contrast, functional feedstock substitution requires downstream customers (e.g. consumer

product manufacturers) to develop products that rely on bio-based plastics, to be sourced directly from bio-based resin manufacturers.

To date, only a handful of studies have addressed the use of renewable energy in the production of bio-based plastics (e.g., refs^{244,299,300}) and none have compared this to renewable energy use in fossil polymer production. This work adapts the stochastic life cycle assessment model described in Posen *et al.* (2016) (Chapter 3)¹⁴⁴ to examine the GHG emissions from a range of scenarios for the production of both conventional and bio-based plastics. Consistent with Chapter 3 this work considers production of bio-based plastics using either corn grain or switchgrass as a feedstock.

4.3. Material and Methods

4.3.1. Model Overview

This chapter develops a set of feedstock and energy substitution scenarios for the plastics industry. The feedstock substitution scenario assumes that all commodity thermoplastics (with a partial exception for polypropylene) will either be produced using bioethylene, or replaced with polylactic acid (PLA), as summarized in Table 4.1. In particular, the model assumes that bioethylene will replace all ethylene in polyethylene (HDPE, LDPE, LLDPE) and PVC; PLA will replace all PET and PS. Further, PLA will replace PP, but only in the subset of pathways where PLA has lower mean GHG emissions than PP. This is an optimistic, bounding case, since a) it is unlikely that PLA can substitute for all applications of PS, PET and PP, and b) it assumes PLA can substitute for fossil plastics on a 1:1 mass basis despite some evidence that PLA products may require a higher mass of plastic.^{252,301} Since PHB is both more expensive, and has higher GHG emissions than other bioplastics, I did not include it in the main feedstock substitution scenarios; for completeness, PHB is included whenever results are presented for individual plastics (sections 4.4.3, 4.4.4 and appendix section C.2.2). The base-case scenario assumes that all bio-based plastics are produced from corn grain, which is currently the dominant feedstock for bio-based products in the U.S. In addition, the model considers two advanced bio-based scenarios: corn-based plastics produced using low carbon energy, i.e. combining feedstock and energy substitution, and plastics made from switchgrass – an illustrative second-generation cellulosic feedstock. In all cases, the model accounts for cradle-to-gate emissions from resin

production, and emissions from end of life, but not product manufacture or use. The model assumes that landfilled PLA and bioethylene plastics act as carbon sinks; alternatively PLA may be composted, releasing much of its stored carbon as carbon dioxide. The model assumes all fossil plastics are landfilled.

In the energy substitution scenario, low-carbon energy provides all process heat and electricity throughout the supply chain for the production of conventional plastics. The baseline low carbon (LC) energy scenarios in this chapter assume RNG²⁹⁸ made from landfill gas (LFG) will provide all fuel requirements, while wind power will provide all grid electricity requirements. In all cases, renewable energy scenarios apply only to unit processes within the chemical industry, and do not extend to natural gas production and processing, crude oil production and refining, or agricultural operations. The grey box in Figures 4.2 and 4.3 show the scope of the energy substitution scenarios within the fossil plastic and corn bio-plastic supply chains respectively. Renewable energy does not displace combustion of waste products (i.e., internal off-gas) produced during steam cracking or benzene production.

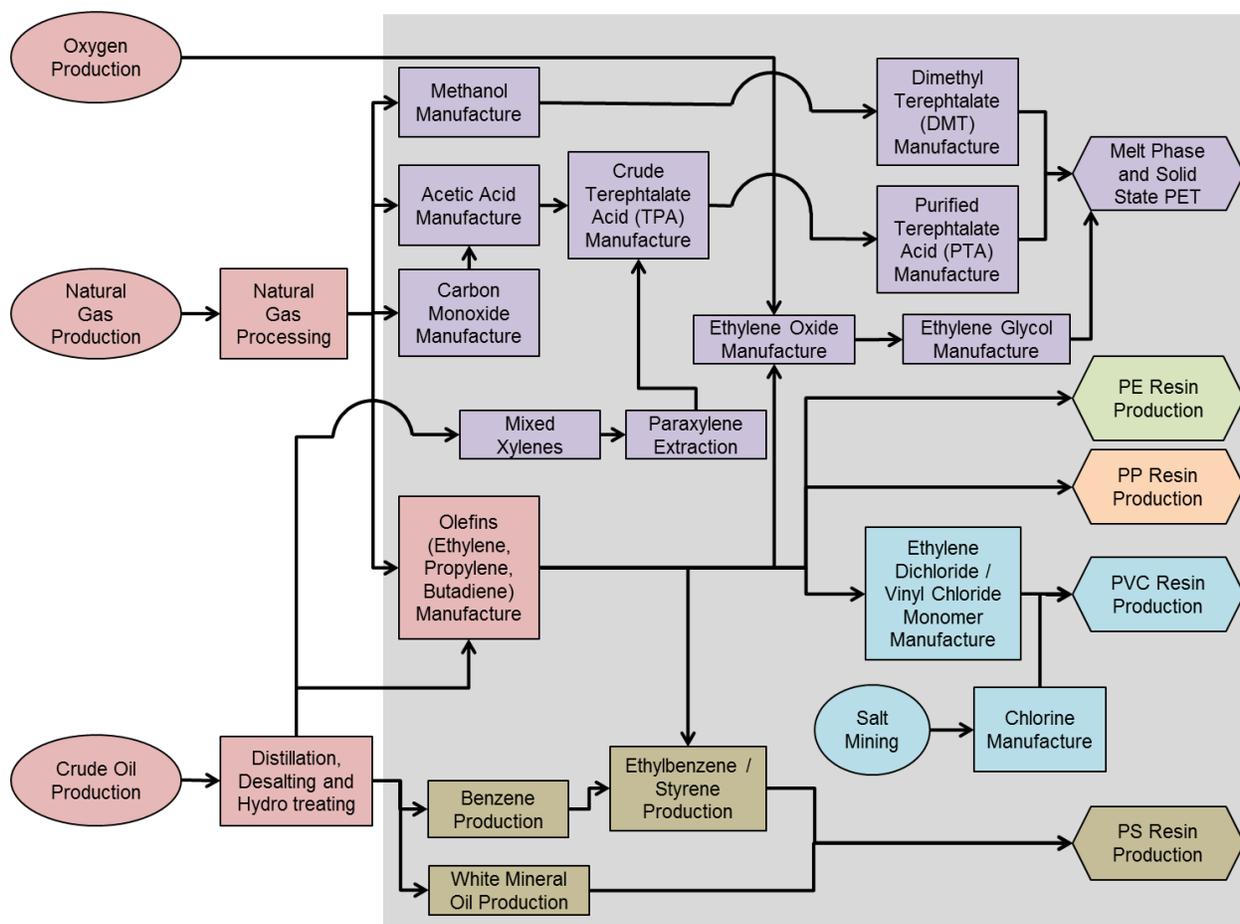


Figure 4.2. Manufacturing processes for commodity thermoplastic polymers: polyethylene terephthalate (PET), polyethylene (PE), polypropylene (PP), polyvinyl chloride (PVC), and polystyrene (PS). Circles represent feedstocks, rectangles production/manufacturing, and hexagons the final manufacture stage. Pink processes are common to multiple polymers, while other colors are unique to each polymer family. Renewable energy scenarios are applied only to processes within the grey background region. End of life emissions (landfilling) are not shown in the figure, but are included in the model. Adapted from Posen *et al.* (2016) (Chapter 3).¹⁴⁴

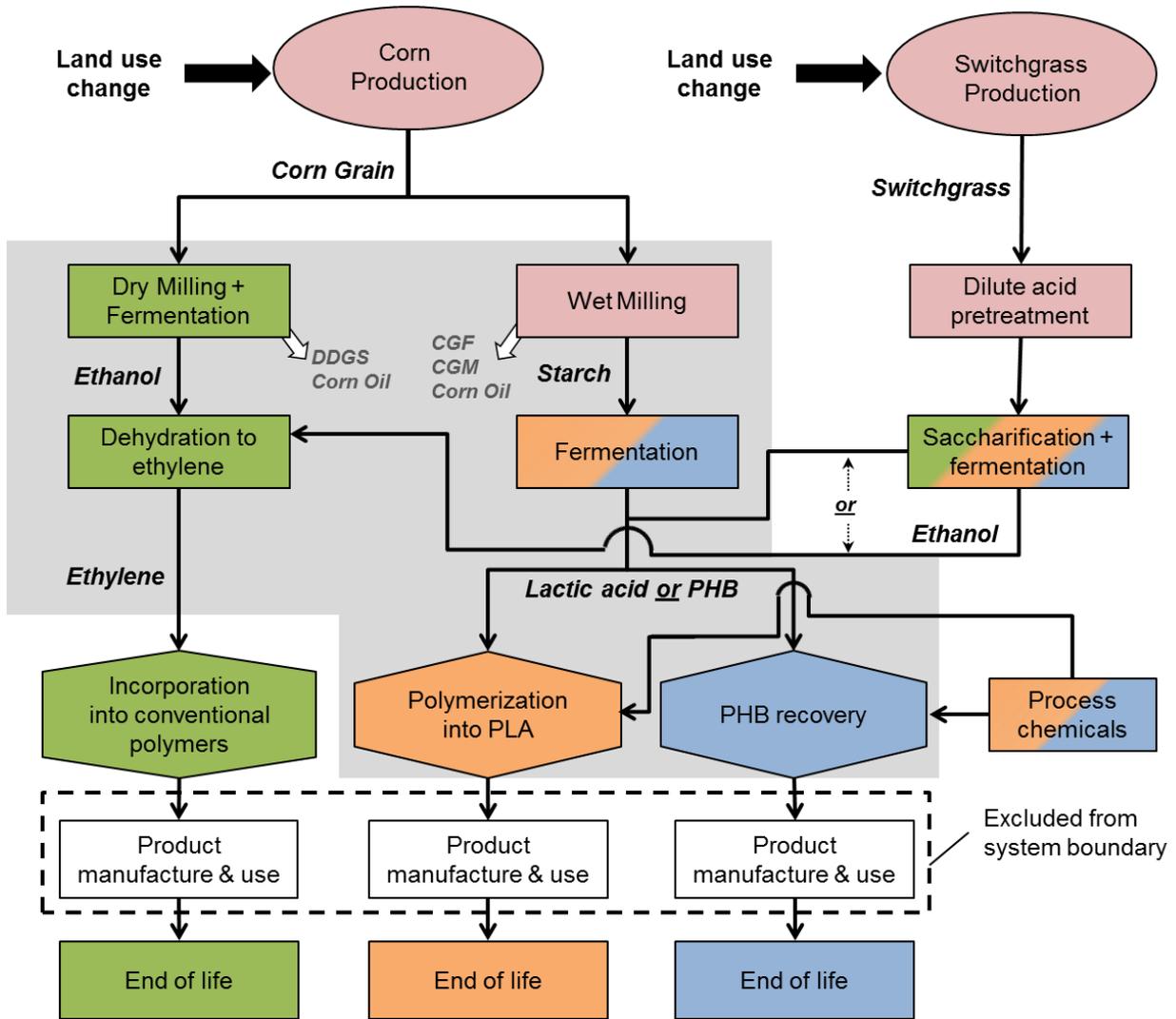


Figure 4.3. Bio-based polymer production processes. Thick black arrows represent market-mediated effects, thin black arrows indicate main reference flows, and white arrows indicate co-product production: dried distillers grains with solubles (DDGS), corn oil, corn gluten feed (CGF), corn gluten meal (CGM), and energy. Circles represent feedstocks, and hexagons are the final manufacture stages, which represent the end of the cradle-to-gate model. All other stages are shown as rectangles. Pink processes are common to multiple polymers and white processes are excluded from the system boundary. Green processes are for producing bioethylene-based polymers, orange for polylactic acid (PLA), and blue for polyhydroxybutyrate (PHB). Boxes with multiple colors indicate equivalent, but separate processes for multiple polymer families. For the LC corn pathway, renewable energy scenarios are applied only to processes within the grey background region. Adapted from Posen *et al.* (2016) (Chapter 3).¹⁴⁴

The primary impact metric in this chapter is the 100-year global warming potential (GWP), modeled using normally distributed equivalence factors (in kg CO₂e) based on the Intergovernmental Panel on Climate Change (IPCC) fifth assessment report (AR5).^{204,205} Posen *et al.* (2016) (Chapter 3)¹⁴⁴ provides a detailed description of the underlying life cycle assessment model. The present chapter uses PLA case 1, based on Groot and Boren (2010)²⁵¹ since the data used for the other cases in Posen *et al.* (2016) (Chapter 3)¹⁴⁴ have insufficient detail to adapt for incorporation of renewable energy. Results for the baseline model (no renewable energy) would be similar (within ~10%) if using Vink *et al.* (2010 or 2015)^{260,262} for the PLA data source. The model for fossil polymers relies on the system expansion scenario (for hydrogen co-product) from Posen *et al.* (2016) (Chapter 3).¹⁴⁴ Similarly, this chapter uses the system expansion scenario for corn-coproducts. For switchgrass pathways, this chapter uses the scenarios from Posen *et al.* (2016) (Chapter 3)¹⁴⁴ that include co-generation of steam and electricity from unfermented residues. To isolate the comparison between feedstock and energy substitution, this chapter does not apply any credit for surplus energy from switchgrass pathways. For switchgrass ethylene, this analysis assumes the more favorable ‘mid-term’ yield scenario.

Key additions to the model, developed for the present study, involve the use of renewable energy (wind, RNG, and/or direct combustion of biomass), discussed in the following section.

4.3.2. Emissions from Renewable Fuels and Electricity

Wind power is one of the most promising and fastest growing sources of renewable generation in the U.S. and worldwide,³⁰² and so is the primary low-carbon electricity source for this case-study. Dolan and Heath (2012)³⁰³ report harmonized estimates of the life cycle GHG emissions from wind power (in g CO₂e/kWh) for 126 estimates representing 49 different studies. I fit a continuous distribution to these 126 point estimates, giving each of the 49 studies the same weight, and equally weighting the different estimates within a given study (e.g. if a study produces 6 different estimates, each of these receives 1/6 the weight of data points from studies that produce only a single estimate). This procedure avoids giving undue weight to studies that produce multiple estimates, since any biases in the method applied are likely to affect each of the

estimates within a single paper. The result is a log-logistic distribution with a mean of 12.4 g CO₂e/kWh and a 90% confidence interval ranging from 4.7-26 g CO₂e/kWh.

For process heat, I assume RNG will be produced from LFG and that it will be transported using existing natural gas transmission infrastructure. RNG is chemically and functionally equivalent to conventional natural gas, and can be produced by isolating methane from the mixture of methane, carbon dioxide, and other contaminants that result from the decay of organic material in landfills. Because its use is easily integrated into existing production processes, RNG is the baseline renewable fuel for on-site heat production in corn and fossil-based pathways in this study.

I model emissions from the production of RNG based on Argonne National Laboratory's Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) 2014 model²⁶⁷ and its supporting documentation.³⁰⁴ Mintz *et al.* 2010³⁰⁴ report the RNG processing efficiency, defined as the ratio of the energy in the final product to the input gas and electricity, to range from 91-97% with a default value of 94.4%. I use these values as the parameters of a triangular distribution. Furthermore, I assume that generation of electricity used to process raw landfill gas (LFG) into RNG relies on the combustion of raw LFG in a reciprocating engine, with an electricity generating efficiency of 30%.²⁶⁷ I calculate emissions from the reciprocating engine using default emissions factors in GREET.²⁶⁷ Additionally, GREET assumes a 2% fugitive emission rate for the input CH₄, at the landfill site. As modeled in GREET, all LFG used as feedstock for RNG, or for energy in the reciprocating engine, receives a credit for avoiding the emissions that would result from just flaring the gas, as is common practice in U.S. landfills.³⁰⁴ I then add in emissions from natural gas transmission, fit approximately to the parameters provided in Tong *et al.* (2015).²⁶⁶ Finally, I model the combustion of RNG the same way as the combustion of conventional natural gas.⁹⁵ Combustion emissions are mostly offset by the credit for avoided flaring. As a result, net emissions correspond predominantly to the emissions from natural gas transmission and from the 2% natural gas leakage during RNG upgrading. The final distribution closely resembles a normal distribution (mean: 17.9, stdev: 4.6 g CO₂e/MJ RNG LHV), with most of the spread stemming from the uncertainty in CH₄ GWP.

Finally, Appendix C (section C.2.1) considers an alternate renewable energy scenario in which switchgrass combustion provides the on-site fuel requirements, instead of RNG. This scenario requires an adjustment for the difference in efficiencies between fossil fuel and biomass boilers. When data sources quote energy requirements in terms of steam energy, I assume that steam was generated from natural gas combustion. Following Abrahams et al. (2015),²⁶⁵ I model natural gas (HHV) boiler efficiency as a triangular distribution (min: 70%, mode: 80%, max: 94%)³⁰⁵⁻³⁰⁷. Biomass boilers have an efficiency between 68% and 75% (HHV), for as-received (wet) biomass.^{305,306,308} Natural gas accounts for a large majority of fuel used in conventional polymer production, and the boiler efficiency range modeled already encompasses the typical range for other fuels like coal.²⁶⁵ Thus, the same efficiency adjustment applies for all fossil energy displaced by biomass. Appendix C, Table C.1 presents key parameters for the modeling of renewable energy pathways in this chapter.

4.3.3. Cost Estimates

Prices of commodity thermoplastics change rapidly with time, and are not generally available in the public domain; this section describes scoping estimates for the cost of the emission reduction strategies considered in this chapter. Sin *et al.* (2013)³⁰⁹ published 2009 average prices (in Euro/kg) for a range of polymers, including PLA, PHB, and most conventional commodity thermoplastics. I convert these estimates to U.S. dollars using the 2009 average exchange rate (0.75 Euro/USD),³¹⁰ and then inflate them to 2015 values (a net increase of 11%).³¹¹ The resulting prices (in 2015 USD/kg) are: 2.82 (PLA), 5.94 (PHB), 1.78 (HDPE), 1.63 (PP), 2.08 (PS), 1.48 (PVC), 2.23 (PET). I assume the average price of LDPE is similar to HDPE. Taking the difference between the price of each biopolymer and each commodity thermoplastic gives the additional cost incurred by end users for converting from fossil polymers to PLA or PHB.

The International Renewable Energy Agency (IRENA) estimated the cost range for producing bioethylene from US corn in 2009 USD/tonne ethylene (min: 1,700, mean: 2,060, max: 2,730).¹⁸⁴ From these values, I subtract \$55/tonne ethanol (~\$95/tonne ethylene) for corn co-products,¹⁸⁴ and inflate the results to 2015 values. I fit the resulting estimates to a triangular distribution (min: 1,780, mode: 2,180, max: 2,930) 2015 USD/tonne bioethylene. The spot price

of fossil ethylene is modeled as a uniform distribution from 35-65 cents/lb (770-1430 \$/tonne), loosely fit to recent market data (from September 2014 to July 2015).³¹²

The cost of converting to low carbon energy relies on estimates of the levelized costs from producing RNG and wind power, which I compare to the case of existing fuel and (wholesale) electricity. The American Gas Foundation (AGF) estimated the cost of producing RNG from LFG on a state by state basis.³¹³ Using their more conservative “non-aggressive” scenario, I fit a distribution to the state-by-state estimates AGF provided. The result is a shifted exponential distribution with mean 2.05 (before shifting), and a minimum value of 5.19 \$/mmbtu. I adjusted this value for inflation (6%) from 2011 (the year of publication) to 2015.³¹¹ The most recently available prices for fossil fuels come from the U.S. Energy Information Administration (EIA) via their excel data add-in tool.³¹⁴ I fit distributions for industrial sector prices for natural gas and residual fuel oil using monthly data and projections from the Short Term Energy Outlook (January 2013-December 2015). I fit quarterly historical coal prices for industrial users to a uniform distribution (January 2013-April 2014). Finally, I treat diesel and distillate as the same, with prices modeled as a triangular distribution fit to historical monthly retail prices, as sold by refiners from January 2013-May 2015.

For the levelized cost of wind energy, I modeled a triangular distribution (min:35, mode: 66, max: 111 \$/MWh), based on data from the Department of Energy’s Open Energy platform.³¹⁵ For grid electricity, I use the 2014 US wholesale price of electricity, fitted to the weighted average price across all dates and regions, as provided by EIA.³¹⁶ The resulting best-fit for US wholesale electricity (in \$/MWh) is a log-logistic distribution (location: 13.7, scale: 31.0, shape: 4.2). The difference between the levelized cost of wind energy, and the US wholesale price of electricity indicates the additional cost incurred by switching to wind power. Appendix C, Table C.2 includes a summary of key parameters used for cost estimation.

4.4. Results

4.4.1. Energy Substitution and Feedstock Substitution: Scale and GHG Emissions

Table 4.1 summarizes production volumes and emissions factors for fossil polymer scenarios, along with the identities of alternative bio-based plastics used for feedstock substitution scenarios. Full energy substitution across the plastics industry would require approximately 12 billion kWh of wind power (~6% of U.S. wind power generation in 2014³¹⁷), and 650 billion MJ of RNG or other suitable renewable fuel. It is worth noting that this value exceeds the approximately 200-400 billion MJ of domestic RNG potential from LFG, but is well within the 1,000-2,500 MJ of RNG potential from all sources.³¹³ Additional analysis also shows that similar or greater GHG reductions can be achieved by supplementing RNG with wind power through increased electrification, or via the combustion of energy crops like switchgrass (Appendix C, section C.2.1). Simply to note the scale of this alternative, full feedstock substitution (i.e., fully transitioning to bio-based polymers) would require approximately 110-120 Mt of dry corn or 130-140 Mt of dry switchgrass. This quantity of corn requires approximately 30-45 million acres and is equivalent to 40% of the 2015 U.S. corn harvest.²⁷⁹ The estimated quantity of switchgrass would require approximately 15-70 million acres of land, with a mean of 30 million acres; this is equivalent to 5-15% of current agricultural land in the U.S.³¹⁸ Switchgrass yields are prospective and thus highly uncertain, which explains the large range for switchgrass land requirements.

Table 4.2 summarizes emissions factors for bio-based plastics. These results combined with those in Table 4.1 produce Figure 4.4, which shows industry-wide GHG emissions for different pathways. Using a 95% confidence interval, adoption of low carbon energy can reduce GHG emissions from plastics production by approximately 50-75% (mean reduction of 38 Mt CO₂e/year). In contrast, corn-based bioplastics (in the lower emission, ‘landfill’ scenario) may result in anywhere from a 50% decrease to a 10% increase in GHG emissions (mean reduction of 16 Mt CO₂e). Emission reductions achieved in the advanced feedstock substitution pathways have wide confidence intervals, but show substantial probability of achieving net negative emissions in the landfill scenario, owing to the GHG emissions credit for carbon stored in the bio-based plastics. Appendix C, section C.2.2 shows more detailed results for individual plastics;

section C.2.3 shows results for select additional scenarios related to allocation and scope of energy substitution.

Figure 4.5 shows a direct comparison of GHG emissions between fossil plastics produced with low carbon energy, and each bioplastic pathway. In over 98% of simulations, producing fossil plastics with low carbon energy results in lower emissions than corn-based bioplastics. Emissions from the corn pathway exceed emissions from the fossil plastic energy substitution pathway by ~20-30 Mt CO₂e (median results) depending on the end of life scenario for PLA. Advanced feedstock substitution likely results in higher GHG savings than energy substitution, but there is more certainty in the landfill scenario (90% of simulations and 99% of simulations, respectively) than in the compost scenario (55% and 75% of simulations, respectively).

These results (Figure 4.4) demonstrate the importance of the stored carbon credit for bio-based products (i.e., it is a large negative contributor to the GHG emissions shown in the figure). In the absence of this credit, all feedstock substitution pathways have higher emissions than the fossil plastic production pathways. Although the stored carbon credit is likely accurate for bioethylene plastics, recent evidence suggests that even when landfilled, PLA does not always act as a carbon sink,^{301,319} as previously assumed.^{144,268,271} Furthermore there is ongoing debate about whether biogenic carbon should receive an emissions credit in the first place;⁹⁹ land use change emissions associated with agricultural production could also greatly surpass those modeled here.^{85,285,286} As a result, the feedstock substitution pathways have a higher degree of inherent uncertainty than presently modeled. In contrast, the low-carbon energy fossil polymer pathways have more steps in common with conventional production, which contributes to fundamentally lower uncertainty for emission differences.

Table 4.1. Summary information for fossil plastics considered in this study.

	Annual North American production volume (Mt)	Conventional emissions factor (kg CO₂e/kg plastic)	Emissions factor with low carbon energy^d (kg CO₂e/kg plastic)	Alternative plastic for feedstock substitution scenarios
High Density Polyethylene (HDPE)	7.9 ^a	1.48 (1.02, 1.96) ^c	0.59 (0.19, 1.01) ^e	bio-HDPE
Low Density Polyethylene (LDPE)	3.2 ^a	1.75 (1.27, 2.25) ^c	0.66 (0.23, 1.1) ^e	bio-LDPE
Linear Low Density Polyethylene (LLDPE)	6.3 ^a	1.48 (1.01, 1.97) ^c	0.65 (0.24, 1.06) ^e	bio-LLDPE
Polypropylene (PP)	7.5 ^a	1.54 (1.14, 1.96) ^c	0.85 (0.5, 1.21) ^e	PP/PLA ^f
Polyethylene (PET)	2.8 ^b	2.39 (2.18, 2.65) ^c	1.03 (0.83, 1.29) ^e	PLA
Polystyrene (PS)^g	2.0 ^a	3.12 (2.78, 3.54) ^c	1.64 (1.28, 2.05) ^e	PLA
Polyvinyl Chloride (PVC)	6.8 ^a	2.19 (1.92, 2.49) ^c	0.63 (0.36, 0.92) ^e	bio-PVC

a) Year 2014 data; source:¹⁴²

b) Year 2012 data; source:¹⁴³

c) Mean and 95% confidence interval (CI) for each plastic; source: ref¹⁴⁴ (Chapter 3)

d) Wind and RNG

e) Mean and 95% CI for each plastic; new estimate, based on model from ref¹⁴⁴ (Chapter 3)

f) PLA only replaces PP in the advanced feedstock substitution scenarios (corn with low carbon energy or switchgrass), since switching to PLA would not reduce emissions in the conventional (corn) pathway

g) PS is modeled as general purpose polystyrene (GPPS). Results for high-impact polystyrene (HIPS) are very similar.

Table 4.2. Mean and 95% CI emissions factors for bio-based plastics considered in this study (kg CO₂e/kg plastic).

	Corn bioplastics^b (kg CO₂e/kg plastic)	Corn bioplastics with low carbon energy^c (kg CO₂e/kg plastic)	Switchgrass bioplastics^d (kg CO₂e/kg plastic)
PLA^a	1.85 (1.43, 2.34)	0.09 (-0.21, 0.46)	0.25 (-0.27, 0.92)
bio-PVC	1.92 (1.52, 2.39)	1.26 (0.91, 1.69)	1.34 (0.81, 2.1)
bio-HDPE	0.89 (0.11, 1.82)	-0.55 (-1.22, 0.29)	-0.38 (-1.46, 1.25)
bio-LDPE	1.14 (0.35, 2.1)	-0.32 (-1, 0.54)	-0.14 (-1.24, 1.52)
bio-LLDPE	0.89 (0.1, 1.83)	-0.57 (-1.24, 0.28)	-0.39 (-1.48, 1.25)

- a) Based on case 1 from;¹⁴⁴ table shows emissions assuming that PLA is landfilled and acts as a carbon sink. Composting PLA releases an additional 1.6 kg CO₂e/kg plastic.
- b) Treating co-products by system expansion; from ref¹⁴⁴ (Chapter 3).
- c) Treating co-products by system expansion; plastic production powered by wind and RNG; new estimates, based on model from ref¹⁴⁴ (Chapter 3).
- d) Assumes non-fermented residues are used to generate steam and electricity; no credit for surplus energy generation; bioethylene-based plastics assume mid-term yield scenario from ref¹⁴⁴ (Chapter 3).

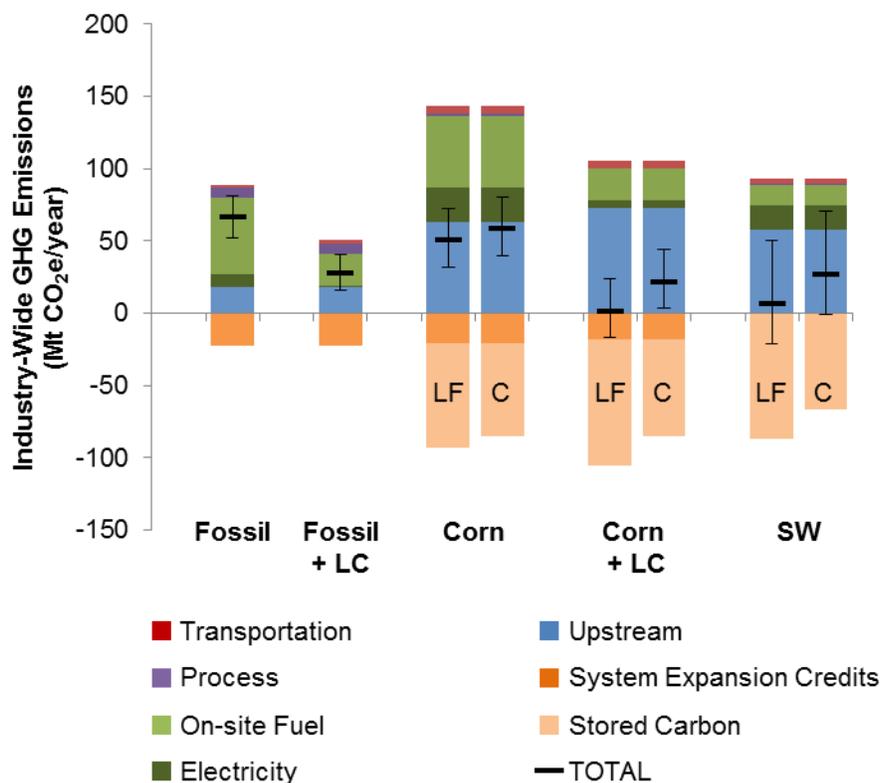


Figure 4.4. Life cycle GHG emissions from aggregate North American production of a) conventional fossil-based commodity thermoplastics (“Fossil”), b) fossil plastics using low carbon energy sources (wind and RNG) across the chemical industry supply chain (“Fossil + LC”), c) corn-based plastics (“corn”), d) corn-based plastics using wind and RNG (“Corn + LC”), or e) switchgrass-based plastics (“SW”). Feedstock substitution scenarios assume all conventional plastics are replaced with alternative plastics as per table 1; these scenarios show results for both landfilled (“LF”) and composted (“C”) PLA. Upstream emissions refer to oil and gas extraction and refining/processing for fossil routes, or land use change and biomass production for bio-based routes. Error bars represent an approximate 95% confidence interval for total emissions, based on Monte Carlo simulation. All results assume current production volumes (production volumes from 2012-2014).

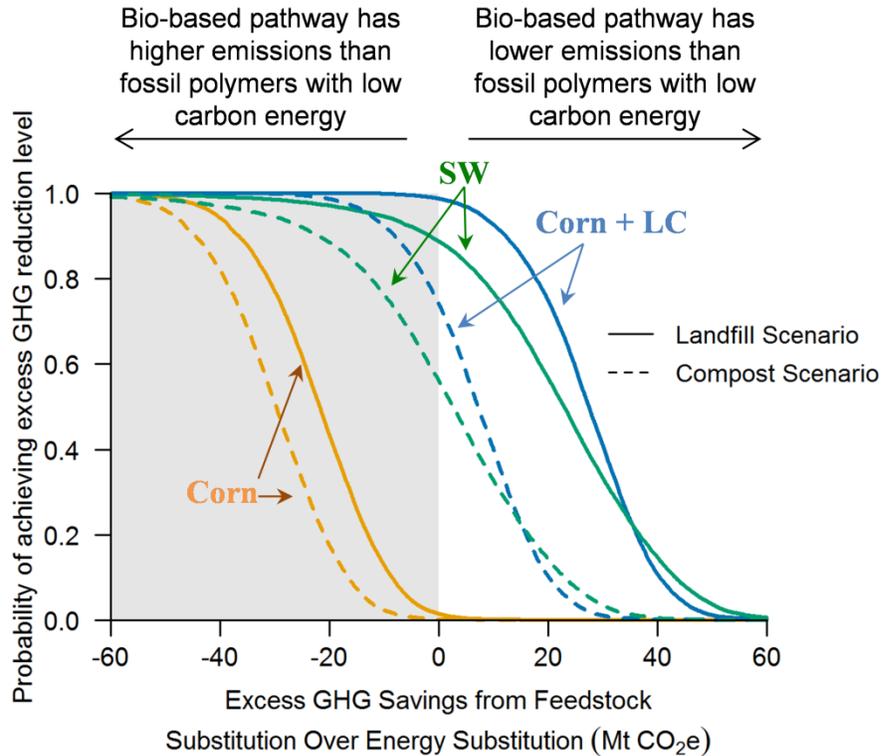


Figure 4.5. Life cycle GHG emissions comparison between energy substitution and different feedstock substitution scenarios, including corn-based plastics (“corn”), corn-based plastics produced using wind and RNG (“Corn + LC”), and switchgrass-based plastics (“SW”), with PLA disposal by either landfill or compost. Positive numbers (white background) indicate the feedstock substitution scenario has lower GHG emissions than the energy substitution scenario. Negative numbers (grey background) indicate the energy substitution scenario has lower GHG emissions than the feedstock substitution scenario.

4.4.2. Cost estimates

Table 4.3 presents results from the first-order cost estimates discussed in section 4.3.3. The cost of converting to low-carbon energy ranges from \$10-\$200/tonne plastic, whereas the cost of switching to bio-based polymers likely ranges from several hundred to several thousand dollars per tonne, depending on the plastic. The cost estimates for bio-based polymers are based on presently available (first generation) feedstocks. It is likely that use of a cellulosic feedstock (like switchgrass) would be even more cost-disadvantaged than these numbers indicate. Thus, adopting low-carbon energy is currently more economic than switching to bio-based polymers, reinforcing the GHG emission results that favor energy substitution for near-term GHG

mitigation. As industry gains experience with these bio-plastics, their costs may decrease through learning-by-doing and economies of scale.

Table 4.3. Cost of emission reduction strategies (\$ additional / tonne of plastic). Values represent additional costs incurred, above those estimated for conventional production. Ranges, where available, span 90% of model runs.

	PET	PS	PVC	HDPE	LDPE	PP
Low carbon energy (full supply chain)	10-120	20-200	30-180	15-120	20-160	10-90
Corn Bioethylene	200-600	300-1000	400-1,500	900-3,000	900-3,000	N/A
PLA	~600	~700	~1,300	~1,000	~1,000	~1,200
PHB	~3,700	~3,900	~4,400	~4,200	~4,200	~4,300

4.4.3. Comparing uses for switchgrass

The potential to use biomass as either a feedstock or energy source also raises questions about the best use of biomass for near-term GHG mitigation. Figure 4.6 presents the results of a first-order test case for uses of switchgrass, structured to provide a relatively optimistic scenario for bioplastics. The model compares switchgrass combustion to the lowest GHG emission fossil fuel, natural gas; it assumes full recovery of all residue from fermentation to make bioplastics, and that this residue also displaces natural gas; it uses the higher yielding and lower energy use scenarios for bioethylene and PHB production from Posen *et al.* (Chapter 3)¹⁴⁴; finally the model is on a cradle-to-gate basis, which implicitly assumes that bioplastics act as a carbon sink. This last assumption is likely accurate for bioethylene, is uncertain for PLA, and likely underestimates emissions from PHB. With the exception of PLA displacing certain high emission polymers (e.g. PS and PET), equal or greater mean emission reductions can be achieved by using a given quantity of switchgrass for energy instead of for bio-based polymers. This is particularly notable since assumptions were deliberately favorable to bioplastics. This result reinforces the main conclusion of the chapter: focusing on energy substitution will likely achieve greater GHG emission reductions in the near-term than feedstock substitution.

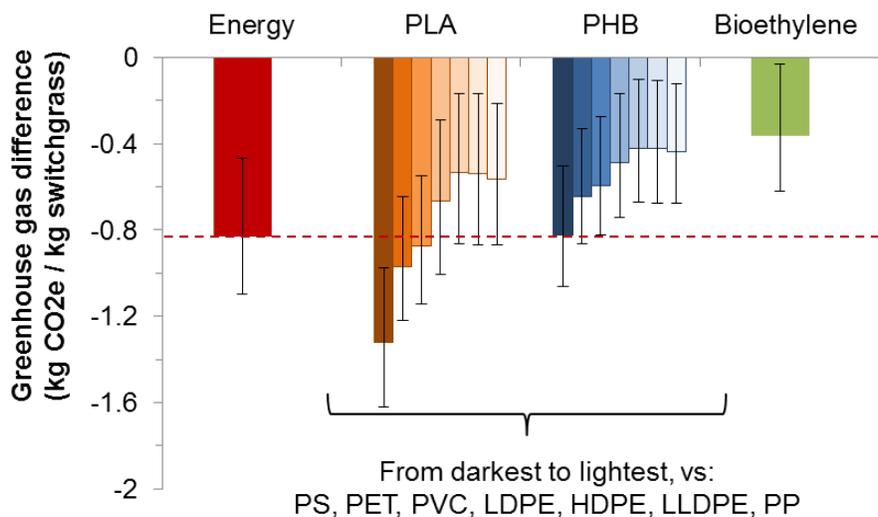


Figure 4.6. Comparison of uses for switchgrass. The graph shows the net change in GHG emissions when 1 kg of switchgrass is i) combusted to displace natural gas, ii) used to produce PLA to displace different thermoplastic fossil polymers, iii) is used to produce PHB to displace different thermoplastic fossil polymers, or iv) is used to produce bioethylene to displace fossil ethylene. Bio-product scenarios show results on a cradle-to-gate basis, and assume that all unfermented switchgrass is also used to displace natural gas. The dotted line is shown as a reference point.

4.4.4. Projected emissions: energy substitution won't be enough

The results presented above make a compelling case to prioritize energy substitution over feedstock substitution. Over the long-run, however, it may be necessary to find other ways to reduce emissions in the plastics industry. Figure 4.7 shows projected GHG emissions due to North American production of commodity thermoplastics, from 2015-2050. The figure shows two scenarios: one in which all plastics are produced using conventional energy, and one in which all plastics are produced using low carbon energy (wind and RNG). The figure shows results based on the mean GHG emissions from the model developed in this chapter.

Additionally, I assume a range of 1-3% in per capita plastics consumption, the upper end of which is consistent with recent historical growth, from 2005-2015.³²⁰ I also project population growth based on the U.S. census.³²¹ As per the results presented above, switching to low carbon energy can produce a substantial and immediate reduction in GHG emissions. If, however, plastics consumption continues to grow at, or even somewhat below historical rates, GHG emissions from the low carbon pathways would once again surpass current levels by 2050. Given

that advanced feedstock substitution scenarios have the potential reduce plastic emissions to zero or less (i.e. becoming a net CO₂ sink), it could be advantageous to develop these pathways in the long run.

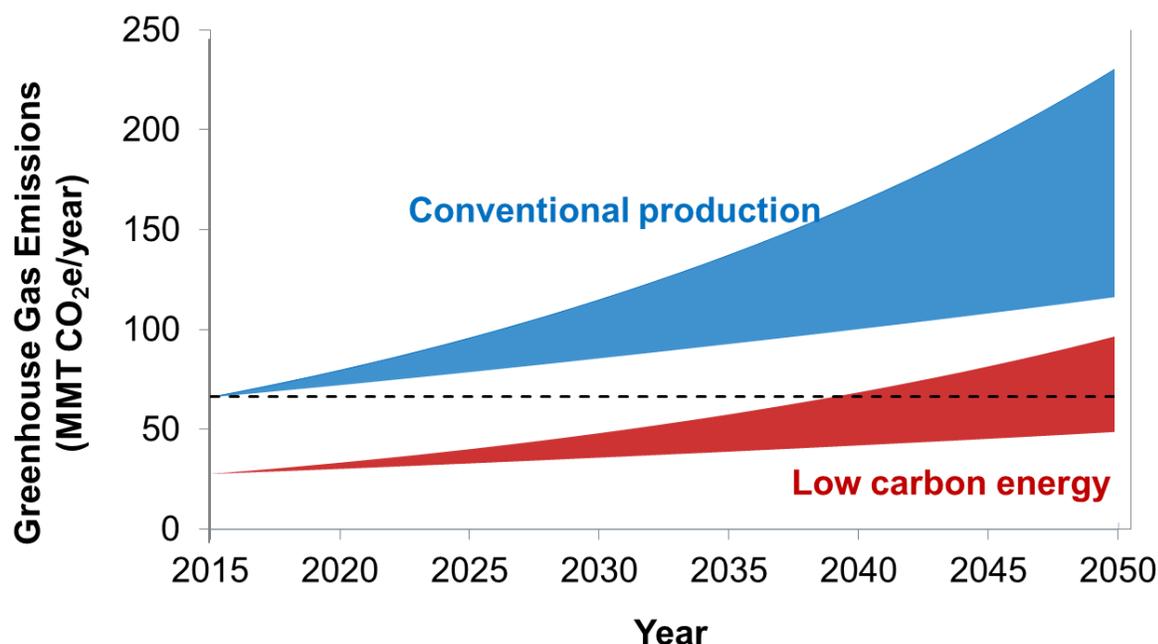


Figure 4.7. Projected emissions from the North American plastics industry under a conventional production and a low carbon energy scenario, respectively. The figure uses mean emissions for each scenario, and shows a future emission range based on a 1-3% annual growth in per capita plastic consumption.

4.5. Discussion

Although a comprehensive sustainability analysis is beyond the scope of this study, there are numerous other factors to consider in comparing feedstock and energy substitution in the plastics industry. The following is a limited discussion of several key considerations:

- Non-GHG environmental impacts: Due to heavy reliance on agriculture, bio-based products tend to score poorly on other environmental metrics, such as ozone depletion,^{152,257} acidification,¹⁵³ eutrophication,^{152,153,257,322} water use,³²³ and food security.^{126,127,324}

- **Substitutability:** Energy substitution results in no change in the final resin produced. The new, ‘greener’ polymer can substitute across the market without any changes in downstream production methods or product functionality. While this is also the case for bioethylene-based plastics, other renewable products like PLA have more limited potential to substitute for existing plastics.
- **Resin Properties:** While biodegradability may be an advantage of PLA (and some other bio-plastics), as this may reduce landfilling requirements, few cities have the required infrastructure for composting,¹⁵² and many organizations using compostable biopolymers continue to send their waste to landfills.³²⁵ Further, biodegradation increases the life cycle GHG emissions of these bio-based plastics, potentially overturning any benefits from their production.^{144,270} As a further caveat, this study does not include emissions from resin foaming or plasticizer and other additives, which may affect the comparison between PLA and fossil plastics. To my knowledge, no prior studies have included these emissions.
- **Market size:** the potential market for renewable energy, and resulting potential emission reductions, is far larger than the potential market for bio-based polymers. Thus, energy is likely a more important target for decarbonization than feedstocks, especially if learning or spillover effects³²⁶ are expected.

The choice for near-term GHG mitigation is clear: switching to low-carbon energy across the chemical industry for conventional polymers achieves greater GHG reductions (in >98% of simulations), at lower cost, and with less uncertainty than corn-based biopolymers (if produced with conventional energy). This energy substitution can be achieved without any fundamental modification to current production methods, existing capital infrastructure in the chemical sector, or additional testing to ensure preservation of product quality, as would be the case for switching to bio-based plastics. In the long-run, if advanced bio-based plastic pathways prove technically and economically feasible, feedstock substitution may substantially reduce or even capture GHG emissions. For these benefits to be realized, however, bio-based production must be coupled with renewable energy – either explicitly (as above), or through recovery of fermentation residues from cellulosic production.¹⁴⁴ Until such advanced bio-plastic pathways are available, energy substitution has the greater potential.

Chapter 5. Biofuels and Indirect Output Use Change: the Role of Refineries

5.1. Abstract

In recent years, there has been a growing awareness that traditional attributional life cycle assessment may not be an appropriate tool for capturing the greenhouse gas emissions that result from biofuel policies. A nascent literature takes a consequential approach toward capturing the indirect change in consumption of petroleum products that results from different policy choices. Common to these prior studies, however, is poor resolution in the modeling of the petroleum refining sector. To address this shortcoming, this chapter develops a model of how petroleum refineries change their product slate in response to market conditions. Using a set of dynamic regression models (e.g., partial adjustment and adaptive expectations models) with monthly data for the United States, I estimate that the relative yield of distillate exhibits price elasticities of approximately 0.40 to 0.50 relative to its own price, and -0.42 to -0.34 relative to the price of gasoline. In contrast, gasoline has smaller yield elasticities of approximately 0.17 to 0.20 relative to its own price, and -0.25 to -0.22 relative to the price of distillate. Using these estimates in a partial equilibrium environment, I show that biofuel share mandates and emission standards can induce refiners to shift toward greater distillate production. This results in a large increase in greenhouse gas emissions, even before accounting for the emissions from biofuel production itself. This work suggests that refiner flexibility is a potentially important source of carbon leakage. As a result, share mandates and emission standards that apply disproportionately to gasoline consumption may be ineffective policies for reducing GHG emissions. Policies like a carbon tax that apply more evenly across petroleum products, and create a price wedge between producers and consumers are far more likely to result in emission reductions.

5.2. Introduction

Much of the analysis presented in chapters 2-4 above follows an attributional life cycle assessment framework (ALCA). Although ALCA is frequently used in policy decisions, it is properly viewed only as a form of environmental accounting; it does not necessarily predict actual changes in emissions that would result from increased production of bio-based products.

The ALCA approach is, however, indicative of the emissions that may be attributed to the products under study (taken in isolation from market forces) and as such provides a simple and consistent basis to establish how pathways perform relative to one another.

Recently, however, the usefulness of ALCA has been called into question, with some authors arguing that policy decisions require a more consequential approach.⁷⁵ The formal distinction between ALCA and consequential LCA (CLCA) was introduced at a 2001 workshop,⁷⁶ and continues to grow in popularity. In brief, while ALCA accounts for environmental flows in a static environment, CLCA attempts to answer how such flows will change in response to new decisions or activities. Elements of CLCA have been incorporated into Chapters 2-4 (e.g. inclusion of emissions from indirect land use change, examining how results vary with marginal electricity emissions as part of a sensitivity analysis, and so on), however only a preliminary analysis of wider market interactions was conducted.

One particularly important and understudied market-mediated interaction is the change in net output for different final products, in response to policy actions. For example although bio-products can often substitute for fossil products on a 1:1 basis in physical terms, the resulting changes in market prices make 1:1 replacement unlikely across the entire market. This effect is rarely addressed in existing LCA studies. A nascent literature examines this effect in fuel markets, in what is alternately termed the indirect fuel use effect (IFUE),²³⁶ market leakage,³²⁷ indirect output use change (IOUC),³²⁷ indirect demand change (IDC),¹⁵⁴ or the rebound effect in fuel markets.³²⁸ Existing modeling efforts to quantify IOUC resulting from US and European biofuel policies are summarized in a review by Smeets *et al.* (2014).³²⁸ Studies have used both partial equilibrium and general equilibrium frameworks, and have considered a wide range of related policy interventions. All but one³²⁹ assume competitive markets. Depending on the specific policy considered, and modeling framework, reported IOUC values range from -20% to 119% (i.e. 1 unit of biofuel may displace up to 1.2 units of fossil fuel, or may cause a net increase in fossil fuel consumption of 0.19 units).³²⁸ An additional study by Rajagopal and Plevin (2013)³³⁰ used a partial equilibrium framework together with Monte Carlo simulation to include parametric uncertainty for key market elasticities and GHG intensities of different fuels (the only

study to do so). The authors report 95% confidence intervals for IOUC ranging from approximately -50% to 70% depending on the policy considered.

Common to all of these prior studies is poor resolution in the modeling of the fossil fuel sector. Most treat the fuel sector either as a single product, or as multiple products (i.e. gasoline, diesel and other) that can only be produced in fixed proportions. Similarly, most treat crude oil as a single commodity, or consider at most two types of crude oil (i.e. conventional crude and oil sands). This chapter provides a better understanding of how market forces affect the change in GHG emissions resulting from biofuel policies by investigating how the oil industry is likely to respond to shifting demand for individual refined products. The remainder of this chapter is organized as follows: section 5.3 discusses the degree to which the petroleum refining industry can and does change its product slate in response to market conditions. Section 5.4 lays out the model that this chapter uses to investigate the importance of refiner flexibility in assessing biofuel policies. Section 5.5 presents the main results for this chapter. Finally section 5.6 provides additional discussion and concluding thoughts.

5.3. Analysis of Refiner Response

The goal of this section is to determine the degree to which the petroleum industry can adjust its product slate in response to market conditions. Section 5.3.1 first presents an overview of historic and potential relative product yields, followed by section 5.3.2, which presents a quantitative assessment of U.S. petroleum product yield elasticities with respect to product prices. Throughout this chapter, all reported yields are on a volume basis; non-liquid products are converted to volumes using default conversion factors from EIA.³³¹ Further, all analysis presented below measures refinery yield as a percent of total refinery production (i.e. relative yield), rather than as a percent of input crude oil (i.e. absolute yield); these two measures can differ due to the ~6-7% volume gain that typically results from petroleum refining. Unless otherwise specified, the term ‘yield’ hereafter refers to relative yield.

5.3.1. Preliminary Analysis

The U.S. Energy Information Administration (EIA) provides data on international production of major petroleum products going back to the 1980s.¹¹⁷ Figure 5.1 provides a graphical representation of this data, as a percent of total refinery production. While there is a notable increase in the yield of diesel over time, the yield of gasoline has been remarkably stable. The aggregated nature of global yields, however, masks large international variations. Figure 5.2 shows the annual breakdown of refinery yields for individual countries going back to 1980, as based on EIA data.¹¹⁷ For reference, the figure also shows the U.S. and global average yields for the year 2007, the year in which the current U.S. Renewable Fuel Standard was established,⁴ and the base year of analysis for the economic modeling described in sections 5.4 and 5.5.

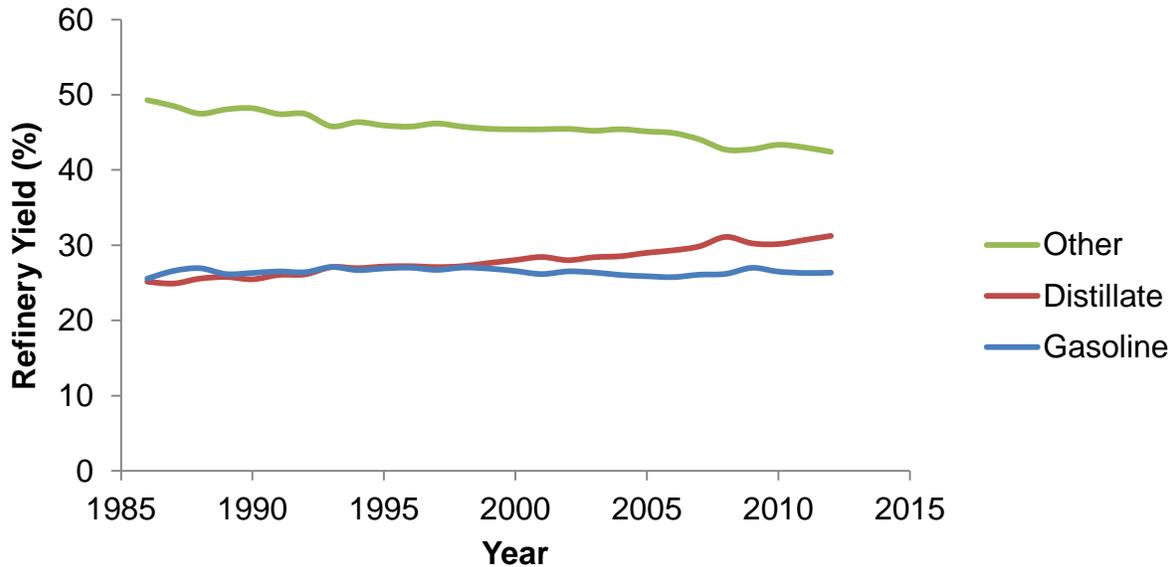


Figure 5.1. Historic volumetric global yields of major refinery product categories. Refinery yield is expressed as a percent of total refinery products. Figure is based on EIA data.¹¹⁷

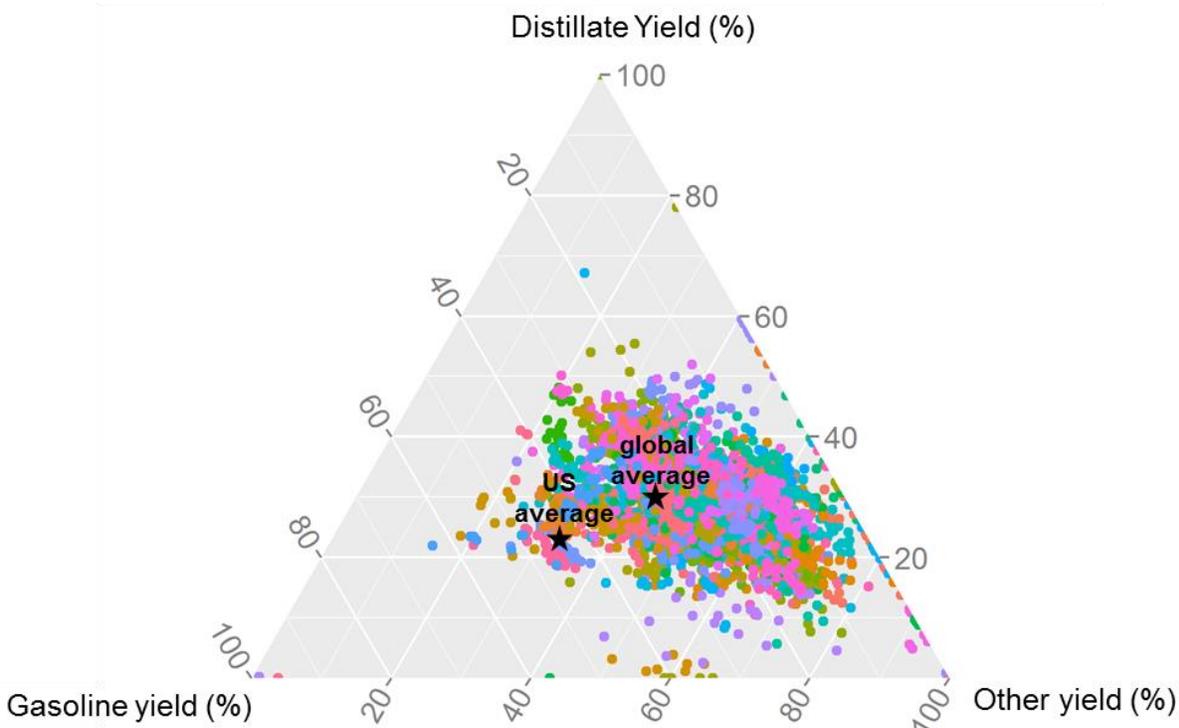


Figure 5.2. International volumetric yields of major refinery product categories for 113 different countries and regions, from 1980-2013. Refinery yield is expressed as a percent of total refinery products. Data is colored by country; each point represents a different country/year combination. The yield of each product is represented by the proximity of each data point to the corresponding vertex. The 2007 US average and global average yields are shown for reference. Figure is based on EIA data EIA data.¹¹⁷

Figure 5.2 clearly demonstrates that refineries can and do achieve a wide range of product slates. To understand how this might be achieved, as well as whether more extreme yields are possible, I investigate product slates predicted by the Petroleum Refinery Life Cycle Inventory Model (PRELIM) refinery model.¹⁶³ The present analysis uses an April 2016 version of the model obtained directly from the model developer. PRELIM simulates refinery yields, energy use and emissions for 10 different refinery configurations with differing levels of complexity: a simple hydroskimming refinery (PRELIM configuration 0), refineries containing medium conversion process units (PRELIM configurations 1-3), deep conversion coking refineries (configurations 4-6) and deep conversion hydrocracking refineries (PRELIM configurations 7-9). The model also contains 103 different built-in crude oil assays, representing different types of petroleum. I run each type of crude oil through each available configuration and record volumetric product yields. The resulting data are plotted in Figure 5.3 Additional refiner flexibility may be possible due to changes in refinery operating conditions, however this is left as a question for future work.

PRELIM was designed primarily with the U.S. refining sector in mind. While it appears to have relatively poor coverage of the low-gasoline yield region, it nevertheless shows a similarly wide feasible region as the actual international data from Figure 5.2. Taken together, these figures suggest that it is possible to produce gasoline yields from below 10% up to nearly 60%, and distillate yields from below 10% up to approximately 50%. While it is unlikely the entire industry could produce at the extremes of these ranges, there nonetheless appears to be substantial room to adjust product yields from the status quo, assuming unlimited access both to different types of crude oil and different refinery process units. In the short run, market sources suggest that individual refineries can only adjust their product slates by less than 5 percentage points.³³² Industry wide flexibility will be higher due to the potential for some refineries to ramp up production while others ramp down; additionally, long-term the industry clearly has access to a wider range of product slates as evidenced by Figure 5.2 and Figure 5.3.

Figure 5.3 also suggests that increasing refinery complexity tends to increase the yields of both gasoline and distillate together (i.e. higher numbered configurations tend to move up and to the left in the ternary plot). In contrast, the choice of crude oil processed allows for a more direct trade-off between gasoline and distillate production – especially within more complex refineries. This conclusion is confirmed quantitatively using product covariance matrices from the PRELIM data (Appendix D, Table D.9 and Table D.10): for most refinery configurations, there is a negative covariance between gasoline and diesel yields across different crude oil types; for most crude oil types, there is a positive covariance between gasoline and diesel yields across different refinery configurations.

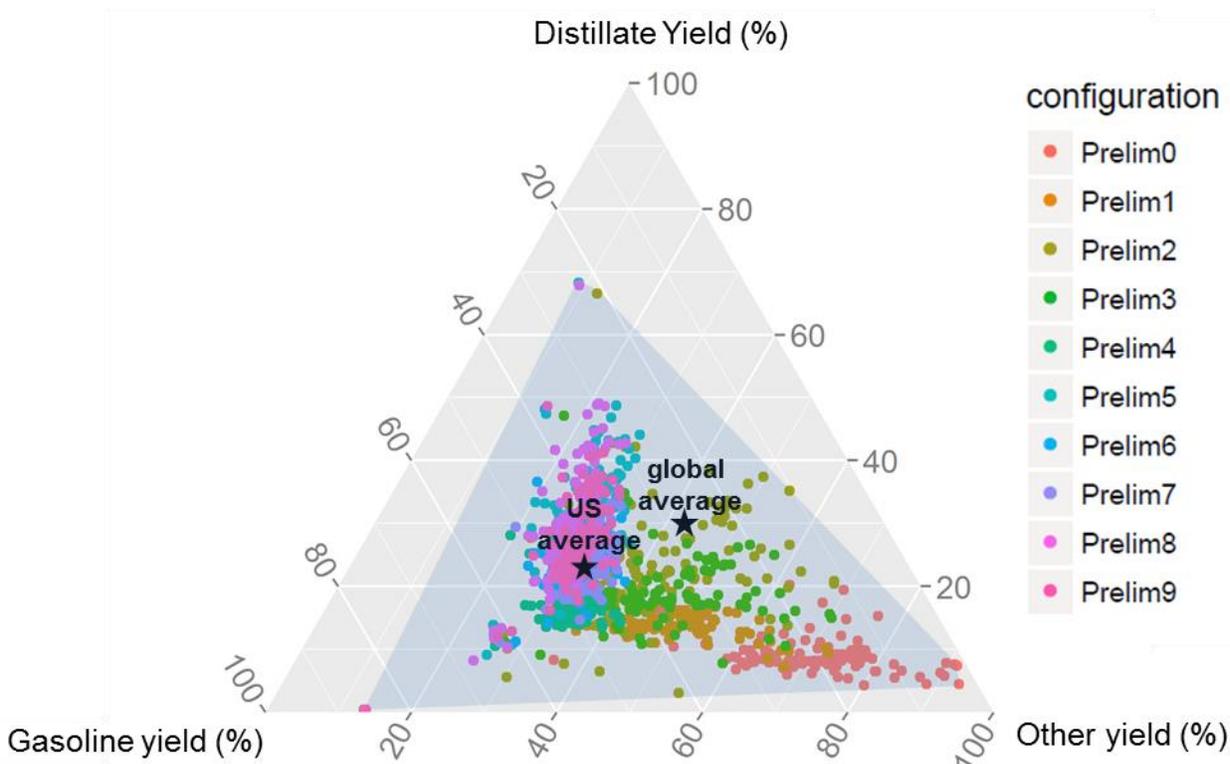


Figure 5.3. Volumetric yields of major refinery product categories predicted by the PRELIM¹⁶³ model. The yield of each product is represented by the proximity of each data point to the corresponding vertex. Each point represents a different crude oil and refinery configuration combination. Different colors represent different refinery configurations, as defined in PRELIM. The light blue polygon indicates the feasible region, for all convex combinations of product slates. The 2007 US average and global average yields are shown for reference.

5.3.2. Quantitative Regression Analysis

Having established that substantial refiner flexibility exists in theory, this section examines specifically how relative yields of petroleum products vary in response to changes in product prices. Existing literature on the subject is extremely limited, especially within the last several decades. Across a series of publications in the early 1980s, Dahl and Laumas used nationally/regionally aggregated annual data to investigate the price responsiveness of gasoline's share of a barrel of crude oil in the U.S., Canada and Europe.³³³⁻³³⁵ These results are summarized in Table 5.1. In a related series, Considine derives a multiproduct cost function for petroleum refining,³³⁶⁻³³⁸ from which yield elasticities can theoretically be derived following the method outlined in Dahl and Duggan (1996).³³⁹ Based on Considine (1992)³³⁶ and ignoring cross-price

elasticities Dahl and Duggan (1996),³³⁹ report gasoline's share elasticity as +0.57 (with respect to its own price); following the same method for distillate gives a share elasticity of +1.20 (with respect to the price of distillate). Correcting the method in Dahl and Duggan (1996),³³⁹ to account for cross-price elasticities and fully applying the chain rule leads to implausibly large yield elasticities, often with unexpected signs. This is likely due to high standard errors among certain input regression coefficients; thus, this method is not pursued further. Various other papers have estimated supply elasticities of petroleum products (e.g., as reviewed in ref³³⁹) or refinery cost functions (e.g., ref³⁴⁰), but from which yield elasticities are not readily derived. Some authors explicitly note their data suggest that refiners alter their product mix in response to price changes (e.g., ref³⁴¹); however, to my knowledge, there have been no recent attempts to quantify this effect using market data.

Table 5.1. Previous estimates of the responsiveness of refinery product yields with respect to petroleum product prices.

Source	Region	Elasticity of gasoline yield with respect to price of			
		<i>Gasoline</i>	<i>Distillate</i>	<i>Residual Fuel Oil</i>	<i>Kerosene</i>
Dahl (1981) ³³⁵	U.S.	+0.20	-0.16	-0.04	NA ^a
	Canada	+0.41	-0.61	+0.20	NA ^a
	Europe	NS ^b	NS ^b	NS ^b	NA ^a
Dahl and Laumas (1981) ³³⁴	U.S.	+0.08	-0.11 ^c	-0.07	NS ^b
Dahl and Laumas (1984) ³³³	Canada	+0.28	NS ^b	+0.27	-0.49

a) NA = not included in regression model

b) NS = Not significant (regression coefficient is not significantly different from zero)

c) Summing the coefficients for distillate and kerosene, and attributing the result primarily to distillate.

This chapter develops new estimates of refiner product yield elasticities based on U.S. data. The U.S. Energy Information Administration (EIA) provides data on product yields from crude oil refining,³⁴² dating back to 1993, along with prices received by refiners for finished petroleum products (for resale).³⁴³ The data is available on a monthly or annual basis, and as both as a national U.S. average, or subdivided by petroleum administration defense districts (PADDs). The

general strategy taken in this chapter is to develop a pair of seemingly unrelated regression equations³⁴⁴ to determine the elasticity of gasoline and diesel yields, as a function of gasoline and diesel prices. The joint yield of all other products is then calculated in function of changes to the gasoline and diesel yields. This decision is justified below. As a simplification, the terms ‘distillate’ and ‘diesel’ will be used interchangeably throughout this section.

As discussed above, the main models estimate the elasticity of gasoline and diesel yields, as functions of gasoline and diesel prices; the joint yield of all other products is then calculated from gasoline and diesel yields. This approach guarantees that yields always balance to 100%, while respecting the product categories (gasoline, diesel and ‘other’) present in the partial equilibrium model described in section 5.4.1. In addition to gasoline and diesel prices, EIA also provides pricing information for a subset of other petroleum products, including residual fuel oil, jet fuel, and propane. Due to high correlations among petroleum product prices, inclusion of these other prices tends to decrease the stability of regression coefficient estimates. Moreover, preliminary analysis suggests that the relationship between product yields and these ‘other’ product prices are generally weak and are often in the reverse direction from what would normally be expected. For example, Figure 5.4 shows that the gasoline/diesel yield ratio responds strongly and essentially monotonically to the gasoline/diesel price ratio. In contrast, Figure 5.5 shows that ratios involving other products are far less regular. The yield ratio of gasoline to ‘other’ products (panel a) actually appears to have a negative relationship with the ratio of the gasoline price to a basket I create of other product prices (weighted by the relative production volumes of these other products). The yield ratio of diesel to ‘other’ appears to be weakly increasing in the corresponding price ratio (panel c), but the relationship is noisy and essentially flat over a large portion of observations. It is possible that these weak relationships simply reflect the noise created by aggregating all other products into a single category. To test this hypothesis, I also compare gasoline and diesel yields to the ‘other’ product with which each has the strongest relationship: liquefied petroleum gases (LPG) and residual fuel oil, respectively (see correlation matrix in Appendix D, Table D.8). These results, presented in Figure 5.5 panels b) and d), once again show only a weak, and potentially unexpected inverse relationship between price ratios and yield ratios. As a result, I conclude that refiners are responding primarily to gasoline and diesel prices, treating other products only as bi-products. Appendix D, section D.1.2

examines sensitivity to the inclusion of other product prices in the main regression model presented below.

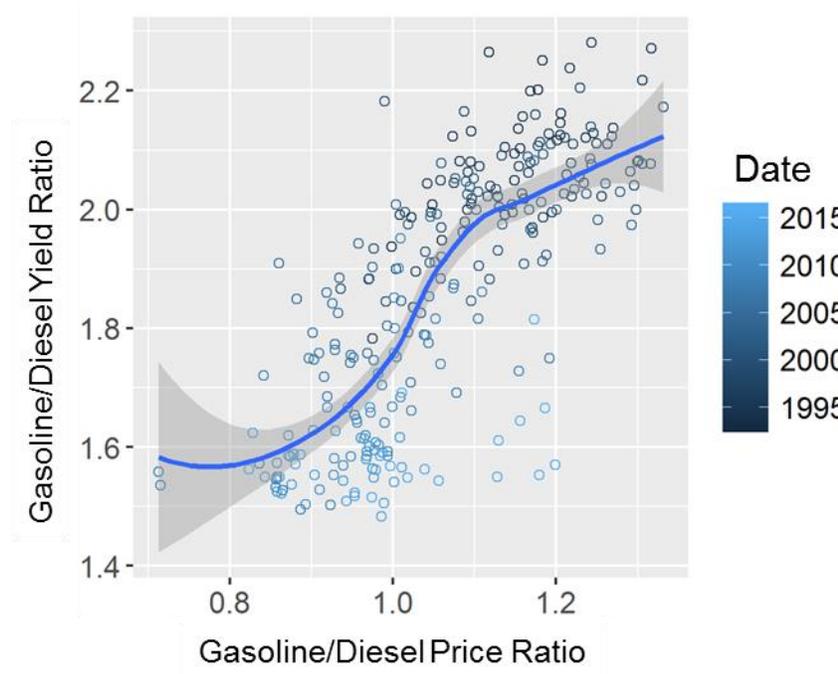


Figure 5.4. Gasoline/diesel yield ratio as a function of the gasoline/diesel price ratio using nationally aggregated U.S. monthly data. A non-parametric smoother is added as a visual aid. Lighter points represent more recent data.

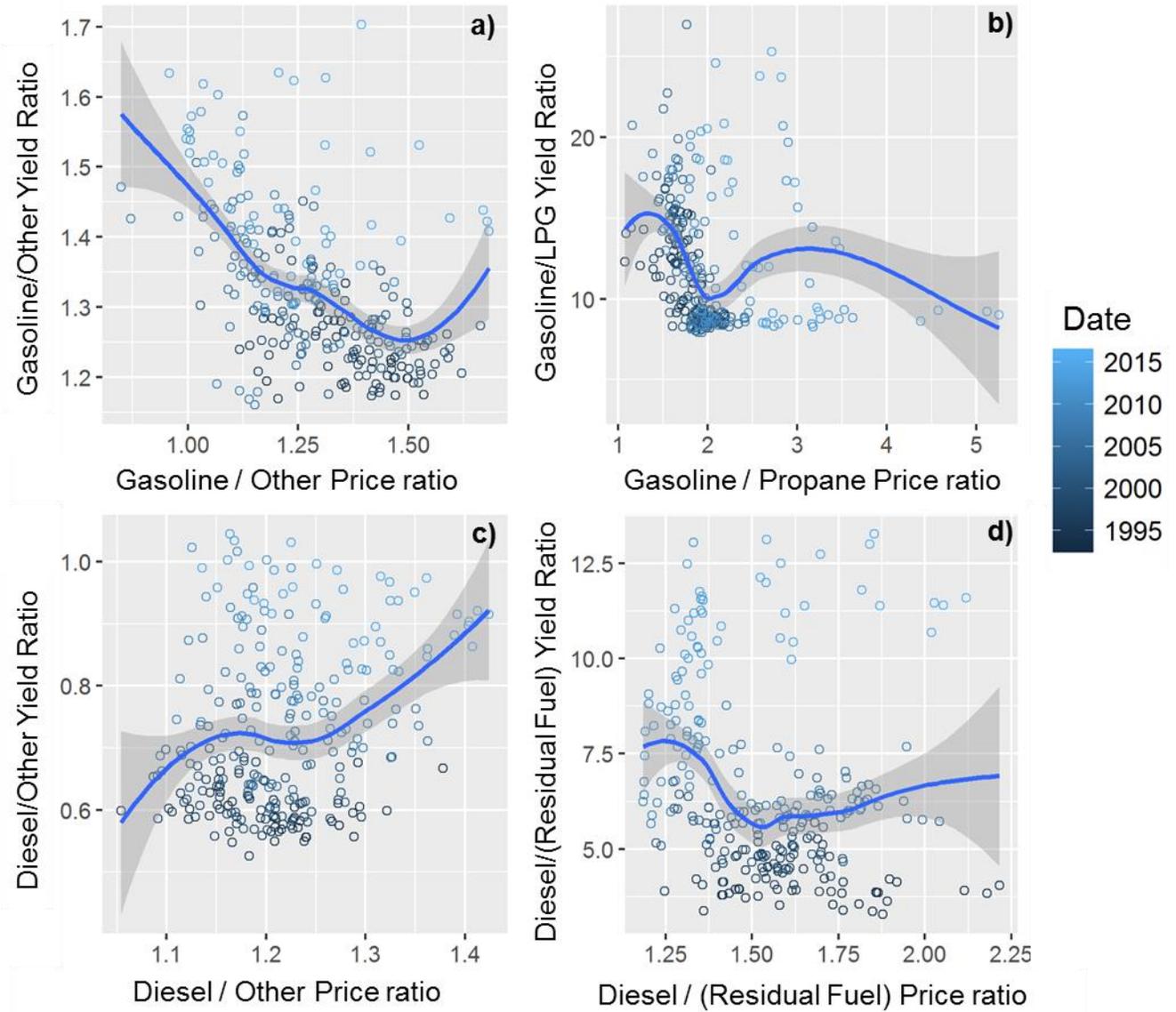


Figure 5.5. Different product yield ratios as a function of their price ratios, using nationally aggregated U.S. monthly data: a) gasoline vs ‘other’ products, b) gasoline vs liquefied petroleum gases (LPG), c) diesel vs ‘other’ products, d) diesel vs residual fuel oil. A non-parametric smoother is added to each plot as a visual aid. Lighter points represent more recent data.

The main models presented in this chapter use monthly data, at the national scale. Additional models are presented in Appendix D, section D.1.2. In its simplest form the regression model appears as follows:

$$\log(\beta_g) = a_0 + a_1 * \log(p_g) + a_2 * \log(p_d) + a_3 * t + a_4 * M \quad (5.1)$$

$$\log(\beta_d) = b_0 + b_1 * \log(p_g) + b_2 * \log(p_d) + b_3 * t + b_4 * M \quad (5.2)$$

where β_g and β_d are respectively the gasoline share and distillate share of total refinery output, p_g is the price of gasoline received by refiners, p_d is the price of distillate received by refiners, t represents a deterministic time trend and M corresponds to a set of dummy variables corresponding to each month of the year (when using monthly data). The resulting coefficients a_1 and a_2 represent the elasticity of gasoline yield with respect to gasoline price and diesel price respectively; coefficients b_1 and b_2 represent the elasticity of diesel yield with respect to gasoline price and diesel price respectively.

The main results presented below introduce two key modifications to the simple models (1) and (2) defined above. First, gasoline and diesel prices are normalized by the refiner acquisition cost of crude oil. This allows the model to better capture the fact that refiners are more likely to respond to changes in production margins than to the absolute price of finished products. Further, the normalized price ratio is unitless, which removes the need to adjust for inflation and allows the model to be run with nominal dollars, as reported by EIA. Second, the regression is modified to include a lag structure that better accounts for the time-dynamics of the model. Three different functional forms are tested, referred to respectively as ‘lagged prices,’ ‘partial adjustment’ and ‘adaptive expectations’ models. These models are described in appendix section D.1.1; their key advantage is that they capture refiner response to price changes that are sustained across multiple time periods. Each model is run both in its basic form, and assuming AR(1) autocorrelation among the residuals. The results, presented in Table 5.2, are stable across all specifications. Appendix section D.1.2 presents results for a number of additional model forms; the results are more or less robust to the functional form of the time controls, the use of direct prices instead of price ratios, the inclusion of other product prices, or the use of annual instead of monthly data. Other functional forms (e.g., including non-linear models, or allowing for asymmetric response to price increases vs price decreases) are beyond the scope of the present analysis.

Table 5.2. Elasticity of diesel and gasoline relative yields from crude oil with respect to the ratio of diesel and gasoline prices to the acquisition cost of crude oil (based on nationally aggregated, monthly, U.S. data). Standard errors are shown in parentheses.

Model	Distillate yield		Gasoline yield	
	Elasticity with respect to distillate price ratio	Elasticity with respect to gasoline price ratio	Elasticity with respect to distillate price ratio	Elasticity with respect to gasoline price ratio
Lagged prices (3 lags)	0.401*** (0.0315)	-0.341*** (0.0230)	-0.218*** (0.0178)	0.170*** (0.0130)
Partial adjustment	0.485*** (0.0614)	-0.404*** (0.0471)	-0.243*** (0.0305)	0.201*** (0.0233)
Adaptive Expectations	0.459*** (0.0403)	-0.410*** (0.0344)	-0.222*** (0.0185)	0.179*** (0.0143)
Lagged prices AR(1)	0.420*** (0.0561)	-0.345*** (0.0438)	-0.229*** (0.0307)	0.176*** (0.0236)
Partial adjustment AR(1)	0.500*** (0.0649)	-0.418*** (0.0504)	-0.245*** (0.0316)	0.203*** (0.0246)
Adaptive Expectations AR(1)	0.467*** (0.0647)	-0.387*** (0.0514)	-0.226*** (0.0319)	0.192*** (0.0255)

***p<0.001

The elasticities presented in Table 5.2 have intuitive signs, and are consistent across the different specifications. Results for gasoline are similar to results reported by Dahl (1981)³³⁵ for the U.S. (see Table 5.1). Own price elasticities (i.e., elasticity of gasoline and diesel with respect to their own prices) are both lower than those derived from Considine (1992).³³⁶ The present model assumes that product prices are exogenous variables to the regression model. To the extent that prices changes are due to exogenous changes in yield (e.g., a yield increase in one product floods the market, driving down the price), the magnitude of the coefficients in Table 5.2 will be biased toward zero. Thus, if anything, Table 5.2 may slightly underestimate relative yield elasticities. Appendix section D.1 provides a more detailed explanation of the regression models presented above, and includes results for additional regressions. It should be emphasized that all results presented here are for the entire industry (rather than individual refineries), and for price changes that are sustained across multiple periods.

For each product, its own price elasticity and cross price elasticity (i.e., elasticity with respect to the other product's price) have approximately the same magnitude, but with opposite signs. Additionally, from Table 5.2, distillate appears to be about twice as responsive as gasoline to price changes; this observation is consistent with results from Considine (1992).³³⁶ These facts imply that if the price of gasoline is driven down (e.g. by biofuel policies) there should be a net shift toward increased diesel production, not only at the expense of gasoline, but also at the expense of other (lower value) petroleum products. This observation is consistent with market sources, which suggest that refiners react to low gasoline prices with an attempt to shore up margins by increasing diesel yields (or vice-versa).^{332,345-347} This shift toward diesel production has important implications for greenhouse gas emissions as discussed in the next section.

The results presented above are nominally only for the U.S. petroleum refining sector. Previous work by Dahl (1981)³³⁵ suggests that the refining industry in other regions, with less cracking capacity (the process by which heavier hydrocarbon chains are transformed into higher value, light molecules), may be less responsive to market prices. Although Dahl found no discernible effect of product prices on product mix in Europe, more recent market sources suggest that even European refiners do respond to product prices.^{164,345} Appendix Table D.5 shows U.S. elasticity estimates broken down by different regions (Petroleum Administration Defense Districts) in the U.S. While the results are not definitive, they appear to support Dahl's claim that regions with more cracking capacity will exhibit larger elasticities. Table D.5 also suggests that elasticities may be correlated with larger average refinery size – perhaps due to greater ease of investing in new processing units.

As of January, 2016, the U.S. was responsible for about 20% of global refining capacity.¹⁵⁸ The U.S. had a combined cracking capacity (thermal cracking, catalytic cracking and catalytic hydrocracking) amounting to 58% of its total crude oil (atmospheric distillation) processing capacity. In contrast, the rest of the world had a combined cracking capacity amounting to only 26% of crude oil processing capacity. Similarly, the U.S. had an average refinery size of 150 thousand barrels per day, compared to 140 thousand barrels per day in the rest of the world.¹⁵⁸ Taken together, these results suggest that the rest of the world could plausibly have a lower responsiveness than the U.S. Thus, in the models that follow I treat U.S. refinery flexibility

(Table 5.2) as an upper bound for global flexibility. As a lower bound, I also run additional scenarios in which only U.S. refiners respond to market prices, while the rest of the world keeps its product slate fixed.

5.4. Implications of Refiner Flexibility: Methods

5.4.1. *The Partial Equilibrium Model*

Using the elasticities determined above, I modify the stochastic partial equilibrium model from Rajagopal and Plevin (2013)³³⁰ to account for flexibility in refinery product mix when relative prices change. The model is a two region representation of global petroleum and biofuel markets: a ‘home’ region, calibrated to approximate U.S. market conditions and a rest of the world (ROW) region, calibrated to global data (excluding the U.S.). The base year for both regions is 2007. The model includes 3 petroleum products (gasoline, diesel and ‘other’) and 2 biofuels (corn ethanol and sugarcane ethanol). Through a set of simultaneous equations, the model provides comparative statics for a world without any biofuel policy, and worlds with eight different biofuel policies: a 10% or 15% biofuel share mandate (SM), a transportation fuel emission standard that requires either a 5% or 10% reduction in emission intensity without accounting for indirect land use change (ILUC) emissions (ES_NoILUC), an equivalent emission standard that accounts for ILUC emissions (ES_ILUC), and a carbon tax (CT) set to 10 or 20 \$/tonne CO₂. Importantly, these policies assume that ethanol is a substitute for gasoline; no other fuel switching is modeled explicitly (though this may occur implicitly through shifts in demand). In all cases, GHG emissions are reported including life cycle emissions from all fossil fuels and biofuels (including ILUC). Detailed model equations and their numerical calibrations are described in Rajagopal and Plevin (2013).³³⁰ The model uses Monte Carlo simulation to model uncertainty among emissions factors, as well as supply and demand elasticities. The present work makes several key modifications to the model and/or documentation, described below:

1. Although the model documentation³³⁰ states that the share mandate is implemented on an energy basis, it is actually implemented on a volume basis. For consistency with the original model I leave the share mandate as originally written (on a volume basis). I note that share mandates are equivalent to appropriately calibrated volume mandates.

2. In the original model, the price of ‘other’ products was determined as the difference between the price of input crude oil and output gasoline and diesel. This neglects refining costs. Thus, in the present iteration, the initial price of ‘other’ products is represented by the 2007 price of residual fuel oil (\$1.38/gal), and a fixed refining cost is added to restore equilibrium to the 2007 status quo.
3. The original model assumed fixed refinery yields from crude oil. The present model allows refinery yields to adjust dynamically, as dictated by the elasticities defined in Table 5.2. The results presented in this section use elasticities from the partial adjustment model (basic version). Each of the 4 required elasticities (gasoline and diesel yield with respect to gasoline and diesel prices) is assumed to be normally distributed, based on mean and standard error of the regression results. The 90% confidence intervals from the partial adaptation model capture the mean coefficient estimates from all models presented in Table 5.2. I assume, subjectively (i.e., based on my own judgment), that the absolute values of the 4 elasticities are pairwise correlated with a coefficient 0.7; this is the same magnitude as the within-region correlation between gasoline and diesel elasticities that the authors subjectively assume in the original model. This assumption does not substantially influence the final results.
4. In the original model, the carbon tax policy was applied only to gasoline. In line with an alternate form of the model developed by the original authors,³⁴⁸ the present work assumes instead that the carbon tax will be applied to all petroleum products.
5. The original model uses life cycle emission factors for gasoline, diesel, and ‘other’ petroleum products. The present model does not use these emission factors, and instead calculates GHG emissions as described below.

5.4.2. Emissions from the Petroleum Industry

Allocation is a common and necessary practice employed when calculating life cycle emission factors for individual products within a multi-product system, such as crude oil refining. These emission factors, however, do not necessarily represent the emissions from increased production of a given product. To avoid the need for emission allocation, this chapter models the total (unallocated) emissions from three different segments of the petroleum industry: extraction, refining, and product combustion.

Crude oil upstream emissions. Distributions for baseline extraction and refining emissions rely on Venkatesh *et al.* (2011),¹⁹⁸ as described in appendix section D.2.2. In addition, these upstream emissions are allowed to vary with product mix. Using the Oil Production Greenhouse Gas Emissions Estimator (OPGEE),³⁴⁹ accessed via Carnegie Endowment’s Oil Climate Index (OCI),³⁵⁰ extraction emissions were retrieved for 30 different types of crude oil from around the world. Each oil from OPGEE was then matched with the corresponding oil in PRELIM.¹⁶³ PRELIM contains 10 different refinery configurations with differing levels of complexity, as discussed in section 5.3.1. I run each type of crude oil through each available configuration and record both the volumetric product yields, and total upstream (extraction + refining) GHG emissions for each run. The resulting data are plotted in Figure 5.6.

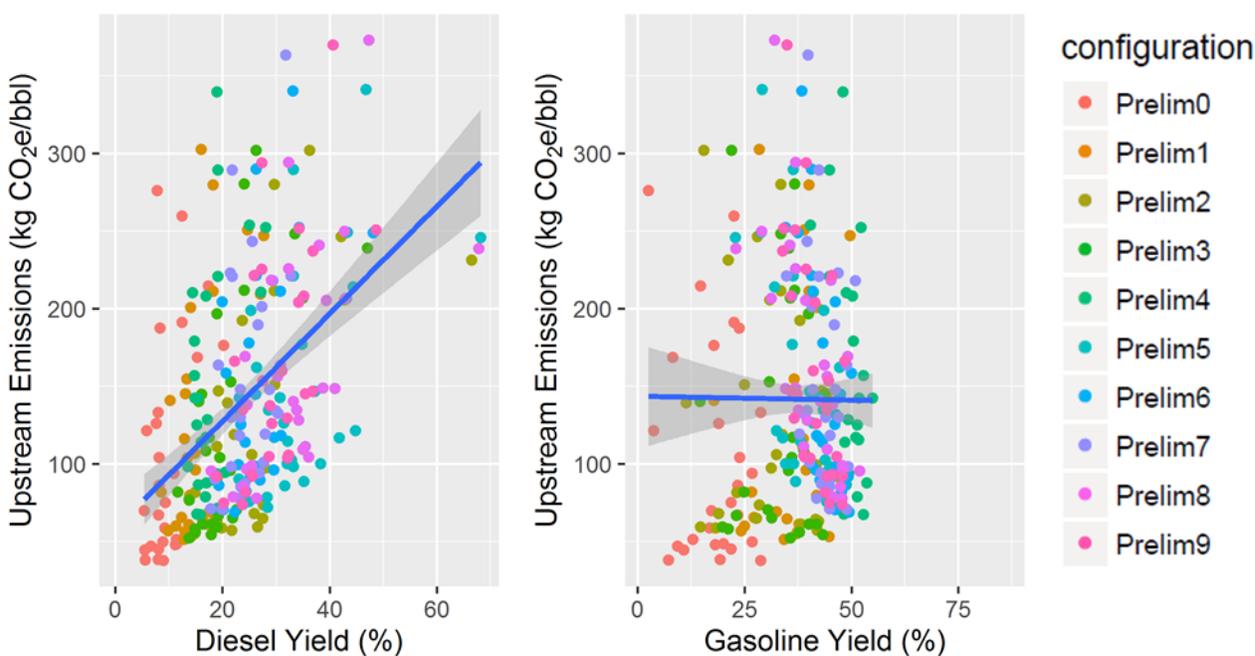


Figure 5.6. Upstream (extraction + refining) GHG emissions from processing different crude oils under different refinery configurations, as a function of product yields. Data are color-coded based on PRELIM refinery configuration. Multiple data points within a configuration represent different types of crude oil. Linear trend-lines are included as a visual aid.

Although product yields are only weakly predictive of upstream emissions, there is a clear positive correlation between diesel yield and upstream emissions. This is confirmed through linear regression, as displayed in Table 5.3. Although these results do not necessarily represent

the actual change in emissions that would occur from shifting the product mix, they are nonetheless highly suggestive. For the present model, the baseline distribution of upstream emissions from Venkatesh *et al.* (2011),¹⁹⁸ is shifted linearly in function of gasoline and diesel yields, as dictated by equation (3); regression coefficients are simulated as normal distributions, in function of the mean and standard errors reported in Table 5.3.

$$\Delta(\text{Upstream Emissions}) = b_{\text{gasYield}} * \Delta\beta_g + b_{\text{dieselYield}} * \Delta\beta_d \quad (3)$$

where β_g and β_d are respectively the gasoline share and distillate share of total refinery output; b_{gasYield} and $b_{\text{dieselYield}}$ are the regression coefficients from Table 5.3. PRELIM and OPGEE do not contain information about how to weight the different oils or refinery configurations (to estimate industry-wide emissions), and do not explicitly account for uncertainty. Thus, I use them only to shift the mean upstream emissions from the distribution based on Venkatesh *et al.* (2011).¹⁹⁸

Table 5.3. Linear regression of crude oil upstream emissions as a function of product yields. Standard errors are shown in parentheses.

	Dependent Variable: Upstream Emissions (kg CO ₂ e/bbl)
Gasoline yield (%)	-0.401 (0.389)
Diesel Yield (%)	3.50*** (0.39)
Constant	72.4*** (17.0)

Observations	270
R ²	0.235
Adjusted R ²	0.229
Residual Standard Error	65.9 (df= 267)
F Statistic	41.1*** (df =2; 267)
***p<0.001	

Combustion Emissions. Although the partial equilibrium model includes only 3 categories of petroleum product (gasoline, diesel and other), finer resolution is required to calculate combustion emissions. The United Nations Energy Statistics Database provides data for year 2007 production of petroleum products on a mass basis, for 97 different countries.³⁵¹ I convert

the mass of each product to a volume using default conversion factors from EIA^{352,353} and use the resulting values to determine the initial 2007 volume share of 12 different individual petroleum products within the ‘other’ (non-gasoline, non-diesel) category. I then simulate combustion emissions for each product using independent triangular distributions, based on emission factors from the Intergovernmental Panel on Climate Change (IPCC).⁹⁵ I assume that bitumen/asphalt, petrochemical feedstocks, lubricants and waxes are not combusted, and therefore have no combustion emissions. From the UN data, I assume that the petrochemical feedstocks are represented by the category ‘naphtha’ (accounting for 6.6% of finished products).

In addition to the baseline composition, it is necessary to establish how the relative yields of these other petroleum products change in function of gasoline and diesel yields. Using monthly average U.S. data from EIA,³⁴² I regress the yield of each finished petroleum product jointly on the yields of gasoline and distillate (diesel). Table 5.4 presents the resulting coefficients. As expected, each column of the table sums to negative one.

Table 5.4. Change in yields (percentage points) of ‘other’ products, for a one percentage point increase in gasoline yield or in distillate (diesel) yield. Each row represents a separate regression, and each column a different regression coefficient.

Dependent variable	Gasoline (%)	Distillate (%)
Jet fuel (%)	-0.028	-0.086
Petroleum coke (%)	+0.045	+0.12
Still gas (%)	-0.041	-0.034
Residual fuel oil (%)	-0.063	-0.29
Liquefied refinery gases (%)	-0.75	-0.31
Asphalt (%)	-0.15	-0.20
Petrochemical Naphtha (%)	+0.015	-0.0049
Petrochemical oils (%)	-0.047	-0.13
Lubricants (%)	-0.020	-0.024
Special Naphthas (%)	-0.0027	-0.020
Kerosene (%)	+0.052	-0.030
Aviation gasoline (%)	-0.0066	-0.01
Waxes (%)	-0.010	-0.014
Miscellaneous (%)	+0.0049	+0.027
SUM	-1	-1

5.4.3. Summary of Model Parameters

Table 5.5 below shows the range of key input parameters used in the Monte Carlo simulation model. Additional details are available in appendix section D.2.

Table 5.5. Key input parameters used for Monte Carlo simulation. “Home” refers to the region implementing the policy, and is approximately calibrated to U.S. conditions. ROW = rest of world; GWI = global warming intensity; ILUC = indirect land use change.

Model Parameter	Distribution	Range ^a
<i>Parameters from the original model^b</i>		
Elasticity of supply of crude oil, home	Normal	(0.12, 0.27)
Elasticity of supply of crude oil, ROW	Normal	(0.08, 0.23)
Elasticity of supply of corn ethanol, global	Normal	(1, 3)
Elasticity of supply of cane ethanol, global	Normal	(1, 5)
Elasticity of demand for gasoline, home	Normal	(-0.6, -0.4)
Elasticity of demand for gasoline, ROW	Normal	(-0.85, -0.5)
Elasticity of demand for diesel, home	Normal	(-0.6, -0.4)
Elasticity of demand for diesel, ROW	Normal	(-0.85, -0.5)
Elasticity of demand for other petrol. prods. home	Normal	(-0.6, -0.4)
Elasticity of demand for other petrol. prods., home	Normal	(-0.85, -0.5)
Corn ethanol GWI (g CO ₂ e / MJ)	Uniform	(55, 70)
Cane ethanol GWI (g CO ₂ e / MJ)	Uniform	(10, 30)
Corn ethanol ILUC (g CO ₂ e / MJ)	Uniform	(5, 100)
Corn ethanol ILUC (g CO ₂ e / MJ)	Uniform	(5, 50)
<i>Parameters adapted for the present chapter</i>		
Elasticity of diesel yield vs normalized diesel price ^c	Normal	(0.36, 0.61) ^d
Elasticity of diesel yield vs normalized gasoline price ^c	Normal	(-0.50, -0.31) ^d
Elasticity of gasoline yield vs normalized gasoline price ^c	Normal	(0.16, 0.25) ^d
Elasticity of gasoline yield vs normalized diesel price ^c	Normal	(-0.30, -0.18) ^d
Crude oil extraction, baseline GWI (kg CO ₂ e/bbl)	Lognormal	(25, 77)
Crude oil refining, baseline GWI (kg CO ₂ e/bbl)	Normal	(37, 64)
Change crude oil upstream GWI vs gasol. yield (kg CO ₂ e/bbl/%)	Normal	(-1.2, 0.36)
Change crude oil upstream GWI vs diesel yield (kg CO ₂ e/bbl/%)	Normal	(2.7, 4.3)
Petroleum product combustion emissions (kg CO ₂ e / bbl)	See appendix Table D.7	
Change in yields of other products vs gasol. and diesel yields	See Table 5.4	

a) Range shows upper and lower bounds for uniform distributions, and 95% confidence intervals for all other distribution families.

b) From Rajagopal and Plevin (2013).³³⁰

c) Elasticities are with respect to the ratio of each product price to the price of crude oil.

5.5. Implications of Refiner Flexibility: Results

There are three main mechanisms through which refiner flexibility may influence GHG emissions in the present model. First, shifting the product slate may allow the petroleum industry to compensate for the drop in gasoline prices, thereby increasing the value of crude oil and averting the scale-back in production and subsequent processing that would have otherwise been expected. Second, as outlined in section 5.4.2, increasing diesel yields may increase upstream petroleum emissions through the choice of crude oil processed, refinery configuration, or both. Finally, Table 5.4 shows, increased diesel yields would likely come, in part, at the expense of non-combusted petroleum products like asphalt and petrochemicals; this would increase the downstream combustion emissions for a fixed quantity of oil. Together, these effects could play an important role in determining the net change in GHG emissions brought about by biofuel policies. All three effects are implicitly or explicitly included in the partial equilibrium model described in section 5.4. In this section, I report changes in global market conditions (e.g. product yields and prices) and GHG emissions induced by different biofuel policies.

I run the partial equilibrium model twice: once assuming that the entire world exhibits the same elasticities as U.S. refineries, and once assuming that only U.S. refineries adjust and that the rest of the world has fixed yields for petroleum products. These serve as upper and lower bounds for the global response. Figure 5.7 shows the resulting change in global refinery yields for diesel and gasoline (note: initial yields differ slightly from the 2007 yields shown in section 5.3.1 because the model uses a different data source). The model predicts that biofuel policies induce an increase in diesel yields (panels a and c), and a decrease in gasoline yields (panels b and d), relative to the initial, ‘no policy,’ case. When comparing the different policies, larger yield changes reflect larger underlying price changes, as discussed below (Figure 5.11). The shift in yields is relatively small – limited to just a few percentage points even in the most extreme cases. Nevertheless, these changes can have dramatic implications for the total change in GHG emissions, as discussed below.

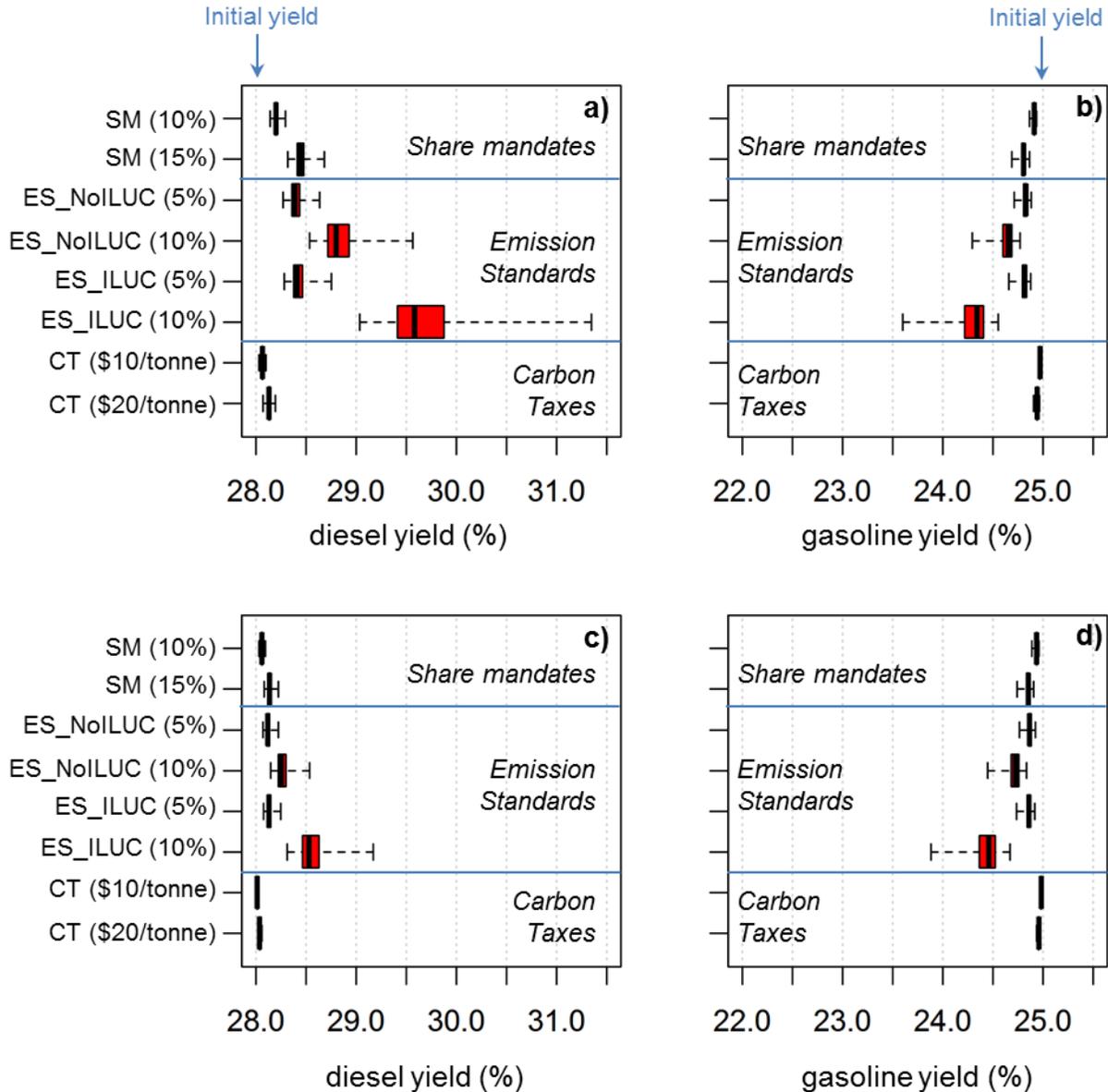


Figure 5.7. Frequency distribution for the resulting average global refinery yields gasoline and diesel (as a volumetric percent of total refined products) under different policy scenarios assuming either that all refineries respond to market prices (panels a and b) or that only refineries in the home region adjust while ROW refineries have a fixed product slate (panels c and d). SM = share mandate, ES = emission standard either with or without ILUC. CT = carbon tax. The box represents the interquartile range, the vertical line represents the median, and the whiskers show the extreme values of the simulation. Figure design based on Rajagopal and Plevin (2013).³³⁰

Figure 5.8 shows the change in global GHG emissions that result from each policy, both assuming fixed refinery shares and assuming that the global refining industry exhibits the same flexibility as US refineries. Figure 5.9 shows the change in global GHG emissions that result from each policy, both assuming fixed refinery shares and assuming that only refineries in the home region adjust their product slate in response to market prices. The figures include changes in emissions due both to the petroleum industry and to the production of biofuels. For each figure, the green boxes (fixed refinery yields) correspond approximately to the original model from Rajagopal and Plevin (2013),³³⁰ subject to modifications discussed in section 5.4.1. The additional emissions from allowing flexible refinery yields (red boxes) are the main contribution of the present study. By comparing the green boxes to the corresponding red boxes in Figure 5.8, it is apparent that the existence of refiner flexibility can substantially influence the net GHG balance from different biofuel policies. As Figure 5.9 shows, the GHG impact of refiner flexibility is still present, though substantially muted if only refineries in the home region respond to market prices. The remainder of the results section focuses on the globally flexible case (represented by Figure 5.8), with the understanding that the effects discussed would be scaled down if ROW refineries are less flexible than the home region.

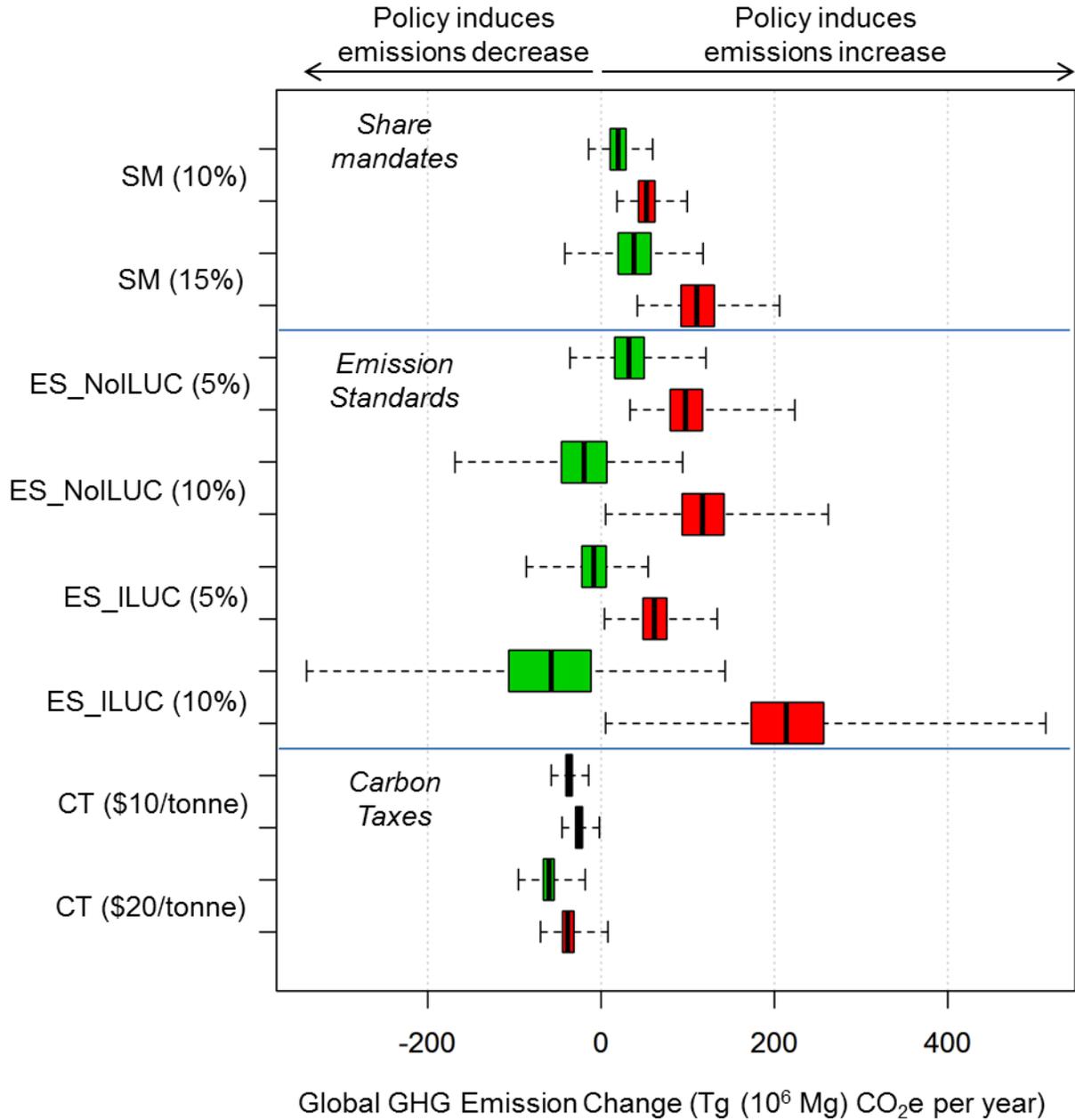


Figure 5.8. Frequency distribution for change in global emissions under different policy scenarios. All values are relative to the ‘no policy’ scenario, represented by 0 on the x-axis. SM = share mandate, ES = emission standard either with or without ILUC. CT = carbon tax. The box represents the interquartile range, the vertical line represents the median, and the whiskers show the extreme values of the simulation. Green boxes (the top member of each pair) represent the results when refinery yields are fixed. Red boxes represent results when all refineries exhibit the same price response as US refineries. Figure design based on Rajagopal and Plevin (2013).³³⁰

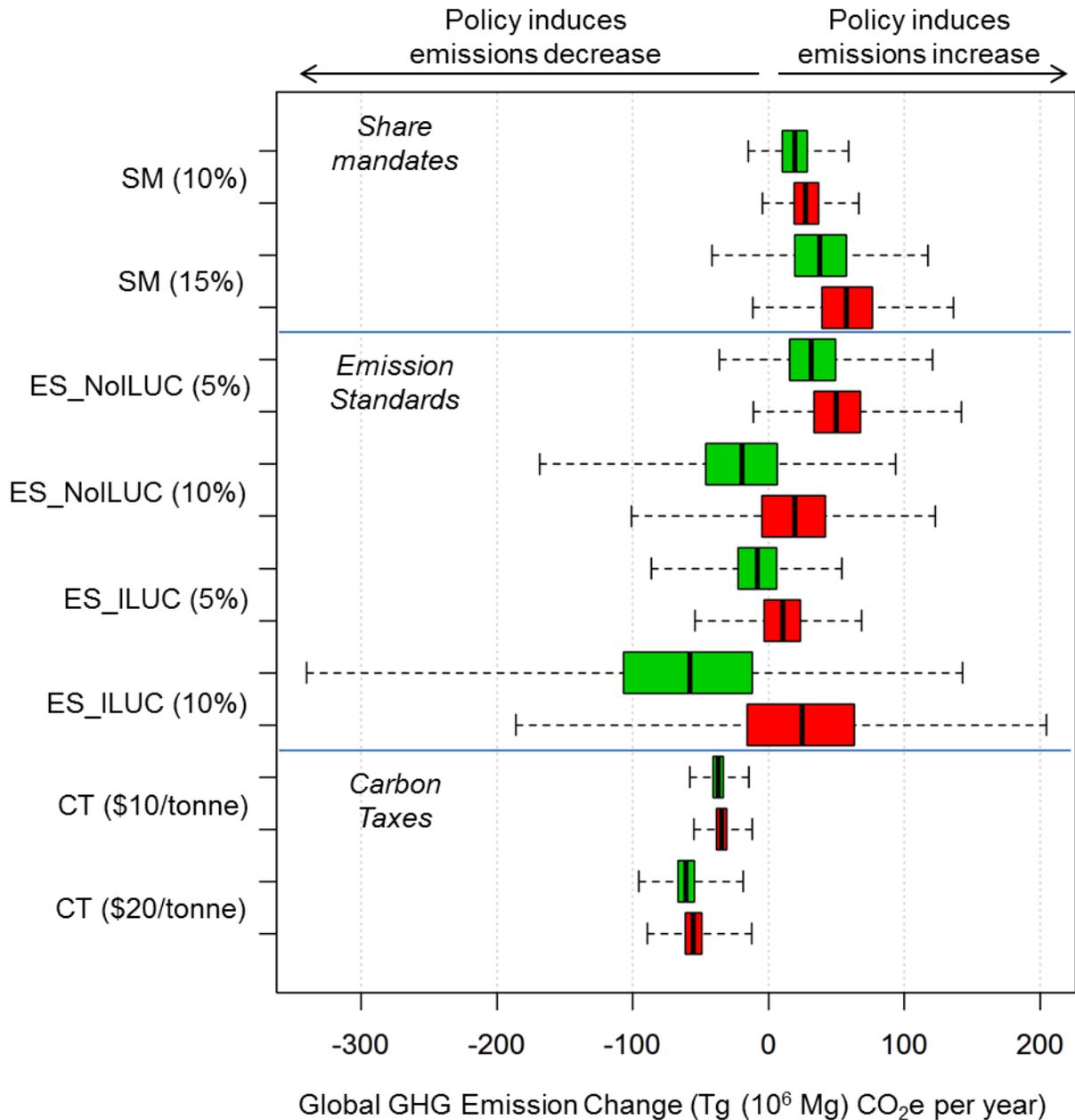


Figure 5.9. Frequency distribution for change in global emissions under different policy scenarios. All values are relative to the ‘no policy’ scenario, represented by 0 on the x-axis. SM = share mandate, ES = emission standard either with or without ILUC. CT = carbon tax. The box represents the interquartile range, the vertical line represents the median, and the whiskers show the extreme values of the simulation. Green boxes (the top member of each pair) represent the results when refinery yields are fixed. Red boxes represent results when U.S. refineries respond to market prices but ROW refineries have fixed product yields. Figure design based on Rajagopal and Plevin (2013).³³⁰

As shown in Figure 5.8, the additional emissions resulting from refiner flexibility differ substantially by policy instrument. The effect is largest for the emission standards, which generally result in the model predicting the use of higher quantities of ethanol and thus larger changes in gasoline prices. Larger share mandates would likely produce similar results. These results rely on the modeling assumption that biofuels compete primarily with gasoline, rather than equally across all fuels. This assumption largely reflects reality; for example, the proposed U.S. Renewable Fuel Standard mandate for 2017 requires that biofuels comprise 10.44% of transportation fuel sales overall, but only 1.67% of diesel sales.³³ Future versions of the present model could account for a biodiesel component to biofuel policies. This would slightly reduce the effect currently predicted by the model; however, unless biodiesel becomes a much larger component of future policies the main conclusions from this chapter will still hold.

In contrast to the other policies, refiner flexibility only adds a small quantity of additional emissions in the case of a carbon tax. This is in part because the carbon tax, at the levels specified, results in a smaller change in the producer price of gasoline than do the other policies. Additionally, the model assumes that the carbon tax applies to all petroleum products (not just gasoline), substantially reducing the incentive for refiners to shift production toward diesel. Nevertheless, the home region initially represents a greater share of global gasoline consumption (41%) than diesel consumption (16%). As a result, the carbon tax implicitly covers a greater proportion of the global gasoline market, and refineries still exhibit a small shift toward diesel production. A separate run of the model in which the carbon tax applies only to gasoline (results not shown) confirms that the additional GHG emissions attributed to refiner flexibility would increase by approximately 50% relative to the present case.

The net result of adding refiner flexibility is that the vast majority of model iterations now predict that the carbon tax is the only policy which achieves a net decrease in global greenhouse gas emissions. Figure 5.10 presents a breakdown of the factors responsible for this observed increase in emissions for each share mandate and emission standard policy (note the change in scale for panels e and f). The figure is built additively. The first row of each panel shows the “naïve” emission reduction that would be expected if biofuels are carbon neutral and perfectly replace gasoline on a 1:1 energy basis. The next 3 rows modify emissions in the petroleum

sector, first by adding emissions from the indirect fuel use effect (“IFUE”), then accounting for the change in upstream (extraction and refining) petroleum carbon intensity (“ Δ upstream”), and finally including the change in downstream petroleum product combustion emissions (“ Δ combustion”). The final 2 rows represent emissions from biofuels, first excluding ILUC (“bio-LCA”), and then including all emission sources (“ILUC”). The net result in all cases presented is a change from expected GHG emission reductions (“naïve”) to a net GHG emission increase in the last row of each panel. In all cases, the model predicts that additional emissions due to the change in carbon intensity within the petroleum industry are actually larger than the emissions caused by IFUE in at least 50% of model runs. In the most extreme case (the 10% emission standard with ILUC, panel f), refiner flexibility is responsible for over double the emissions of IFUE in the median case. For most model runs of the non-tax policies, the results with globally flexible refineries even suggest a net increase in emissions within the petroleum sector alone (i.e. excluding emissions from the production of biofuels). For the case where only home refineries adjust their production slate (appendix Figure D.1), emissions from refiner flexibility still amount to between 25% and 72% of IFUE emissions in the median iteration. Thus, internal adjustments within the refining sector are potentially critical to the net GHG balance of biofuel policies.

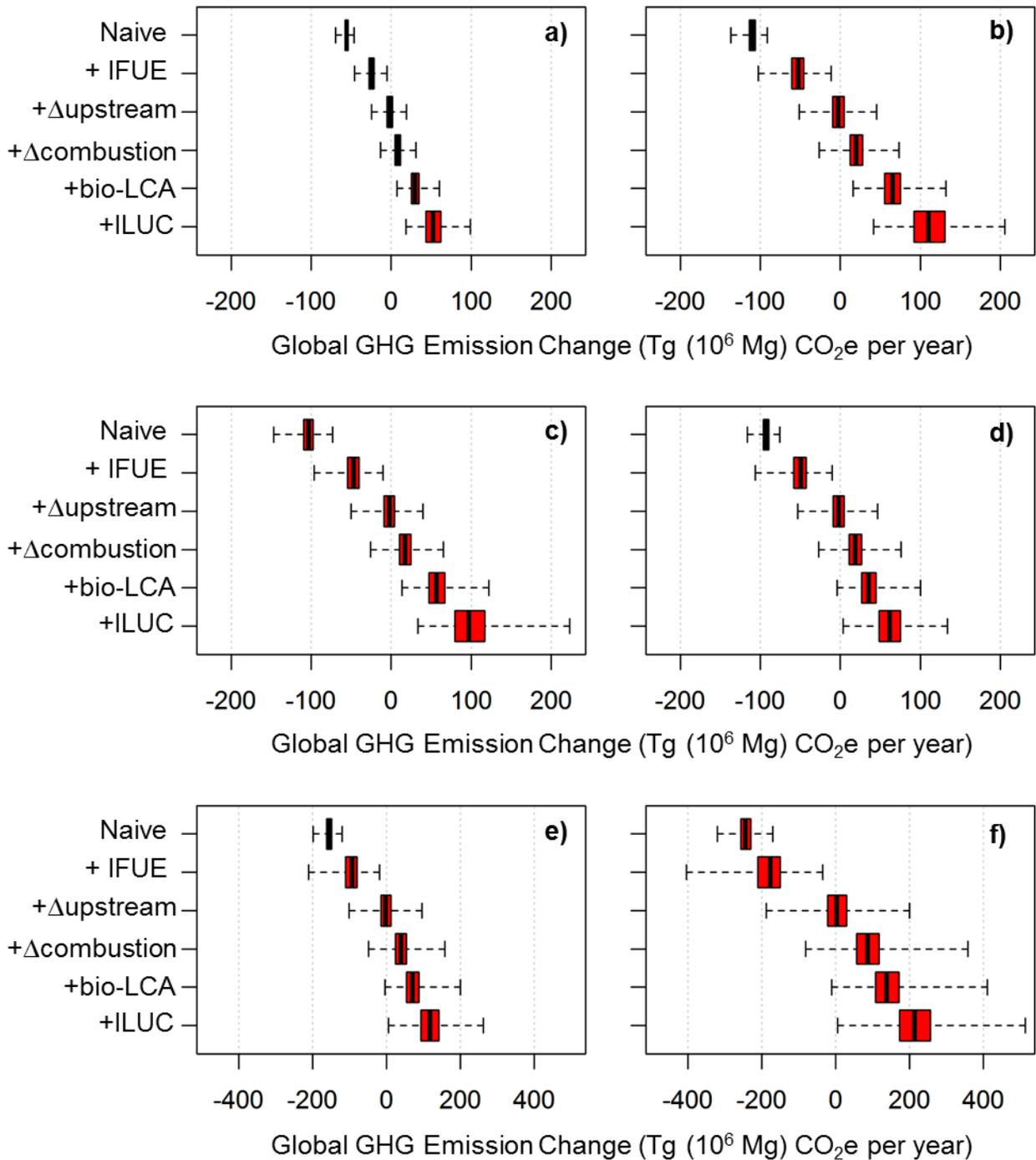


Figure 5.10. Breakdown of emission changes from different policies, assuming globally flexible refineries: a) 10% share mandate, b) 15% share mandate, c) 5% emission standard without ILUC, d) 5% emission standard with ILUC, e) 10% emission standard without ILUC, f) 10% emission standard with ILUC. Note the change in scale for the final 2 panels (e and f). The boxplots in each panel are built additively: “Naïve” represents the change in fossil fuel emissions, assuming biofuels are carbon neutral and displace gasoline

perfectly without any market rebound. The next row adds the market rebound / indirect fuel use effect (IFUE), assuming no change in carbon intensity within the petroleum industry. The next line adds the additional upstream emissions (crude oil extraction and refining) predicted due to the change in product yields. The next line adds the change in combustion emissions resulting from the shift in refinery yields. The final 2 rows represent emissions from biofuels, first excluding ILUC, and then including all emission sources. Each box represents the interquartile range, the vertical line represents the median, and the whiskers show the extreme values of the simulation.

Intriguingly, the ability of refiners to shift production toward the higher value (diesel) product makes little difference in the total quantity of oil processed (appendix Figure D.3 and Figure D.4). In brief the increased diesel yields predicted by the model are offset by a decrease in the price of diesel. Figure 5.11 shows the change in wholesale diesel and gasoline prices induced by the different policies. Due to reduced processing of crude oil, the model with fixed refinery yields predicts a small increase in diesel price for non-tax policies (panel a). In contrast the model with globally flexible refineries predicts a net decrease in the price of diesel for all policies (panel c), implicitly sharing the burden of biofuel policies across both gasoline and diesel markets. Additionally, by shifting away from gasoline production, refineries can blunt the decrease in gasoline prices (compare panels b and d). Appendix Figure D.2 shows equivalent results for the case where only U.S. refineries respond to market conditions. As a result of these changes, the shift toward diesel, though sensible for an individual (price-taking) refinery, does nothing to boost the value of petroleum when applied across the industry. This observation is consistent with casual industry market analysis.³³² Thus, while refiner flexibility increases the GHG emission intensity of the petroleum industry, the model predicts that such flexibility may not affect the magnitude of IFUE itself.

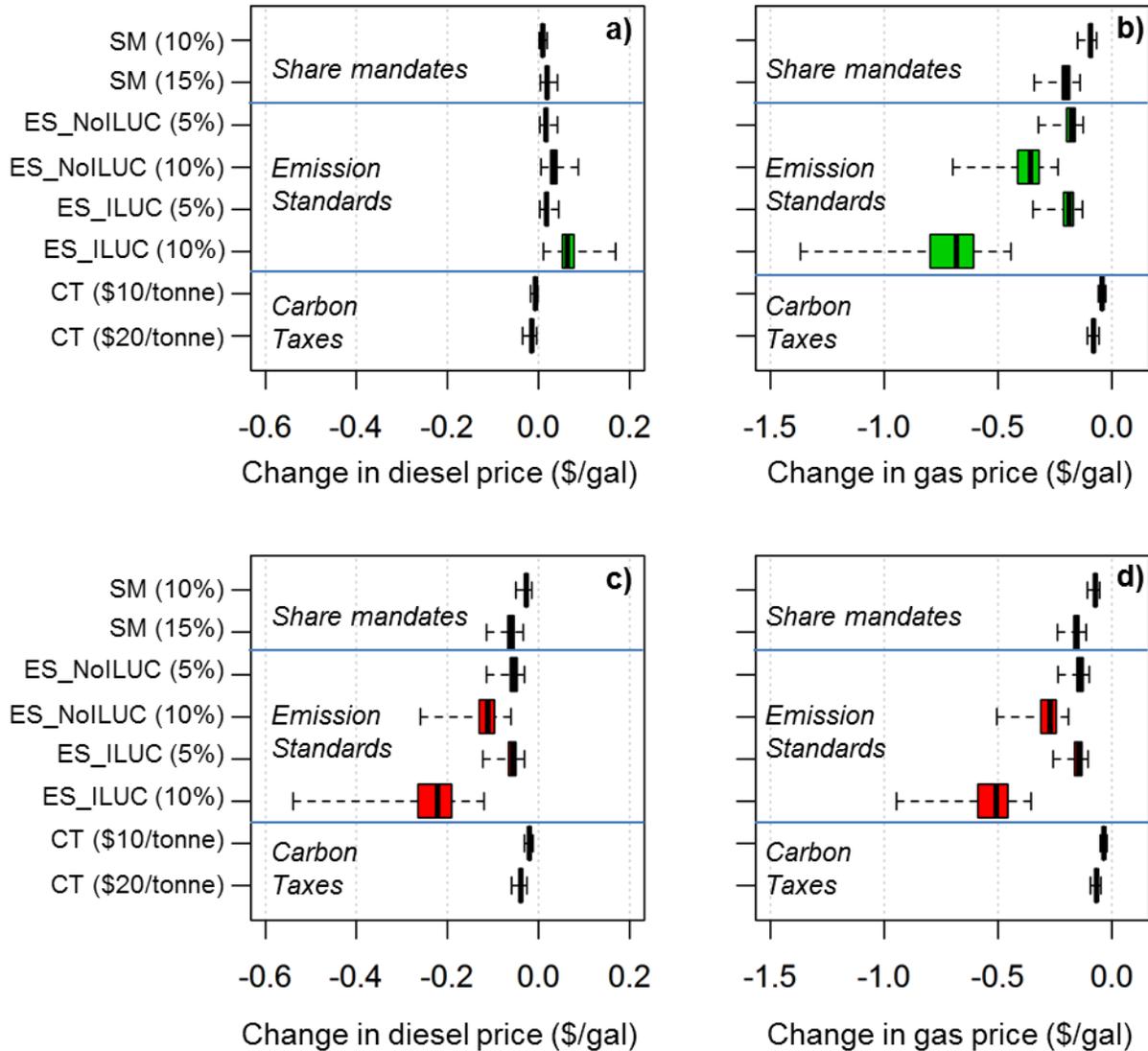


Figure 5.11. Frequency distribution for change in wholesale diesel and gasoline prices induced by the different policies, with fixed refinery yields (panels a and b), or globally flexible refinery yields (panels c and d). Policies include: SM = share mandate, ES = emission standard either with or without ILUC. CT = carbon tax. The box represents the interquartile range, the vertical line represents the median, and the whiskers show the extreme values of the simulation.

5.6. Discussion

Contrary to assumptions in previous consequential assessments of biofuel policies, this work shows the relative yields of final products in the petroleum industry are not fixed. International historical analysis suggests that refining industries can evolve to produce product slates that differ by tens of percentage points. The U.S. petroleum refining sector exhibits relative yield elasticities for gasoline and diesel of approximately 0.2 and 0.5, respectively, relative to their own prices (normalized by the price of crude oil). The U.S. refining sector also exhibits cross price elasticities for gasoline and diesel (relative to each other's price) of around -0.2 and -0.4, respectively.

This work demonstrates refiner flexibility can substantially impact the net change in GHG emissions that result from biofuel policies. Although the model predicts only small changes in relative product yields, these can have dramatic consequences for the total GHG emission changes induced by the different biofuel policies, on the order of tens or hundreds of megatonnes of CO₂e/year. In the upper bound cases where all refineries exhibit the same yield elasticities as U.S. refineries, share mandates and emission standards likely result in a net increase in GHG emissions even before accounting for emissions from biofuel production. The present chapter considers only how refiner flexibility changes the net GHG emissions from biofuel policies; however, the model framework could be applied to any policy that disproportionately targets gasoline consumption (e.g., electrification of the light duty vehicle fleet, fuel economy standards, and so on). Future work can, and should, also examine interactions between different policies such as the simultaneous application of a biofuel mandate, carbon tax, fuel economy standard, and so on.

The results presented above, while compelling, should only be taken as an indication of the potential impact of refiner flexibility on the success of different fuel policies. The partial equilibrium model employed is a very highly simplified representation of global fuel and petroleum markets. The world is divided into only two regions; supply and demand elasticities cover only 2 different biofuels (both ethanol), 3 types of petroleum products, and production of a generic crude oil. Additionally, the different policies considered are introduced to the home region in isolation, without accounting for interactions with existing policies (e.g. corporate

average fuel economy standards³²), or parallel fuel policies around the world. The data used to determine elasticities of refinery yields is a highly aggregated time series data set specific to the United States. Greater resolution (e.g. at the level of individual refineries) and a deeper market analysis of both the U.S. and international refining sectors would provide more confidence in the refiner response elasticities presented in section 5.3.2. At present, the model imposes a top-down (essentially exogenous) refiner response to price changes without explicitly modeling costs within the refining industry. As a result, the model implicitly assumes that refiners are behaving non-competitively (i.e. since they can costlessly shift toward higher value products). This assumption introduces a theoretical inconsistency, since the model also calculates the price of crude oil based on a no-arbitrage condition between crude oil and final petroleum products. The reality is likely between those 2 extremes, and so the direction of any bias is difficult to predict. Finally, while results from PRELIM and OPGEE suggest that increasing diesel yields correlate with higher upstream petroleum emissions, the data are insufficient to make a causal prediction of how emissions would actually change as refiners boost diesel yields.

Despite the above caveats, this work nevertheless provides several important lessons for evaluating biofuel policies. The share mandates considered in this chapter closely resemble the U.S. Renewable Fuel Standard, which currently requires that ethanol make up approximately 10% of gasoline sales,³³ an amount that is mandated to double by 2022,⁴ unless biodiesel begins to account for a much larger share of biofuel consumption in the U.S. than it currently does. As such, it is instructive to consider what lessons this work holds for U.S. policy.

First, the ability of refineries to adjust their product slate can substantially increase the GHG emissions resulting from increased biofuel use – potentially surpassing the emissions caused by the more classic IFUE. Second, contrary to the original model, which suggests a small decrease in world diesel consumption across the different policies (i.e. a negative IFUE for diesel), the present model predicts a rebound in both diesel and gasoline consumption in response to all the policies considered. In essence, refiner flexibility allows the IFUE to be shared across petroleum products. Although the model predicts that product switching has little influence on the economic value of crude oil (and thus on the total quantity produced/consumed), that finding depends heavily on the relative elasticities of different petroleum products and should be

explored further in future work. Taken together, these results provide yet another reason for governments to be leery of policies with incomplete market coverage. The effect of product shifting could be mitigated if regulators adopt policies which apply equally across linked markets (e.g. a broad carbon tax) as opposed to narrower biofuel policies, which disproportionately target gasoline. Alternatively, policies may be designed to take advantage of these indirect effects; for example, the present chapter suggests that policies targeting diesel use may be more effective at reducing emissions than those targeting gasoline. Such an approach would, however, be vulnerable to other, as-yet unidentified market effects. As a result, and in line with conventional economic wisdom, the author recommends policies with broad coverage as the lowest risk approach to carbon mitigation.

Chapter 6. Conclusions and Future Work

This chapter begins by providing brief answers to each of the main research questions outlined in the introduction, followed by a more general discussion, a list of deliverables and research contributions, and finally a discussion of possible directions for future work.

6.1. Research Questions Revisited

Chapter 2: Changing the Renewable Fuel Standard to a Renewable Material Standard: Bioethylene Case Study.

- *What are the life cycle GHG emissions from corn, switchgrass and sugarcane ethanol, and how uncertain are these numbers?*

The chapter developed a life cycle assessment model, using Monte Carlo simulation to characterize uncertainty for key parameters. Mean GHG emissions from U.S. corn ethanol are 97 g CO₂e/MJ, with a 90% confidence interval from 79 to 120 g CO₂e/MJ – a range that spans roughly 40% of the mean value. Mean GHG emissions from U.S. switchgrass ethanol are -18 g CO₂e/MJ (including a credit for surplus electricity production), with a 90% confidence interval from -59 to +18 g CO₂e/MJ – a range nearly double that from corn ethanol. Mean GHG emissions from Brazilian sugarcane ethanol are 33 g CO₂e/MJ, with a 90% confidence interval from 24 to 43 g CO₂e/MJ – the tightest range of the three feedstocks, but one that nevertheless spans nearly 60% of the mean value.

- *What are the life cycle GHG emissions from conventional low density polyethylene (LDPE), produced in the U.S.?*

Ethylene produced from natural-gas derived ethane is the dominant feedstock for conventional LDPE in the U.S. Mean emissions for this pathway are 1.8 kg CO₂e/kg LDPE, with a 90% confidence interval from 1.3 to 2.4 kgCO₂e/kg LDPE – a range that spans roughly 60% of the mean value.

- *What are the life cycle GHG emissions from corn, switchgrass and sugarcane LDPE, and how uncertain are these numbers?*

Mean GHG emissions from U.S. corn LDPE are 2.6 kg CO₂e/kg LDPE, with a 90% confidence interval from 1.7 to 3.6 kg CO₂e – a range that spans over 70% of the mean value. Mean GHG emissions from U.S. switchgrass LDPE are -2.9 kg CO₂e/kg LDPE (a value that remains negative even if credits for surplus electricity are removed), with a 90% confidence interval from -4.9 to -1.2 kg CO₂e/kg LDPE – a range nearly double that from corn LDPE. Mean GHG emissions from Brazilian sugarcane ethanol are -1.3 kg CO₂e/kg LDPE, with a 90% confidence interval from -1.8 to -0.8 kg CO₂e/kg LDPE – roughly half the range from corn LDPE.

- *Can ethanol used for bio-LDPE production meet the GHG reduction targets for ethanol set by RFS2? With what degree of confidence?*

Corn pathways (ethanol or LDPE) have effectively no chance of meeting the 20% RFS2 GHG emission reduction target (relative to gasoline), unless emissions from land use change are far lower than expected, and/or each unit of corn-based product somehow displaces substantially more than one unit of fossil-based product. Sugarcane and Switchgrass pathways (ethanol or LDPE) meet the 50% and 60% RFS2 GHG emission reduction targets (relative to gasoline), respectively, in nearly all iterations of the Monte Carlo simulation. LDPE pathways are particularly robust to assumptions about displacement rate and indirect output use change.

- *Does bio-LDPE achieve similar (or better) GHG benefits to bioethanol used for fuel? With what degree of confidence?*

In approximately 90% of model runs, ethanol produced in the U.S. achieves greater GHG reductions than LDPE, if both displace their fossil counterparts on a 1:1 physical basis. Similarly, in approximately 90% of model runs, LDPE produced in Brazil, and imported to the U.S. achieves greater GHG reductions than imported ethanol. The difference is a result of the weight reducing process of ethanol dehydration to ethylene, and the lower GHG intensity of the Brazilian grid relative to the U.S. In either event, the difference in emissions between feedstocks far surpasses differences in how the ethanol is used.

- *What are appropriate policy recommendations for RFS2 in light of the above results?*
From a GHG perspective, incentives for corn ethanol should be discontinued. In a demand constrained environment, switchgrass ethylene-based products are a promising alternative to switchgrass ethanol used for fuel. For imported Brazilian products, bioethylene-based products will generally be preferred over the fuel ethanol currently incentivized by RFS2. This analysis suggests a strong case for expanding the scope of RFS2 to include credits for chemical use of ethanol. In its narrowest form, a renewable material standard could simply add bioethylene as an approved use for bio-ethanol in RFS2. It would be a simple matter (conceptually, not politically), to allow bioethylene producers to sell credits into the existing RIN market. A more complex scheme could also establish GHG equivalence factors between different uses of ethanol. Long term, replacing RFS2 with a more comprehensive renewable material standard has the potential to provide increased flexibility without compromising GHG reduction targets.

Chapter 3: Uncertainty in the Life Cycle Greenhouse Gas Emissions from U.S. Production of Three Bio-based Polymer Families.

- *What are the cradle-to-gate GHG emissions from producing each of the major commodity thermoplastics (polyethylene terephthalate (PET), polystyrene (PS), polyvinyl chloride (PVC), polypropylene (PP), high density polyethylene (HDPE) and low density polyethylene (LDPE)) in the U.S.? How uncertain are these numbers?*

In the base case (treating the hydrogen co-product by system expansion), mean emissions range from a low of 1.4 kg CO₂e/kg HDPE to a high of 3.1 kg CO₂e/kg PS. HDPE and LDPE exhibit the widest 95% confidence intervals: ~1 kg CO₂e/kg plastic from the low end to the high end, representing 60-70% of mean emissions. PET exhibits the narrowest 95% confidence interval with a span of ~0.5 kg CO₂e/kg PET, representing 20% of mean emissions. Some of the differences in uncertainty can be attributed to data availability: uncertainty is more fully characterized for polyolefin pathways than for the other plastics, for which some intermediate stages used a single point estimate for energy requirements.

- *What are the cradle-to-gate GHG emissions from producing polylactic acid (PLA), polyhydroxybutyrate (PHB), and bioethylene-based plastics in the U.S., using either corn grain or switchgrass as a feedstock? How uncertain are these numbers, and how do modeled emissions differ depending on the data source for fermentation and recovery (for PHB and PLA) and treatment of co-products?*

The model develops a wide range of scenarios for the cradle-to-gate emissions from the production of PLA, PHB and bioethylene or bioethylene based plastics. Results are summarized below:

- Mean emissions from corn PLA range from 1.0 kg CO₂e/kg PLA to 2.9 kg CO₂e/kg PLA, depending on both the fermentation and polymerization data source (responsible for ~60% of this range) or treatment of co-products (responsible for ~40% of this range). In each case, 95% confidence intervals span a range from 50-70% of the mean value.
- Mean emissions from corn PHB range from 2.1 kg CO₂e/kg PLA to 7.8 kg CO₂e/kg PLA, depending on both the fermentation and recovery data source (responsible for ~25-30% of this range) or treatment of co-products (responsible for ~70-75% of this range). In each case, 95% confidence intervals span a range from 45-65% of the mean value.
- Mean emissions from corn bioethylene-based plastics depend on treatment of co-products and range from -0.15 to 1.5 for Bio-HDPE on the low end, to 2.6 to 3.1 for Bio-PS on the high end. Similar to the fossil-plastic cases, bio-PET exhibits the narrowest 95% confidence interval, with an interval length of ~0.45 to 0.6 kg CO₂e/kg PET depending on treatment of co-products; bio-HDPE and bio-LDPE exhibit the widest 95% confidence intervals, with interval lengths of 1.3 to 2.2 kg CO₂e/kg plastic, depending on the treatment of co-products.
- Mean emissions from switchgrass PLA (single data source for fermentation and polymerization) range from -0.19 kg CO₂e/kg PLA to 1.3 kg CO₂e/kg PLA, depending on the treatment of co-products. The length of the 95% confidence intervals range from 0.6 kg CO₂e/kg PLA to 1.4 kg CO₂e/kg PLA, depending on the treatment of co-products.

- v. Mean emissions from switchgrass PHB range from -0.97 kg CO₂e/kg PHB to 5.1 kg CO₂e/kg PLA, depending on both the fermentation and recovery data source (responsible for ~10-55% of this range) or treatment of co-products (responsible for ~45-85% of this range). The width of the 95% confidence intervals vary from a low of 0.78 kg CO₂e/kg PHB to a high of 4.36 kg CO₂e/kg PHB, with most falling in the range from 2 to 3.5 kg CO₂e/kg PHB.
 - vi. Mean emissions from switchgrass bioethylene-based plastics depend on both treatment of co-products and assumptions about reaction yields. These means range from lows of -0.4 for the most optimistic polyethylene (HDPE and LDPE) scenarios to highs of 3.6 for the most pessimistic scenarios of PS and LDPE. Bio-PET scenarios exhibit the narrowest 95% confidence intervals, ranging in length from 0.6 to 1.1 kg CO₂e/kg PET; bio-HDPE and bio-LDPE exhibit the widest 95% confidence intervals, with lengths varying in magnitude from a total of 2.7 to 5.7 kg CO₂e/kg plastic, depending on the scenario.
- *What are the expected end of life emissions from each of the fossil-based and bio-based polymers listed above?*
 Mean emissions from incineration with energy recovery range from a low of 0.9 kg CO₂e/kg plastic for PLA, to a high of 2.1 kg CO₂e/kg plastic for PS. Only PLA and PHB are compostable; the former produces approximately 1.7 kg CO₂e/kg PLA, while the latter produces 1.9 kg CO₂e/kg PHB, when composted. Landfilling likely causes low emissions (0.04 kg CO₂e/kg plastic) for all polymers with the exception of PHB, for which landfilling releases between 2.2 and 4.8 kg CO₂e (90% confidence interval). Due to applied emissions credits, GHG emissions from recycling are highly correlated to the virgin cradle-to-gate emissions for each polymer; with the exception of switchgrass-based polymers, which can have negative life cycle emissions, recycling results in a net emission savings up to a mean of 1.9 kg CO₂e/kg plastic (for PS).
 - *Accounting for uncertainty, how do GHG emissions from each of the modeled bio-based plastics compare to emissions from each of the modeled fossil-based plastics?*

In general, PHB (from either feedstock) is unlikely to have lower emissions than fossil polymers once end of life emissions are included. PLA generally has the lowest emissions when compared to high emission fossil polymers, such as polystyrene (mean GHG savings up to 1.4 kg CO₂e/kg corn PLA and 2.9 kg CO₂e/kg switchgrass PLA). In contrast, bioethylene is likely to achieve the greater emission reduction for ethylene intensive polymers, like polyethylene (mean GHG savings up to 0.60 kg CO₂e/kg corn polyethylene and 3.4 kg CO₂e/kg switchgrass polyethylene). In many scenarios (though not all) there is a non-trivial probability that a given bioplastic will have higher GHG emissions than a given fossil plastic.

Chapter 4: Greenhouse Gas Mitigation for U.S. Plastics Production: Energy First, Feedstocks Later.

- *What GHG emission reductions are possible if fossil-plastics are produced using renewable energy (e.g. wind power and renewable natural gas) in place of conventional fuels?*

Adopting low-carbon energy (wind and renewable natural gas) across the chemical industry supply chain for all conventional thermoplastics can reduce GHG emissions in that industry by 50-75%, with mean annual savings of 38 Mt CO₂e/year across the North American industry.

- *In the U.S. plastics industry, how do the GHG savings from energy substitution (i.e. using renewable energy in place of conventional energy) compare to the GHG savings achieved by feedstock substitution (i.e. replacing fossil-plastics with PLA, PHB or bioethylene based bio-plastics, produced from either corn or switchgrass, and using either conventional or renewable energy)?*

In over 98% of simulations, producing fossil plastics with low carbon energy results in lower emissions than switching to baseline corn-based bioplastics. Emissions from the corn pathway (with conventional energy) exceed emissions from the fossil plastic energy substitution pathway by ~20-30 Mt CO₂e (median results) depending on the end of life scenario for PLA. Advanced feedstock substitution (using switchgrass, or corn processed with renewable energy) likely results in even lower GHG emissions than energy

substitution, but with more certainty in the landfill scenario (90% of simulations and 99% of simulations, respectively) than in the compost scenario (55% and 75% of simulations, respectively).

- *How might other factors such as cost and market size influence the choice between feedstock substitution and energy substitution?*

These factors tend to favor energy substitution: bio-based products are likely more expensive than low-carbon energy, may have high non-GHG environmental impacts, can be difficult to substitute for conventional products, and serve a smaller overall market than does renewable energy. In some cases, however, bio-based plastics may have properties (e.g. biodegradability) that will make them attractive to certain consumers.

Chapter 5: Biofuels and Indirect Output Use Change: the Role of Refineries.

- *Over the long run, what flexibility does the petroleum industry have to choose its product slate (i.e. the mix of finished petroleum products it produces)?*

The findings suggest that refineries can achieve yields of gasoline that range from below 10% up to nearly 60%. Distillate yields can likewise range from below 10% up to 50% or more in extreme cases. While it is unlikely that the industry average could ever reach the extreme ends of these ranges, even a simple comparison between the U.S. and the rest of the world suggests the petroleum industry can swing its yields of gasoline by more than 20 percentage points. Comparing either the U.S. and rest of world, or U.S. production over time suggests distillate yields can vary by at least 10 percentage points. Individual refineries are likely far less flexible in the short-run.

- *How responsive is the crude oil refining sector to relative shifts in price among its major products?*

Analysis suggests that refineries in the U.S. respond primarily to gasoline and distillate prices, which I normalize by the price of crude oil. Regression results indicate that distillate has mean yield elasticities of approximately 0.40 to 0.50 relative to its own price, and -0.42 to -0.34 relative to the price of gasoline. In contrast, gasoline has smaller mean yield elasticities of approximately 0.17 to 0.20 relative to its own price, and -0.25

to -0.22 relative to the price of distillate. The numbers represent an upper bound for the global petroleum industry, since it is likely that the American refineries used in the analysis are more responsive than less complex refineries in the rest of the world.

- *How is the petroleum industry likely to respond to shifts in demand for individual products, such as reduced demand for gasoline brought about by policies like the RFS2?*
The biofuel policies considered in this thesis likely induce price changes on the order of cents to tens of cents per gallon of gasoline and diesel respectively (Figure 5.11). This induces the global petroleum sector to shift its relative yields of gasoline and diesel by several tenths of a percentage point in most policies considered. A couple of extreme scenarios predict yield changes of up to 3 percentage points.
- *How does the existence of refiner flexibility affect the balance of GHG emissions and petroleum consumption that result from different policies aimed at reducing consumption of petroleum fuels?*

Although the model predicts only small changes in relative product yields, these can have dramatic consequences for the total GHG emission changes induced by the different biofuel policies, on the order of tens or hundreds of megatonnes of CO₂e/year. In the upper bound cases where all refineries exhibit the same yield elasticities as U.S. refineries, share mandates and emission standards likely result in a net increase in GHG emissions even before accounting for emissions from biofuel production!

- *What recommendations does this analysis suggest for policies aimed at reducing petroleum use, and GHG emissions through the use of biofuels?*

This analysis suggests that share mandates and emission standards that apply disproportionately to gasoline consumption may be ineffective policies for reducing GHG emissions. Policies like a carbon tax that apply more evenly across petroleum products, and create a price wedge between producers and consumers are far more likely to result in emission reductions. If nothing else, this work suggests that additional research is needed to understand how biofuel policies affect the dynamics of the global petroleum market.

6.2. Discussion

This thesis examines a series of questions on whether and how to use biomass for GHG mitigation: fuel, feedstock, or neither? Internationally, policies tend to focus on using biomass as a transportation fuel. This narrow scope skews the market and risks producing a suboptimal allocation for uses of biomass, while leaving policies vulnerable to idiosyncratic hurdles like the ethanol blend wall. If biofuels and bio-based products are to continue playing a role in decarbonizing the transportation sector, it will be critical to move away from first generation feedstocks, like corn, toward more advanced feedstocks, like switchgrass. These markets are unlikely to develop without a strong and stable demand, which the world's largest biofuel policy – the U.S. renewable fuel standard – is presently failing to provide. In Chapter 2, I examine the GHG impact of expanding the scope of RFS2 to include credits for bioethylene-based products. I conclude that replacing RFS2 with a broader mandate can provide increased flexibility to obligated parties and shore up the flagging standard without compromising GHG reduction targets. Having concluded that bio-based plastics are a reasonable extension to RFS2, Chapters 3 and 4 then take a step back and ask whether these plant-based plastics make sense in the first place. Chapter 3 demonstrates that there are large uncertainties involved in the life cycle GHG emissions from bio-based plastics, and that only a subset of pathways is likely to be preferable to conventional plastics. Chapter 4 further demonstrates that greater GHG reductions are possible in the near term by focusing on energy substitution rather than feedstock substitution. Thus, while a fixed quantity of ethanol may just as well be used as fuel or to produce plastics, the plastics industry itself can have a larger, more immediate impact on GHG emissions by focusing on renewable energy rather than bio-based plastics. That is not, however, where the story ends. Adopting low carbon energy can reduce the GHG emissions from plastics production only by 50-75%. The remaining emissions stem primarily from upstream oil and gas operations that will be far more difficult to decarbonize. The plastics industry is one of the few industries that has a built-in potential for negative life cycle GHG emissions. Thus, in the long run, it could be advantageous to transition toward bio-based plastics with a combination of advanced feedstocks and low carbon process energy. Doing so would, however, require careful management of land, water and fertilizer to avoid creating new problems for global hunger, water scarcity, water quality and ecosystem health.

Finally, Chapter 5 returns to the dominant form of biomass-related government incentives: biofuel policies. Chapters 2-4 have already highlighted some fundamental uncertainties in the GHG emission from bio-based products. For the most part, however, these models exclude a potentially large class of model uncertainty related to how market factors can change the GHG balance that results from adopting bio-based products. This is traditionally the domain of consequential LCA. While a nascent literature quantifies indirect output use change resulting from biofuels production, flexibility in the refining sector has traditionally been ignored altogether. Chapter 5 demonstrates that biofuel policies may induce a shift toward greater diesel production at the expense of both gasoline and non-combustion petroleum products. This has the potential to result in a large increase in GHG emissions, even relative to other CLCA models of the global petroleum sector. This effect dramatically increases the chance that biofuel policies will actually increase GHG emissions, even before accounting for emissions from biofuel production. A simple fix would be to craft policies in a way that does not disproportionately target the gasoline market, as RFS2 currently does. This conclusion echoes the results from Chapter 2: policies with a broad base run a lower risk of creating unexpected or unfavorable distortions.

In the long-run, different GHG mitigation measures and different uses for biomass need not be mutually exclusive. In the meantime, however, financial, political and physical resources are limited. Thus, it is imperative to set mitigation priorities, and to craft policies that produce favorable results in the short-run, while creating an appropriate long-term trajectory. This dissertation demonstrates that existing policies and private ventures are potentially failing in those objectives. Biomass systems continue to be fraught with uncertainty, including some important market dynamics that have previously been ignored altogether. Biofuels and bio-based plastics may indeed have an important role to play in future GHG mitigation, but this dissertation suggests they are not currently the low-hanging fruit. It is prudent and advisable to continue developing technologies for advanced biofuels and bio-based plastics, however, market deployment should not yet be a priority.

6.3. Deliverables

The key deliverables from this work are peer-reviewed journal publications. Chapters 2 and 3 have been published in *Environmental Science and Technology*.^{144,154} Chapters 4 and 5 will be submitted for publication in the near future. Additionally, the results of chapters 2-4 have all been presented at domestic and international conferences, and have won several conference awards. The results of chapters 2 and 3 have also been disseminated through CMU press releases, an *Energy Collective* blog post, and an interview and subsequent article in *Chemical & Engineering News*. I will seek out similar outlets to disseminate the results of chapters 4 and 5 once that work is published.

6.4. Research Contributions

This thesis answers an important subset of questions regarding how, or even if, to use biomass for GHG mitigation. To my knowledge, it is the first to propose expanding the scope of the renewable fuel standard and to quantify the GHG implications of doing so. It is the first work that systematically harmonizes and quantifies uncertainty in the GHG emissions from a range of fossil-based and bio-based plastics, and the first to consider the potential role for low-carbon energy in the production of conventional plastics. It is also the first work in decades to quantify how refiners are likely to respond to relative changes in market prices, and it is the first either to use monthly data, or to apply dynamic regression models like the partial adjustment and adaptive expectations models. To my knowledge, this is also the first work to highlight the potentially large GHG consequences of refiner flexibility in evaluating policies for reducing the use of petroleum fuels. In conducting this work, I have continued to extend and develop methods for quantifying uncertainty in LCA, and have proposed new ways of crafting policy or private sector decisions that better account for the existence of uncertainty.

6.5. Future Work

6.5.1. Continued Analysis of Best use of Biomass for GHG Mitigation

This dissertation has examined an important subset of the ways in which biomass may be used for GHG mitigation: ethanol biofuel and bio-based plastics. Biomass can also be used to generate

heat or electricity, as feedstocks for other organic chemicals, for other biofuels such as biodiesel and bio-jet fuel, or as a carbon storage/sequestration medium (e.g. via afforestation). Several studies have shown that biomass resources, while substantial, will likely be insufficient to meet global energy demand. Thus, there is an ongoing need to establish which uses of biomass are either a) most likely to achieve GHG reductions, or b) which end uses have the greatest need for bio-based products in order to meet long-term GHG emission goals. The techniques used in this dissertation can be extended to a wide range of additional product systems and coupled with a deeper analysis of mitigation alternatives in those sectors. It would also be instructive to consider specifically how these different low-carbon futures might evolve and to investigate the impact of different bio-based products in a dynamic fashion, for example, with a reduced form climate model.

6.5.2. Quantification of Non-GHG Impacts from Bio-based Products

The present work evaluated primarily the GHG implications of biofuels and bio-based plastics. Increased use of bio-based products is well known for the risk of environmental burden shifting: GHG reductions, but at a cost to air and water quality, water scarcity, global hunger and ecosystem health among others. Much of the existing literature has focused exclusively on GHG emissions. Significant gaps exist in quantifying other environmental impacts, particularly with respect to the characterization of uncertainty and providing spatial resolution for these impacts; unlike GHGs, the importance of other pollutants depends on local conditions surrounding the emissions source. Final recommendations must also depend on how much weight to assign to each of these competing impacts. These are all critical areas for future work.

6.5.3. Extensions to Chapter 5: a Deeper Look at the Global Petroleum Refining Industry.

The results from Chapter 5 suggest several avenues for future research, either as part of the current paper, or as part of a longer-term research agenda. Adding a more explicit refinery cost model is among the most important enhancements that could be made to the overall model. In the short-term, it is possible to use relatively simple refinery economics models to compare the capital and operating costs of different refinery configurations (e.g. based on refs^{354,355}). Further the partial equilibrium model could be updated to include multiple different types of crude oil,

including separate supply curves, product slates and upstream emissions; together these two steps would allow for increased bottom-up modeling of refinery response that could be compared to the top-down model presented here. A more complete picture of refiner response would also require an explicit model of how refineries can make operational adjustments to change their product slate without changing the type of crude oil processed or the installed process units. While PRELIM has some limited functionality for adjusting refinery operating conditions, these modules are fairly minimal, and are still under development. A limited investigation using either PRELIM or existing literature (e.g. ref³⁴⁰) could be added to the present paper; greater detail would require either access to data from individual refineries, or a professional simulated distillation program.

Other relatively minor adjustments to the present work could include a more in depth treatment of the relationship between different petroleum product yields using international data (e.g. ref³⁵¹), or a more detailed analysis of how demand elasticities differ between petroleum products and the implications for biofuel policies; currently the model simply assumes the same range of demand elasticities for all three categories of petroleum product. EIA data³⁵⁶ could also be used to probe further the potential relationship between refining emissions and product yields discussed in section 5.4.2. Additionally, it may be worthwhile to create a new range of policy scenarios to explore the benefits of adopting policies with broader coverage (e.g. a biofuel mandate with equally stringent biodiesel and bioethanol requirements).

As part of a separate project, there is also a need to work toward validating/ground truthing the different models of indirect output use change (IOUC) in response to biofuel policies. It has already been over 10 years since the first U.S. Renewable Fuel Standard was established.¹¹⁹ Without a clear counterfactual for the last decade, it is impossible directly to compare the results of theoretical models, like the one developed here, to observed outcomes. Nevertheless, these theoretical models do make general predictions, which, with the right set of additional control variables, can and should be tested.

Longer term, an even more detailed bottom-up refinery model will be required to examine the potential impact of much larger shifts in product demand than can be predicted by historical

observation. At present the existing models for exploring IOUC in the petroleum sector all rely (to varying degrees) on the assumption that there will be no irreversible upheavals in the structure of the industry. To meet the stringent GHG reduction targets that will be required to avert catastrophic warming will require far more than the marginal changes the existing models assume. There will thus be a need to envision what a much reduced petroleum industry will look like in such a future, to explore changes that must occur to keep crude oil in the ground (as compared simply to slowing its extraction), and to reassess which finished products will be the most important bottlenecks.

An additional extension could involve developing new IOUC models with non-competitive markets. Although some existing models include logistical constraints (e.g. the ethanol blendwall), only Hochman *et al.* (2010)³²⁹ considered the possibility of market power in the form of a cartel of nations model. There exist, however, a host of other models for characterizing the international oil industry, including multiple different oligopolistic models (e.g. Cournot with or without market sharing, Bertrand, Stackelberg), as well as target revenue models and target price models, among others.³⁵⁷ Adapting one or more of these models to calculate the resulting IOUC from biofuel policies would add new insight into the range of possible market responses to increased use of biofuels. If estimates vary considerably across model choices, the different possibilities could be used as part of a robust decision making framework for policies aimed at reduced use of petroleum products or GHG emissions

The results of Chapter 5 suggest it may be worth investing time to develop a more complex model of the global fuels market that accounts for refiner behavior in substantially more detail.

6.5.4. Indirect Output Use Change Model for the Chemical Sector

Chapter 5 and the extensions discussed in section 6.5.3 focus on the petroleum sector, with particular emphasis on liquid fuels. There is potentially even wider scope for modeling IOUC in the chemical sector, which would directly complement analyses presented in chapters 2-4. Although several papers have now examined IOUC from biofuels, no equivalent analysis yet exists for bio-based chemicals. Following a partial equilibrium framework such as the one used in Chapter 5, one could characterize IOUC resulting either from the production of a single bio-

based chemical intermediate like bioethylene, or more broadly from the production of various bio-based plastics. The North American petrochemical industry is heavily dependent on natural gas liquids (NGLs), which are the primary feedstock for the production of olefin intermediates in the U.S.¹⁵⁴ Thus, in addition to elasticities from the petroleum sector, one would also need to develop supply and demand elasticity estimates for the natural gas sector. While there exist elasticity estimates for natural gas used as fuel (e.g. refs^{358,359}), I am not aware of any prior work that quantifies elasticities related to natural gas liquids.

Beyond the simple partial equilibrium analysis described above, there is some scope for investigating the detailed workings of natural gas and NGL markets. One could investigate the extent to which natural gas producers can change their product slate, for example by developing different wells, or by simply leaving more NGLs in the final natural gas product. Unlike petroleum products, NGLs are not globally traded commodities. Nevertheless, the U.S. shale gas boom has brought about increasing exports of even the most unwieldy (volatile) NGL, ethane.³⁶⁰ Investigation of export costs, and potential NGL markets abroad (e.g. steam cracking facilities, heating fuel, etc.) would also help bound the market response to a reduction in domestic demand for NGLs. Finally, an economic analysis of U.S. natural gas operations could help predict the response of domestic producers to a drop in price of NGLs resulting from increased use of bio-based chemicals. My own preliminary analysis of EIA data suggests that NGLs make up approximately 30% of value from natural gas wells, explaining why they may actually be the driving force behind continued production in the current climate of low natural gas prices.³⁶¹ A particularly salient question would be: how far do NGL prices have to fall before natural gas wells begin to shut down?

6.5.5. Robust Decision Making for Biofuel Policies

Existing attempts to quantify the uncertainty related to life cycle GHG emissions from biofuels and bio-based products have focused on assigning probability distributions to key parameters and using Monte Carlo simulation to characterize outcomes (e.g. refs^{74,144,154}). Given the large, difficult to characterize, and potentially irreducible uncertainties associated with biofuels, particularly with respect to indirect land use change,^{85,286} and IOUC, a robust decision making framework³⁶² may be more appropriate for evaluating policies like RFS2.

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Appendix A. Supporting Information for Chapter 2

A.1. Model and Data

A.1.1 Allocation

Production volumes for each natural gas co-product are established as follows. EIA reports annual production by state for dry natural gas,²¹¹ lease condensate,³⁶³ and combined natural gas plant liquids^a (NGPLs)³⁶⁴ as well as annual production of disaggregated NGPLs^b by refining district.^c The combined NGPLs from each state are assumed to be distributed among individual products in the same (volumetric) proportion as the refining district(s) to which that state belong(s). Unless otherwise specified, all data used in this chapter pertains to reporting year 2011 (the most recent available data). Allocation is performed on a state by state basis and integrated into a discrete distribution for each process modeled, as discussed in the main text. Mass and energy densities of relevant substances can be found in Table A.7.

A.1.2 Global Warming Potential

Whenever possible, GHG emissions were modeled explicitly by gas before conversion to CO₂ equivalent. For natural gas pre-production emissions (well pad construction, well drilling, hydraulic fracturing chemicals and water management),²⁰⁹ and life cycle emissions for fuels,^{198,201,206} only the total GWP was available. Emissions from natural gas used as fuel, fugitive CH₄ from production, liquids unloading, processing, transmission, distribution and combustion were modeled explicitly as per Venkatesh *et al.*²⁰¹ and used to update the life cycle GHG estimate accordingly. No adjustment was made to the other inputs listed above.

^a Data is by state of origin of the gas (as opposed to state of processing).

^b Categories reported are: ethane, propane, isobutane, normal butane and pentanes plus.

^c Refining districts are subdivisions of petroleum administration for defense districts (PADDs).

A.1.3 Fuels and Electricity

As indicated in the main text, emissions from U.S. electricity production are modeled by North American Electric Reliability Corporation (*NERC*) region.²⁰⁸ For corn ethanol, the majority of existing ethanol biorefineries are located in the region spanned by the Midwest Reliability Organization (MRO).²³⁰ For switchgrass, the EPA predicts production primarily in the regions spanned by the Southwest Power (SPP), the Texas Regional Entity (TRE) and the Southeast Electric Reliability Council (SERC),¹²⁸ and so it is assumed these are the regions where most switchgrass biorefineries will be located. Finally, the majority of existing ethylene production capacity is located in the region spanned by TRE and SERC.²³¹ Due to difficulties in transporting ethylene gas and the large scale of existing chemical manufacturing complexes, it is assumed that bioethylene production and ethylene polymerization will take place near existing ethylene infrastructure (i.e. in TRE and SERC). For each region, multiple sources were consulted and a uniform distribution was employed that spans the ranges of the different estimates. For aggregated regions, distribution bounds represent the extreme estimates for any of the constituent regions. For electricity consumption, emissions factors account for transmission line-losses; when grid electricity is displaced, it is assumed that line-losses still occur, resulting in lower emissions savings. Line losses are taken to be 5.8% for U.S activities (representative of the Eastern Interconnect)³⁶⁵ and 16% for Brazil.³⁶⁶

Electricity emissions factors employed in this chapter are nominally for average electricity generation.^{202,207,272-274} Nevertheless, the range employed for each U.S. region encompasses the marginal electricity emissions factor for that region as reported by Siler-Evans *et al.* (2012),³⁶⁷ after adjusting for line-losses and upstream emissions from coal and natural gas.^{201,206,365,366} Following Liptow and Tillman,¹⁹¹ natural gas is assumed to be the marginal electricity source in Brazil; this is examined further in the sensitivity analysis below.

A.1.4 Natural Gas Pre-Production

Emissions (in CO₂e/unit gas produced) from well pad construction, well drilling, production of chemicals for hydraulic fracturing, and water management from fracturing employ the same inputs as Weber and Clavin²⁰⁹ and are modeled as triangular distributions. The two distributions

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pertaining to hydraulic fracturing are multiplied (on a state by state basis) by the percentage of gross gas withdrawals that are from unconventional wells.²¹¹

Weber and Clavin report their distributions as g CO₂e/MJ, which results from allocating all emissions to dry natural gas. These figures are converted to CO₂ emissions per unit volume assuming the same energy density as Weber and Clavin (35.95 MJ/m³) and then allocated across products (and normalized per unit mass of each product).

Further, for both conventional and unconventional wells, there is the potential for a release of fugitive natural gas emissions during the final pre-production phase (well completions) or from remedial operations to increase production (workovers). Well completions and workovers are divided into 3 categories according to EPA nomenclature: conventional wells, unconventional^d wells (uncontrolled emissions) and unconventional wells (controlled emissions^e) as outlined below.

Fugitive emissions from conventional completions and workovers are taken from 2010 revised estimates by EPA³⁶⁸. These are coupled with conservative (low) estimates for well lifetime and daily production, from Venkatesh *et al.*,²⁰¹ to obtain emissions per MMscf of gross withdrawals. Further, a conservative (high) number of workovers (1 per year) is assumed. Even with conservative assumptions in place, conventional well workovers and emissions amount to less than 1% of the total emissions from ethylene production and so the uncertainty was not characterized further.

For unconventional wells, potential emissions from uncontrolled completions or workovers are much higher and could have a large effect on the final results. Following a 2012 EPA background technical support document, an uncontrolled completion or workover is assumed to

^d Following the U.S. EPA, unconventional wells are assumed to involve hydraulic fracturing, and include tight sand, shale, and coal bed methane formations. ^{368 p.84}

^e Controlled completions are also known as ‘green completions’ and ‘reduced emission completions’ (RECs)

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release a normally distributed volume of methane.³⁶⁹ This is converted to release of whole gas using the EPA assumed methane content of 83.24%. The result is coupled with a distribution for estimated ultimate recovery from Weber and Clavin²⁰⁹ to normalize the emissions of whole gas per volume of gas produced. Finally, whole gas released is converted to emissions of methane and carbon dioxide per MMscf of production, assuming respective methane and carbon dioxide contents in each state equal to that of the hydraulically fractured wells in the National Energy Modeling System (NEMS) region²¹³ to which that state belongs^f (tables A-130 and A-139 of ref²¹²). For reduced emission completions (RECs), it is assumed that 90% of flowback emissions are captured³⁷⁰; all other calculations are the same as for uncontrolled emissions. Finally, following Jiang *et al.*,³⁷¹ a uniform distribution is assumed for the percent of released gas which is flared; flare efficiency is taken to be 98%. For the base case, EPA projects that, in the absence of regulations, 51% of completions would be performed with reduced emissions in 2015.³⁶⁹ However, current regulation requires flaring for all new completions, and green completions with flaring for all completions subsequent to January 2015. Simulating a ‘regulated scenario’ assuming 100% RECs, and 100% flaring had no noticeable effect on the final results.

For unconventional workovers, the well pad will already be fitted with appropriate gathering equipment, and so I assume that any refractures will be performed with reduced emissions as described above. Using various data sources, the U.S. EPA finds that the annual refracture rate among unconventional wells is approximately 1%.³⁶⁹ Although the number of workovers is likely positively correlated with the estimated ultimate recovery, employing a correlation parameter had little effect on the final results.

Workover and completion emissions are multiplied by the corresponding (conventional or unconventional) percent of gross withdrawals on a state by state basis for 2011.²¹¹ Completion

^f For states that belong to multiple NEMS regions (Texas and New Mexico), CO₂ and CH₄ contents are modeled as uniform distributions across the values for the relevant regions.

emissions from oil well completions are much smaller overall³⁷⁰ and it is assumed that the portion allocated to the associated gas will be negligible.

A.1.5 Natural Gas Production

The annual EPA GHG Inventory provides data on CH₄ emissions from the natural gas production phase.²¹² From the 2013 EPA GHG Inventory, table A-124 is used to determine potential production emissions by NEMS region. Workovers and completions are removed, as these have been accounted for in the above pre-production analysis. Reductions by the Natural Gas STAR program (table A-132) and from other regulations (table 1-133) are allocated to each NEMS region in proportion to that region's share of total emissions from the relevant category.^g Because production volumes are only known by state and some states (New Mexico and Texas) are covered by more than one region, it was necessary (for normalization by production volumes) to merge certain NEMS regions, leaving 3 regions in all: West Coast, North East and the combined Midcontinent, Rocky Mountains, Gulf Coast and South West region. EPA further reports uncertainty from -19% to +30% for CH₄ emissions from the entire natural gas system,²¹⁴ for which field production is the single largest category (accounting for just over a third of system wide emissions). It is assumed that the relative uncertainty on production emissions within each region is on the same order as for system wide emissions, and so a triangular distribution is used for the emissions within each region. Production CH₄ emissions from each region are then normalized by gross withdrawals for all states within that region;²¹¹ these emissions are then allocated across products (and normalized per unit mass of each product) on a state by state basis.^h The overwhelming majority of CO₂ emissions from the natural gas production phase reported in the EPA GHG Inventory are from gas flaring, which has already been taken into account above using direct EIA data.

^g For example, the North East region accounts for 33.5% of all potential emissions from Kimray pumps (table A-124), and so 33.5% of CH₄ reductions for Kimray pumps (Table A-132) are likewise attributed to the North East.

^h Each state is assumed to have the same emission intensity as the region to which it belongs. Alaska, which is not part of any region, is assumed to have the same emission intensity as all regions combined (i.e. national emission intensity).

A.1.6 Natural Gas Processing

The following is an account of statistical methods that were used in analyzing the data from the EPA GHG inventory after matching with EIA processing flows.

Using ordinary least squares (OLS) regression of normalized emissions on plant flow confirms there is no overall trend for normalized emissions in function of plant flow ($p=0.12$) – suggesting that the data may be drawn from a static distribution. Visual inspection of the data (in tonnes CO₂e/MMcf processed) suggested a small number of outliers with abnormally high emissions. This is confirmed with a number of statistical tests, as described below.

In the end, the five points with the highest normalized emissions were removed from the dataset as they are believed to represent data errors rather than true heterogeneity in emissions. All such points were more than 3 times the interquartile range above the 75th percentile of the distribution. One of the outliers was driven by exceedingly high normalized CH₄ emissions – 4 times higher than the next highest entry and nearly 14 standard deviations above the mean.

Initial attempts to fit the data suggested that a lognormal distribution would be appropriate, and indeed a Shapiro-Wilk test on the log-data (post-removal of outliers) does not reject the null hypothesis of normality at the 5% level. Thus, further tests were run on the natural logarithm of the normalized emissions. The remaining four suspected outliers are all greater than 1.5 times the interquartile range above the 75th percentile in the log data. Further all were beyond 3 standard deviations away from the mean, giving less than 0.3% chance they belong to the (assumed normal) distribution.

Of five eliminated outliers, three were for the lowest plant flows in the dataset (1.22, 1.7 and 2 MMcf/day), and the 4th was among the 11 smallest (9 MMcf/day). While it is possible that these results suggest a steep upward trend in normalized emissions for small plants, plants below the size of 9 MMcf/day account for less than 1% of all natural gas processing (according to the complete EIA dataset). A more likely explanation is that the facilities with low plant flow have

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processing as a secondary operation in a larger facility, thereby falsely inflating emission estimates for natural gas processing. The 5th outlier was close to average plant flow (145 MMcf/day), but had well below average utilization (21%), suggesting that the EIA reported plant flow may not be representative of the true processing flows for the (slightly mismatched) time period of the EPA reported emissions. Inclusion of all outliers would increase mean processing emissions by approximately 20%, which represents only a small (<2%) increase in life cycle GHG emissions for LDPE.

Upon removal of the outliers OLS regression of normalized emissions on plant flow now predicts a significant downward trend in normalized emissions in function of plant flow, but with an absolute coefficient so small as to be irrelevant.

Through a series of OLS regressions and Goldfeld-Quandt tests for heteroskedasticity, it is determined that the variance of total emissions increases approximately linearly with plant flow; this result is as expected if one imagines total emissions in each plant to be the result of a sum of emissions from multiple discrete unit plant flows for that plant.

Normalized emissions of greenhouse gases for each plant are then used to fit continuous distributions (weighted by the plant flow for each facility) as shown in Figure A.1. This has the advantage of accounting for the fact that larger plants yield more efficient estimates for normalized emissions. To the extent that normalized emissions may not actually be constant with increasing plant size, this method will also weight each observation in proportion to the likelihood that gas was processed at the corresponding plant.

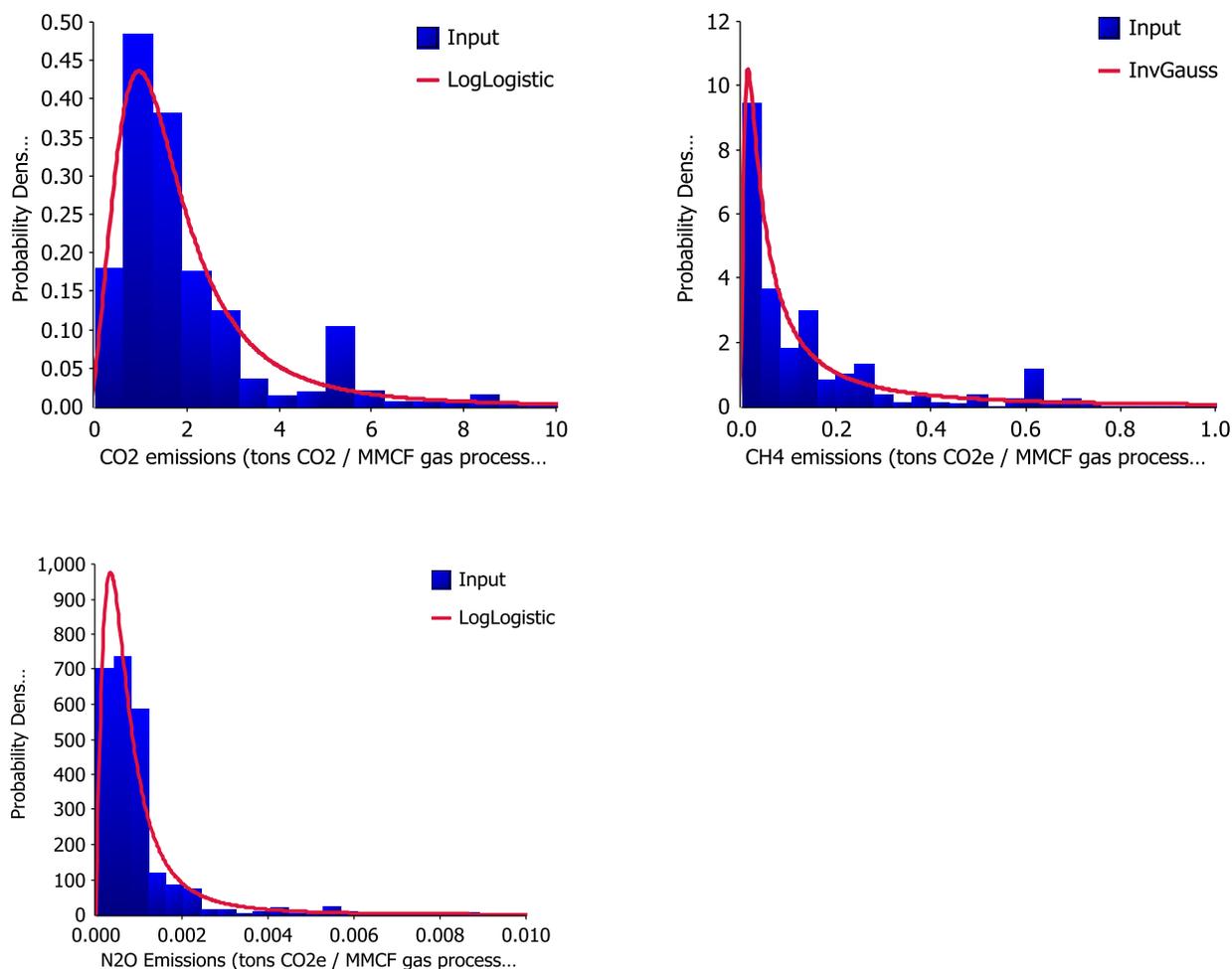


Figure A.1. Input data (histogram) and fitted distributions for emissions from natural gas processing

A.1.7 Steam Cracking

Specific energy requirements (lower heating value) for the production of a tonne of ethylene via steam cracking of ethane are estimated by a number of sources.²¹⁷⁻²¹⁹ The ranges given are very similar, and are used as the parameters of a uniform distribution. The resulting distribution is renormalized per tonne of ethane input using the stochastic output of ethylene determined below.

Volumes for each product resulting from steam cracking ethane are also given by a variety of sources.²¹⁷⁻²²¹ Production volumes from each source are normalized to 1 tonne of ethane input (using the stochastic distribution for product losses across sources if the original value is given only as a ratio of products). From these estimates are formed distributions for each product (triangular if there is a modal clustering across sources, or uniform otherwise). Since

product/loss draws are performed independently, there is no guarantee of mass balance; all products (and losses) are scaled equivalently to restore mass balance for each Monte Carlo draw.

It is assumed that methane, C4 components (i.e., butanes) and C5/C6 (i.e., pentanes, hexanes) components are all used to power the steam cracking process. Combustion is assumed to be complete, and so CO₂ emissions are determined stoichiometrically for each product. Lower heating values for each component (Table A.7) are used to determine the quantity of energy provided. Any residual energy needs are assumed to be provided by natural gas, with a stochastic life cycle emission factor set to approximate the results reported by Venkatesh et al.²⁰¹ Finally, direct CH₄ emissions are modeled as reported by the IPCC GHG guidelines.²²²

A.1.8 Ethanol Production

Sugarcane ethanol is co-produced with electricity from the combustion of bagasse. Seabra *et al.*¹⁹⁹ report both co-production of electricity and an additional quantity of bagasse which they assume displaces fuel oil. This chapter takes a more conservative approach assuming that this additional bagasse is instead used for electricity generation, which is in line with existing trends toward greater electricity export from ethanol mills.¹⁹⁹ This produced bagasse is assumed to have a moisture content of 50%;²⁰² electricity generation is assumed to take place with a LHV efficiency of 30%³⁰⁷ and to displace Brazilian grid electricity.

A.1.9 Ethanol Dehydration

Following Liptow and Tillman,²⁰⁰ modeled emissions from ethanol dehydration to ethylene are limited to fuel and electricity use reported by Kochar *et al.*¹⁸⁰ for polymer grade bioethylene. As no other published estimates are readily available, generic uncertainty factors were applied. Following Geisler *et al.*,²²⁷ both fuel and electricity requirements were assumed to follow a lognormal distribution with dispersion factor (ratio of 97.5th percentile to the median) of 2, which is typical of the uncertainty in energy requirements for chemical production.

A.1.10 Polymerization

For U.S. pathways, polymerization is modeled using average U.S. industry data as reported by Franklin Associates.¹⁴⁵ Grid electricity, natural gas, LPG and residual oil are treated on a life cycle basis. Following the recommendation of Franklin Associates, recovered energy from waste gas is treated as LPG (excluding upstream emissions) with combustion emissions as in Venkatesh *et al.*,¹⁹⁸ for bio-based pathways, waste gases are assumed to be biogenic (no net emissions). Primary energy for electricity cogeneration is divided between natural gas (59%), coal (28%) and waste gases (13%) as reported by Franklin Associates; these percentages were used in a probability mixture model as the probabilities for each fuel type (drawn from a discrete distribution).

Following Liptow and Tillman, polymerization in Brazil is assumed to follow European parameters,^{191,200} involving higher electricity use and lower on-site fuel use than in the United States.^{200,228} Due to the low emissions factor for Brazilian electricity, this results in relatively low emissions for Brazilian polymerization, consistent with the values reported by Kikuchi *et al.*¹⁹⁴

A.1.11 Model Parameters

The following tables present a list of the key parameters for each of the models developed in this chapter. Table A.1 shows parameters specific to the production of ethylene from natural gas derived ethane. Table A.2 shows parameters specific to the production of ethanol from U.S. corn starch. Table A.3 shows parameters specific to the production of ethanol from U.S. switchgrass. Table A.4 shows parameters specific to the production of ethanol from Brazilian sugarcane. Table A.5 shows parameters for life cycle stages that are common across models. Table A.6 shows employed global warming potentials along with emission factors for fuels, electricity and agrochemicals. Table A.7 shows the energy and mass densities used throughout this chapter.

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Table A.1. Summary of key parameters for ethylene production pathway via natural gas derived ethane

Parameter	Value or distribution	Units	Source
<i>Pre-Production</i>			
Well pad construction	Triangular (0.05, 0.13, 0.3)	g CO ₂ e/MJ	ref ²⁰⁹
Well Drilling	Triangular (0.1, 0.2, 0.4)	g CO ₂ e/MJ	ref ²⁰⁹
Hydraulic Fracturing Chemicals	Triangular (0.04, 0.23, 0.5)	g CO ₂ e/MJ	ref ²⁰⁹
Hydraulic Fracturing Water Management	Triangular (0.04, 0.07, 0.1)	g CO ₂ e/MJ	ref ²⁰⁹
Gas venting for conventional well completions	0.71	tonnes CH ₄ /completion	ref ³⁶⁸
Gas venting for conventional well annual workovers	0.05	tonnes CH ₄ /workover	ref ³⁶⁸
Conventional well workovers	1	workover/year	ref ²⁰¹
Operating Lifetime of Conventional well	5	Years	ref ²⁰¹
Daily production for conventional well	0.15	MMscf/day	ref ²⁰¹
Uncontrolled gasvented/flared for unconventional completions and workovers	Normal (8900,2006067)	Mcf “CH ₄ ”/completion	ref ³⁶⁹
Unconventional Well Estimated Ultimate Recovery	Triangular (0.5, 2, 5.3)	Bcf	ref ²⁰⁹
Flowback Captured in Reduced Emission Completions	90%	%	ref ³⁷⁰
Percent of released gas which is flared	Uniform (51,100) (100% for regulated scenario)	%	ref ³⁷¹ ref ³⁷²
Flare Efficiency	98%	%	ref ³⁷¹
Number of refractures per unconventional well	Bionomial (p = 0.01, n= 30)	#	ref ³⁶⁹ for p ref ³⁷³ for n
Green Completion Percentage	51% 100% (for regulated scenario)	%	ref ³⁶⁹ ref ³⁷²
Conventional and unconventional percent of growth withdrawals	State by state	%	ref ²¹¹
2011 CO ₂ and CH ₄ content in raw natural gas	By NEMS region for each state	%	ref ²¹² (data from 2011 reporting year)
<i>Production</i>			

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Lease Fuel Consumed	State by state (discrete distribution)	MMcf/year	ref ²¹⁰ (data from 2011 reporting year)																
Gas Vented and Flared	State by state (discrete distribution)	MMcf/year	ref ²¹¹ (data from 2011 reporting year)																
Production CH ₄ Emissions	Triangular (.81*best, best, 1.30*best) by (aggregated) NEMS region(s)	Mg CH ₄ /year	ref ²¹² (data from 2011 reporting year)																
Processing																			
CO ₂ Emissions	Log-logistic(-0.089,1.59,2.28) (truncated at 0)	tonnes CO ₂ /MMcf processed	Own Analysis of refs ^{215,216}																
CH ₄ Emissions	Inverse Gaussian (0.00880,0.00284,-0.000287) (truncated at 0)	tonnes CH ₄ /MMcf processed	Own Analysis of refs ^{215,216}																
N ₂ O Emissions	Log-logistic (9.08*10 ⁻¹⁰ , 2.12*10 ⁻⁶ , 1.66) (truncated at 0)	tonnes N ₂ O/MMcf processed	Own Analysis of refs ^{215,216}																
Correlation Matrix for processing emissions	<table border="1"> <tr> <td></td> <td>CO₂</td> <td>CH₄</td> <td>N₂O</td> </tr> <tr> <td>CO₂</td> <td>1</td> <td></td> <td></td> </tr> <tr> <td>CH₄</td> <td>0.36</td> <td>1</td> <td></td> </tr> <tr> <td>N₂O</td> <td>-0.03</td> <td>-0.05</td> <td>1</td> </tr> </table>		CO ₂	CH ₄	N ₂ O	CO ₂	1			CH ₄	0.36	1		N ₂ O	-0.03	-0.05	1	N/A	Own Analysis of refs ^{215,216}
	CO ₂	CH ₄	N ₂ O																
CO ₂	1																		
CH ₄	0.36	1																	
N ₂ O	-0.03	-0.05	1																
Steam Cracking																			
Specific Energy Required	Uniform (15,25)	GJ/t ethylene	refs ²¹⁷⁻²¹⁹																
Ethylene Produced	Triangular (764, 803, 840)	kg/tonne ethane	refs ²¹⁷⁻²²¹																
Propylene Produced	Triangular (14.1, 16, 29.9)	kg/tonne ethane																	
Butadiene Produced	Triangular (17.4, 19.9, 23)	kg/tonne ethane																	

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Aromatics Produced	Uniform (0, 19.9)	kg/tonne ethane	
Hydrogen Produced	Triangular (57.9, 60, 89.7)	kg/tonne ethane	
Methane Produced	Triangular (58.8, 61, 70.1)	kg/tonne ethane	
C4 Components Produced	Triangular (0, 6, 8.1)	kg/tonne ethane	
C5 and C6 Components Produced	Uniform (0, 26)	kg/tonne ethane	
Product Losses	Uniform (5, 20)	kg/tonne ethane	
Emissions from Hydrogen Production via steam reforming (for system expansion)	Uniform (9.3, 14.2) ^a	kg CO ₂ e/kg H ₂	Multiple sources consulted. Lower bound from ref ³⁷⁴ as cited in SimaPro software. Upper bound from ref ²⁰²
Direct CH ₄ emissions from ethane cracker	Triangular (5.45, 6, 6.6)	kg CH ₄ /t ethylene	ref ²²²

Distributions are written as: Triangular (lower, mode, upper), Normal (mean, standard deviation), Uniform (lower, upper), Binomial (p = probability of event, n = number of draws), Log-Logistic (location, scale, shape), Inverse Gaussian (mean, shape, shift)

(a) Mean bounds are shown. Actual bounds are stochastic due to uncertainty in GWP.

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Table A.2. Summary of key parameters for ethanol/ethylene production pathway via U.S. Corn Starch

Parameter	Value or Distribution	Units	Source
Land-use Change			
Domestic Land Use Change	-4	kg CO ₂ e/mmBtu	ref ¹²⁸
International Land Use Change	Triangular (20.9, 31.8, 44.7)	kg CO ₂ e/mmBtu	Fit to confidence interval given by ref ¹²⁸
Agricultural Operations			
Corn Yield	Beta ($\alpha=21.62, \beta=5.86, [0,14.3]$)	Mg dm/ha	ref ⁷⁴
Nitrogen Application	Triangular (141, 150, 160)	kg N / ha	ref ³⁷⁵ as cited in ref ⁷⁴
Crop residue applied	Triangular (73, 80, 86)	kg N / ha	From ref ²²⁵ as modeled by ref ⁷⁴
CaCO ₃ applied	1150	g / bushel	ref ²⁰²
K ₂ O applied	172	g / bushel	ref ²⁰²
P ₂ O ₅ applied	148	g / bushel	ref ²⁰²
Herbicides applied	4.75	g / bushel	ref ²⁰²
Insecticides applied	0.4	g / bushel	ref ²⁰²
Fossil Fuel Use	894 1.97 0.023	g CO ₂ / bushel g CH ₄ / bushel g N ₂ O / bushel	ref ²⁰²
Dry matter fraction of bushel	87%	%	ref ²²⁵
Ethanol Production			
Corn starch content	Triangular(62.6, 67.3 ,72)	%w of dry matter	ref ³⁷⁶ and ref ³⁷⁷ as used in ref ⁷⁴
Heat input	Triangular (0.32, 0.42, 0.51)	MJ heat / MJ EtOH	ref ^{376,378,379} as cited in ref ⁷⁴
Electricity input	Triangular (0.023,0.038,0.049)	MJ elec/MJ EtOH	
Co-product credit	7.4 0.017 0.018	g CO ₂ /MJ EtOH g CH ₄ /MJ EtOH g N ₂ O / MJ EtOH	ref ²⁰²

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Transportation			
Feedstock transportation	434 0.549 0.007	g CO ₂ / bushel g CH ₄ / bushel g N ₂ O / bushel	ref ²⁰²
Trucking distance for ethanol to ethylene plant	Uniform(1000,1800)	km	Approximate distance from existing corn ethanol refineries ref ²³⁰ to gulf states ethylene infrastructure ref ²³¹
Truck fuel consumption	0.0203	L diesel / t-km	ref ²²⁹

Distributions are written as: Triangular (lower, mode, upper), Normal (mean, standard deviation), Uniform (lower, upper), Beta (α , β , [lower bound, upper bound]).

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Table A.3. Summary of key parameters for ethanol/ethylene production pathway via U.S. Switchgrass

Parameter	Value or Distribution	Units	Source
Land-use Change			
Domestic Land Use Change	-2.5	kg CO ₂ e/mmBtu	ref ¹²⁸
International Land Use Change	Triangular (7.9, 15.1, 23.7)	kg CO ₂ e/mmBtu	Fit to confidence interval given by ¹²⁸
Agricultural Operations			
Switchgrass Yield	Beta ($\alpha=21.62$, $\beta=5.86$, [0,21.6])	Mg dm / ha	ref ⁷⁴
Nitrogen Application	Triangular (55, 74, 100)	kg N/ ha	ref ^{380,381} as cited in ref ⁷⁴
Crop Residue Applied	Triangular (133.5, 171.7, 210)	kg N / ha	From ref ²²⁵ as modeled by ref ⁷⁴
K ₂ O Applied	227	g / tonne dm	ref ²⁰²
P ₂ O ₅ Applied	114	g / tonne dm	ref ²⁰²
Herbicide	31.8	g / tonne dm	ref ²⁰²
Fossil Fuel Use	20.7 0.314 26.7	g CO ₂ / kg SW g N ₂ O / kg SW g CH ₄ / kg SW	ref ²⁰²
Ethanol Production			
Glucan Content	Triangular (31, 34.4, 37.2)	% w	ref ³⁸² as cited in ref ⁷⁴
Xylan Content	Triangular (20.6, 23.0, 26.0)	% w	
Mannan Content	Triangular (0.29, 0.32, 0.36)	% w	
Galactan Content	Triangular (0.67, 1.0, 1.2)	% w	
Arabinan Content	Uniform (2.6, 3.4)	% w	
Lignin Content	Triangular (17.3, 19.2, 21.1)	% w	
Energy Input	Uniform (0.44, 0.72)	MJ / MJ EtOH (treated as HHV)	refs ^{305,383} as cited in ⁷⁴
Percent of energy to electricity, heat	10% / 90%		
Boiler efficiency	68%		
Turbine Efficiency	85%		
Transportation			

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Feedstock Transportation	15	g CO ₂ e/ kg SW	Calculated from ²⁰²
Trucking distance for ethanol to ethylene plant	Triangular (0,1000,1500)	km	Approximate distance from projected switchgrass ethanol facilities ¹²⁸ to gulf states ethylene infrastructure ²³¹
Truck fuel consumption	0.0203	L diesel / t-km	ref ²²⁹

Distributions are written as: Triangular (lower, mode, upper), Normal (mean, standard deviation), Uniform (lower, upper), Beta (α , β , [lower bound, upper bound]).

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Table A.4. Summary of key parameters for ethanol/ethylene production pathway via Brazilian Sugarcane

Parameter	Value or Distribution	Units	Source
<i>Land-use Change</i>			
Land-use change (total)	Triangular (-5.8, 4.3,13)	g CO ₂ e/MJ EtOH	Fit to confidence interval given by ¹²⁸
<i>Agricultural Operations</i>			
Harvest Yield	Normal(86.7,13.4)	t cane / ha	ref ¹⁹⁹
Diesel Consumption	Normal (274,75)	L diesel /ha	ref ¹⁹⁹
Nitrogen Application	Triangular (39, 777, 1515)	g N/t cane	ref ¹⁹⁹
CaCO ₃ applied	Triangular (162,5183,13755)	g / t cane	ref ¹⁹⁹
K ₂ O applied	980	g / t cane	ref ²⁰²
P ₂ O ₅ applied	249	g / t cane	ref ²⁰²
Herbicides applied	44	g / t cane	ref ²⁰²
Insecticides applied	3	g / t cane	ref ²⁰²
Trash burning	Triangular (3,82,126)	kg CO ₂ e/t cane	ref ¹⁹⁹
Emissions from Trash Burning	113	g CO ₂ e / kg straw	ref ²⁰²
<i>Ethanol Production</i>			
Ethanol yield	Normal (81.1, 4.3)	L EtOH/ t cane	ref ¹⁹⁹
Surplus Electricity	Exponential (10.7)	kWh/t cane	ref ¹⁹⁹
Surplus Bagasse	Exponential (8.7)	kg/t cane	ref ¹⁹⁹
Bagasse moisture content	50%	%	ref ²⁰²
Bagasse boiler LHV Efficiency	30%	%	ref ³⁰⁷
<i>Transportation</i>			
Field to ethanol mill, fuel use	10300	kcal diesel/t cane	ref ³⁸⁴ as cited in ²⁰⁰
Ethanol to ethylene plant, fuel use	0.217	MJ diesel / kg ethanol	ref ²⁰⁰
Shipping distance, Brazil (Parangua) to U.S. (Houston)	10700	Km	ref ²³³
Ship fuel consumption (Ocean Freighter)	4.93 *10 ⁻³	L residual fuel oil/t-km	ref ²³²

Distributions are written as: Triangular (lower, mode, upper), Normal (mean, standard deviation), Uniform (lower, upper), Exponential (mean).

Table A.5. Summary of key parameters for processes which are common across models

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Parameter	Value	Units	Source
<i>Ethanol Production</i> <i>(used for switchgrass and corn)</i>			
Hydrolysis yield	Uniform (0.85, 0.95)	%	ref ³⁸⁵ as cited in ⁷⁴
Fermentation yield from glucose	Uniform (0.85, 1)	%	
Fermentation yield from other sugars	Uniform (0.75, 0.9)	%	
<i>Ethanol Fuel Distribution</i>			
Emissions from fuel distribution	1.2	g CO ₂ e/MJ	Calculated from ²⁰²
<i>Ethanol dehydration to ethylene</i>			
Ethylene yield	0.58	kg ethylene / kg ethanol	Calculated from ¹⁸⁰
Fuel used	Lognormal (1.67, 0.611)	MJ /kg ethylene (Assumed to be LHV)	Mean from ¹⁸⁰ ; standard deviation calculated based on ²²⁷
Electricity Used	Lognormal (1.12, 0.41)	MJ electricity/ kg ethylene	Mean from ¹⁸⁰ ; standard deviation calculated based on ²²⁷
<i>U.S. Polymerization</i> <i>(used for switchgrass and corn)</i>			
Fuel for electricity cogeneration	5.66	MJ HHV / kg LDPE	ref ¹⁴⁵
Natural gas (additional)	2.02	MJ HHV / kg LDPE	ref ¹⁴⁵
LPG	9.64*10 ⁻⁴	MJ HHV/ kg LDPE	ref ¹⁴⁵
Residual oil	0.064	MJ HHV / kg LDPE	ref ¹⁴⁵
Recovered energy	0.4	MJ HHV / kg LDPE	ref ¹⁴⁵
<i>Brazilian Polymerization</i> <i>(used for sugarcane only)</i>			
Electricity required	Uniform (3.4,4.0)	MJ electricity / kg LDPE	Lower bound calculated based on ³⁸⁶ as per ²⁰⁰ . Upper bound from ²²⁸ .
Emissions from fuel use: <i>estimate 1</i>	57 1.9 6.5*10 ⁻⁴	g CO ₂ / kg LDPE g CH ₄ / kg LDPE g N ₂ O / kg LDPE	Calculated from ³⁸⁶ as per ²⁰⁰ .

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Emissions from fuel use: <i>estimate 2</i> (net heat required; treated as natural gas)	-0.25	MJ HHV / kg LDPE	ref ²²⁸ for energy required; emissions calculated as per Table A.6
Emissions from fuel use: total	Uniform (<i>estimate 2, estimate 1</i>)	g CO ₂ e/kg LDPE	Calculated from ³⁸⁶ as cited in ²⁰⁰

Distributions are written as: Uniform (lower, upper), lognormal (mean, standard deviation)

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Table A.6. Global warming potentials and emission factors for fuels, electricity and agrochemicals

Parameter	Value	Units	Source
Global warming potentials			
CH ₄ GWP	Normal (36, 8.5)	g CO ₂ e / g CH ₄	ref ^{204,205}
N ₂ O GWP	Normal (298, 52.5)	g CO ₂ e / g N ₂ O	
Fuel Emissions			
Gasoline life cycle emissions	Log-logistic (2.2, 0.2, 80)	g CO ₂ e/MJ (LHV)	ref ¹⁹⁸
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)	
LPG combustion emissions	Triangular (66.7, 68.4, 71.2)	g CO ₂ e/ MJ (LHV)	
Natural gas life cycle emissions (prior to updating GWP)	Normal (66, 3.5)	g CO ₂ e/MJ (HHV)	Approximate fit to parameters from; ²⁰¹ ;
Natural gas CH ₄ and N ₂ O emissions (for updated GWP)	Various	Various	See ref ²⁰¹
Natural gas life cycle emissions (after updating GWP)	Normal (70, 5.0) Normal (78, 5.5)	g CO ₂ e/MJ (HHV) g CO ₂ e/MJ (LHV)	Fit to modeled distribution based on ref ²⁰¹
Coal life cycle emissions	Log-logistic (3.05, 0.14, 74)	g CO ₂ e/ MJ (HHV)	ref ²⁰⁶
Electricity Emissions			
Brazilian electricity (average)	Uniform (20, 81) ^a	g CO ₂ e/MJ	Lower bound from. ²⁰² Upper bound from. ²⁰⁷
Brazilian electricity (marginal): Natural gas turbine	Uniform (179, 207) ^a	g CO ₂ e/MJ	Lower bound from. ²⁰² Upper bound from ³⁸⁷ and ³⁸⁸ as cited in ¹⁹¹ supporting information.
MRO electricity	Uniform (200, 313) ^a	g CO ₂ e/MJ	Lower bound from ²⁰² . Upper bound from ²⁷³
TRE and SERC electricity	Uniform (164, 220) ^a	g CO ₂ e/MJ	Lower bound from ²⁰² for TRE. Upper bound from ²⁷² .
TRE, SERC and SPP electricity	Uniform (164, 308) ^a	g CO ₂ e/MJ	Lower bound from ²⁰² for TRE. Upper bound from ²⁷⁴

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<i>Agrochemicals</i>			
U.S. production of CaCO ₃	0.0137 ^a	kg CO ₂ e / kg CaCO ₃	Calculated from ²⁰²
U.S. production of K ₂ O	0.688 ^a	kg CO ₂ e / kg K ₂ O	
U.S. production of P ₂ O ₅	1.83 ^a	kg CO ₂ e / kg P ₂ O ₅	
Brazilian production of CaCO ₃	0.0205 ^a	kg CO ₂ e / kg CaCO ₃	
Brazilian production of K ₂ O	0.371 ^a	kg CO ₂ e / kg K ₂ O	
Brazilian production of P ₂ O ₅	0.630 ^a	kg CO ₂ e / kg P ₂ O ₅	
Corn Herbicides	21.4	kg CO ₂ e / kg herbicide	
Corn Insecticides	25.0	kg CO ₂ e / kg insecticide	
Switchgrass Herbicides	21.3	kg CO ₂ e / kg herbicide	
Switchgrass Insecticides	25.0	kg CO ₂ e / kg insecticide	
Sugarcane Herbicides	15.6	kg CO ₂ e / kg herbicide	
Sugarcane Insecticides	18.0	kg CO ₂ e / kg insecticide	
Direct CO ₂ emissions from CaCO ₃	0.44	kg CO ₂ / kg CaCO ₃	
Direct N ₂ O from synthetic fertilizer and crop residue	Triangular (0.003, 0.01, 0.03)	kg N ₂ O-N/kg N applied	ref ²²⁵
Volatilization from synthetic fertilizer	Triangular (0.03, 0.1, 0.3)	(kg NH ₃ -N + kg NO _x -N) / kg N	
Indirect N ₂ O from volatilized N	Triangular (0.002, 0.01, 0.05)	kg N ₂ O-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 ₂ O from runoff	Triangular (0.0005, 0.0075, 0.025)	kg N ₂ O-N/kg N runoff	

Distributions are written as: Triangular (lower, mode, upper), Normal (mean, standard deviation), log-logistic (location of the underlying logistic, scale of the underlying logistic, shift)

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

Table A.7. Energy and mass densities used throughout this chapter.

<u>Liquids</u>			
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, etc.	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
Ethane (liquefied)	-	-	546.5 ^d kg/m ³
Propane (liquefied)	84,250 ^a	91,330 ^b	582 ^d kg/m ³
<i>n</i> -Butane (liquefied)	94,970 ^a	103,000 ^b	601.4 ^d kg/m ³
Isobutane (liquefied)	90,060 ^a	94,620 ^b	593.4 ^d kg/m ³
Pentanes plus	-	110,000 ^b	651 ^c kg/m ³
<i>n</i> -Hexane	105,125 ^a	-	655 ^a kg/m ³
<u>Gasses</u>			
Item	LHV Energy Density (btu/ft³)	HHV Energy Density (btu/ft³)	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
<u>Solids</u>		<u>Solids</u>	
Item	HHV Energy Density (MJ/kg)	Item	HHV Energy Density (MJ/kg)
Glucan/Cellulose	16.9 ^e	Glucose	15.6 ^f
Xylan	17.4 ^e	Xylose	15.6 ^f
Mannan	16.6 ^e	Mannose	15.6 ^f
Galactan	17.2 ^e	Galactose	15.5 ^f
Arabinan	16.9 ^e	Arabinose	15.6 ^f
Lignin	25.1 ^e	Non-sugar, non- lignin switchgrass components	11.8 ^e
Sugarcane Bagasse	14.4 ^e (LHV)		

(a) Data from Wang 2013²⁰²(b) Calculated from¹⁸²(c) Calculated using composition data from³⁸⁹ and standard density information(d) Liquid density at boiling point (kg/m³) from³⁹⁰(e) Calculated from³⁰⁵(f) ref³⁹¹

A.2. Additional Results and Discussion

A.2.1 Summary Statistics

The following tables present summary statistics for 10,000 simulations of each of the pathways modeled in this chapter. For the tables in this section, “lower 90% CI” and “upper 90% CI” is constructed as a percent of model runs, and should not be interpreted as a traditional statistically based confidence interval.

Table A.8. Summary Statistics for the GHG emissions from the life cycle stages for production of LDPE from natural gas derived ethane in the U.S.

Life cycle Stage	Mean (kg CO ₂ e/kg LDPE)	Standard Deviation	Coefficient of Variation	Lower 90% CI	Upper 90% CI
Pre-Production	0.04	0.01	0.26	0.03	0.06
Production	0.27	0.09	0.34	0.17	0.37
Processing	0.13	0.16	1.26	0.02	0.33
Steam Cracking	0.65	0.27	0.42	0.20	1.10
Polymerization	0.74	0.08	0.11	0.64	0.87
Ethylene Subtotal	1.1	0.34	0.31	0.58	1.6
LDPE Total	1.8	0.35	0.20	1.3	2.4
Fitted Distribution	Log-logistic (location = 1.04, scale = 2.84, shape = 14.8)				

Table A.9. Summary Statistics for the GHG emissions from the life cycle stages for production of U.S. corn ethanol fuel

Life cycle Stage	Mean (g CO ₂ e/MJ)	Standard Deviation	Coefficient of Variation	Lower 90% CI	Upper 90% CI
LUC	27	4.6	0.17	19	35
Corn Farming	43	9.8	0.23	30	61
Co-Product Credits	-13	0.9	-0.07	-14	-12
Ethanol Production	35	4.7	0.13	27.7	43
Transportation	4.0	0.2	0.05	3.7	4.3
Ethanol Fuel Total	97	12	0.12	79	120
Fitted Distribution	Gamma (shape = 17.3, scale = 2.77, shift = 48.8)				

Table A.10. Summary Statistics for GHG emissions from the life cycle stages for production of U.S. corn LDPE

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Life cycle Stage	Mean (kg CO ₂ e/kg LDPE)	Standard Deviation	Coefficient of Variation	Lower 90% CI	Upper 90% CI
LUC	1.3	0.22	0.17	0.91	1.6
Corn Farming	2.0	0.46	0.23	1.40	2.9
Co-Product Credits	-0.61	0.04	-0.07	-0.68	-0.54
Ethanol Production	1.7	0.22	0.13	1.3	2.0
Ethanol Dehydration	0.34	0.09	0.28	0.21	0.51
Polymerization	0.71	0.08	0.11	0.62	0.85
Transportation	0.31	0.03	0.10	0.26	0.36
EOL (growth credit)	-3.1	-	-	-	-
LDPE Total	2.6	0.57	0.22	1.7	3.6
Fitted Distribution	Gamma (shape = 21.0, scale = 0.123, shift = -0.0209)				

Table A.11. Summary Statistics for the GHG emissions from the life cycle stages for production of U.S. switchgrass ethanol fuel

Life cycle Stage	Mean (g CO ₂ e/MJ)	Standard Deviation	Coefficient of Variation	Lower 90% CI	Upper 90% CI
LUC	12	3.1	0.25	7.4	18
Switchgrass farming	12	2.8	0.24	8.2	17
Ethanol production & electricity credit	-45	24	-0.52	-87	-9.4
Transportation	3.2	0.1	0.04	3.1	3.4
Ethanol fuel Total	-18	23	-1	-59	18
Fitted Distribution	Weibull (shape = 6.18, scale = 135, shift = -143)				

Table A.12. Summary Statistics for the GHG emissions from the life cycle stages for production of U.S. switchgrass LDPE

Life cycle Stage	Mean (kg CO ₂ e/kg LDPE)	Standard Deviation	Coefficient of Variation	Lower 90% CI	Upper 90% CI
LUC	0.58	0.14	0.25	0.35	0.83
Switchgrass Farming	0.57	0.13	0.24	0.38	0.81
Ethanol Production & electricity credit	-2.1	1.1	-0.52	-4.1	-0.44
Ethanol Dehydration	0.34	0.09	0.28	0.21	0.51
Polymerization	0.71	0.08	0.11	0.62	0.85
Transportation	0.20	0.04	0.20	0.13	0.26
EOL (growth credit)	-3.1	-	-	-	-
LDPE Total	-2.9	1.1	-0.39	-4.9	-1.2
Fitted Distribution	Weibull (shape = 5.64, scale = 5.90, shift = -8.34)				

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Table A.13. Summary Statistics for the GHG emissions from the life cycle stages for production of Brazilian sugarcane ethanol fuel

Life cycle Stage	Mean (g CO ₂ e/MJ)	Standard Deviation	Coefficient of Variation	Lower 90% CI	Upper 90% CI
LUC	4	3.7	1.0	-2.6	10
Sugarcane farming	20	4.5	0.23	13	28
Ethanol production & electricity credit	-1.4	1.3	-0.9	-3.8	-0.20
Transportation	11	0.65	0.06	11	12
Ethanol fuel Total	33	6.0	0.18	24	43
Fitted Distribution	Normal (mean = 33.3, standard deviation = 5.95)				

Table A.14. Summary Statistics for the GHG emissions from the life cycle stages for production of Brazilian sugarcane LDPE

Life cycle Stage	Mean (kg CO ₂ e/kg LDPE)	Standard Deviation	Coefficient of Variation	Lower 90% CI	Upper 90% CI
LUC	0.2	0.17	1.0	-0.1	0.5
Sugarcane Farming	0.93	0.21	0.23	0.62	1.3
Ethanol production & electricity credit	-0.067	0.059	-0.9	-0.18	-0.01
Ethanol Dehydration	0.2	0.05	0.31	0.1	0.3
Polymerization	0.2	0.08	0.33	0.1	0.4
Transportation	0.5	0.03	0.06	0.4	0.5
EOL (growth credit)	-3.1	-	-	-	-
LDPE Total	-1.3	0.30	-0.22	-1.8	-0.8
Fitted Distribution	Normal (mean = 1.34, standard deviation = 0.299)				

Table A.15. Summary Statistics for the net GHG emissions from each bio-based pathway. Reported emissions include 1:1 displacement of the relevant fossil fuel product (gasoline or fossil LDPE). The functional unit is scaled so that equivalent volumes of ethanol are considered, resulting in 1kg LDPE or 46.9 MJ energy.

Pathway	Mean net emissions (kg CO ₂ e/functional unit)	Standard Deviation	Coefficient of Variation	Lower 90% CI	Upper 90% CI
Corn ethanol	0.33	0.57	1.73	-0.54	1.3
Corn LDPE	0.74	0.63	0.85	-0.22	1.8
Switchgrass ethanol	-5.0	1.13	-0.22	-7.0	-3.3
Switchgrass LDPE	-4.7	1.16	-0.25	-6.7	-2.9
Sugarcane ethanol	-2.6	0.33	-0.12	-3.2	-2.1
Sugarcane LDPE	-3.2	0.45	-0.14	-3.9	-2.5

Table A.16. Summary Statistics for comparing GHG reductions achieved by bio-LDPE to those achieved by bio-ethanol (as per Figure 2.4 of the main text). Positive values imply that bio-LDPE achieves greater GHG reductions than bio-ethanol. Negative values imply that bio-ethanol achieves greater GHG reductions than bio-LDPE. Results assume bio-products achieve 1:1 displacement of the relevant fossil fuel product (gasoline or fossil LDPE). The functional unit is scaled so that equivalent volumes of ethanol are considered, resulting in 1kg LDPE or 46.9 MJ energy.

Pathway	Mean difference in net emissions (kg CO ₂ e/functional unit)	Standard Deviation	Coefficient of Variation	Lower 90% CI	Upper 90% CI
U.S. Production	-0.41	0.39	-0.96	-1.0	0.2
Brazilian Production	0.51	0.41	0.79	-0.13	1.1

A.2.2 CDF of Net GHG Emissions

Figure A.2 presents, the cumulative probability distribution functions for net GHG emissions from each bio-based pathway. Net GHG emissions are calculated by subtracting the emissions of the relevant fossil counterpart from the emissions for each bio-based product. Each curve thus represents the net increase (positive values) or decrease (negative values) in GHG emissions from replacing a fossil product with its bio-based counterpart. Key conclusions from this figure are already discussed in the main text.

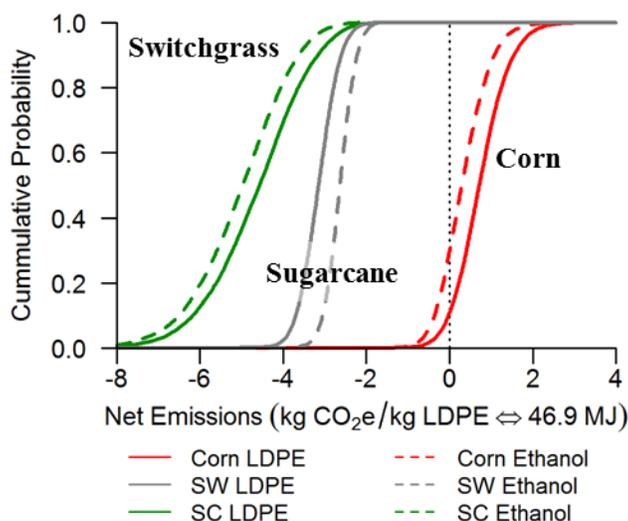


Figure A.2. Net emissions from examined bio-based pathways. The figure shows the cumulative distribution function for net emissions from both chemical (LDPE) and fuel use of bio-based ethanol, including any savings from 1:1 displacement of the relevant fossil fuel product (gasoline or fossil LDPE). The functional unit is scaled so that equivalent volumes of ethanol are considered. For clarity, the y-axis refers to ‘probability’, but should only be interpreted as a proportion of modeled runs.

A.2.3 Uncertainty Importance Analysis

The following figures show sensitivity of mean *net* GHG emissions to model inputs for each of the 6 biomass pathways modeled in this chapter. The results include 1:1 displacement of the relevant fossil fuel product (gasoline or fossil LDPE). The tornado plots are generated using Palisade's @Risk™ software. The edges of the tornado bars show the output mean for the simulations representing lowest (respectively highest) 10% of values for the selected input. The model is first run for 10,000 iterations. Each input is then divided into deciles (10 ascending bins). The output mean is calculated for each of these bins. The lowest of the 10 output means becomes the left edge of the tornado plot for that input; the highest of the 10 output means becomes the right edge of the tornado plot for that input. This method implicitly accounts for correlations and non-linearities in the output response.

For corn and switchgrass pathways, modeled uncertainty in emissions from the bio-based pathways is larger than modeled uncertainty in emissions from the displaced fossil fuel counterparts. The reverse is true for sugarcane pathways. Top uncertainties in corn and sugarcane pathways are related to fertilizer N₂O emissions, and emissions from land-use change. For switchgrass, key uncertainties are all related to emissions reductions from displaced electricity. In several pathways, important contributors to uncertainty are the global warming potentials for CH₄ and N₂O – parameters whose uncertainty is often overlooked.

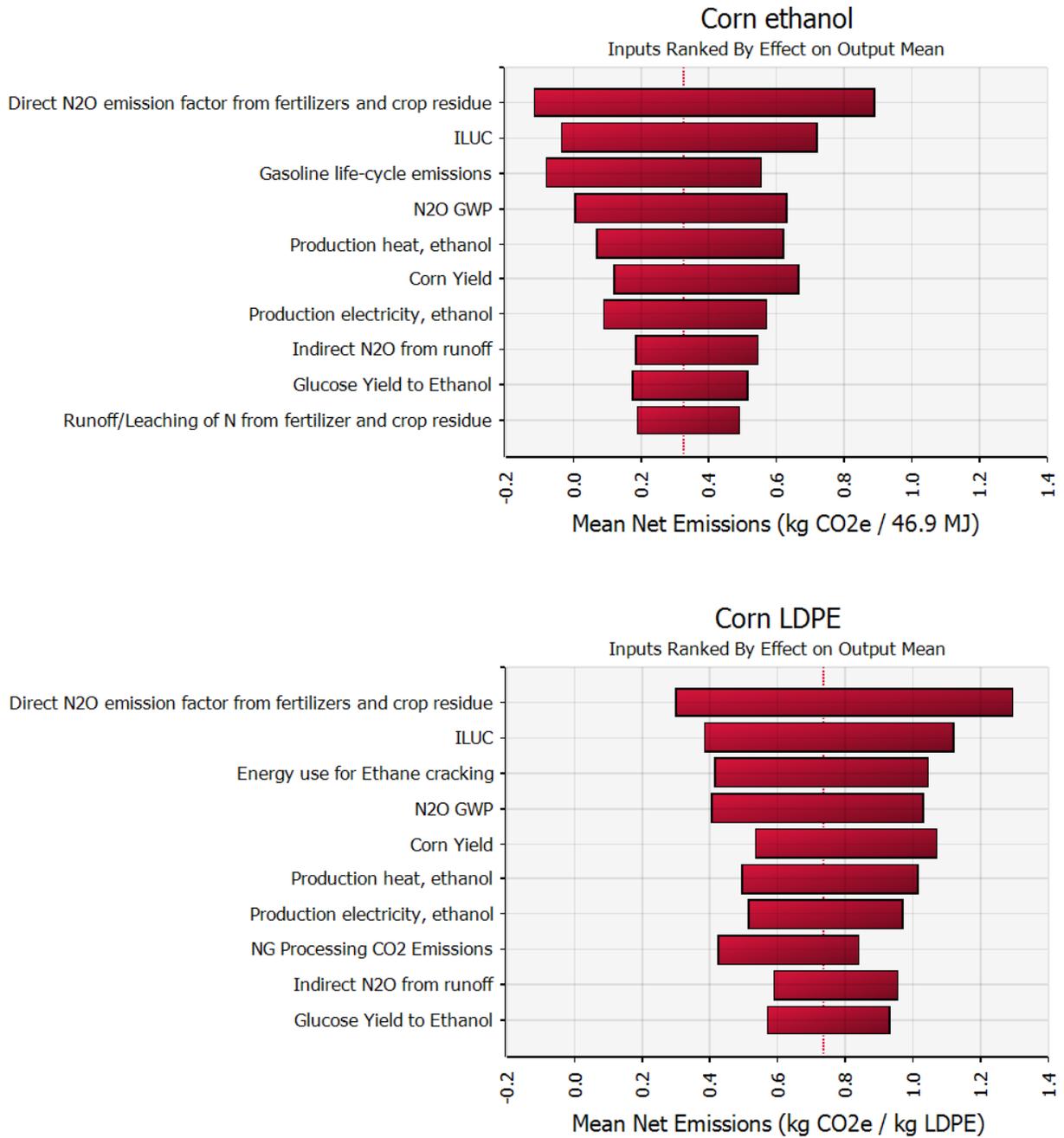


Figure A.3. Sensitivity of mean net GHG emissions of corn pathways to model inputs. The results include 1:1 displacement of the relevant fossil fuel product (gasoline or fossil LDPE). The edges of the tornado bars show the output mean for the simulations representing lowest (respectively highest) 10% of values for the selected input.

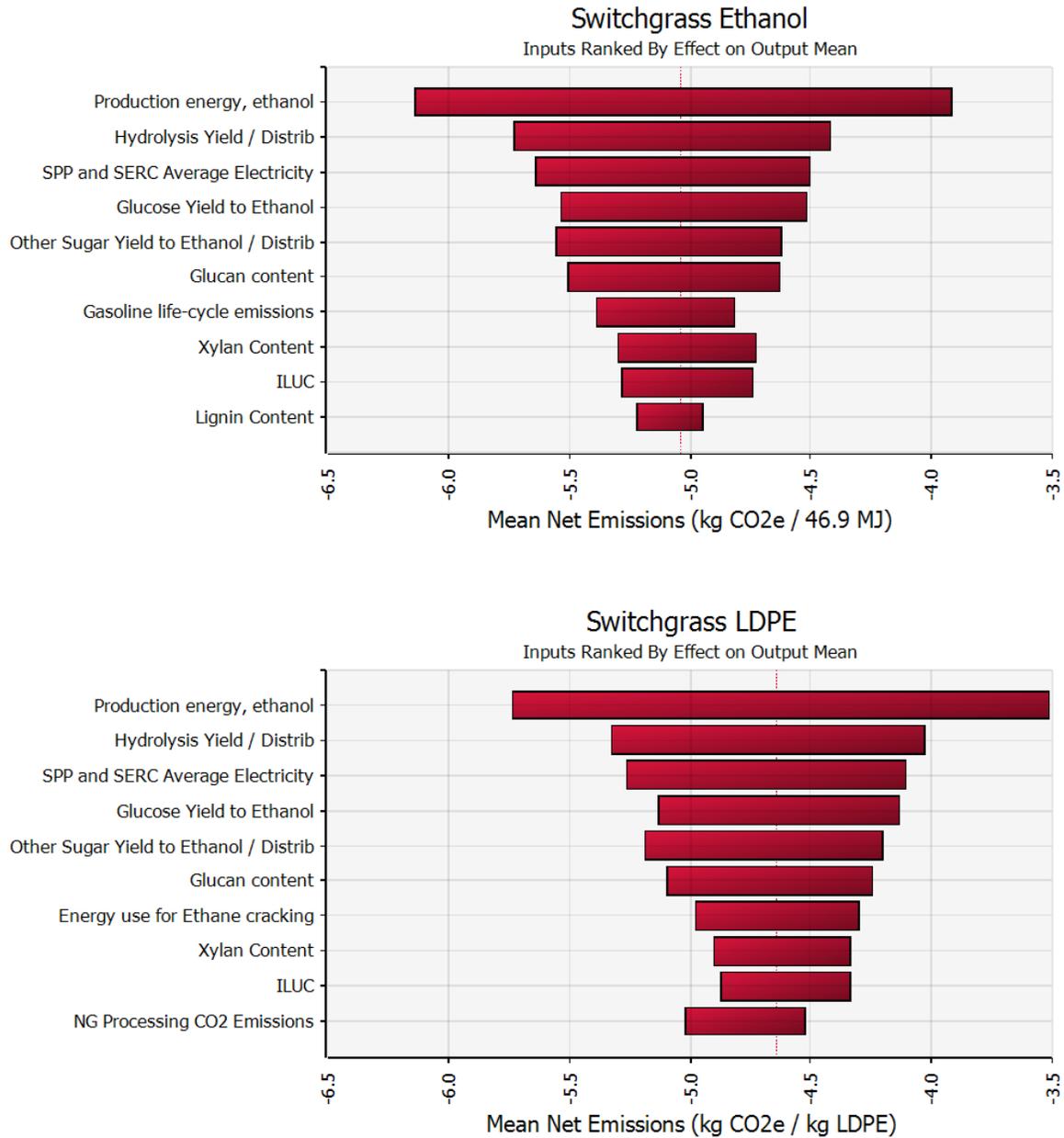


Figure A.4. Sensitivity of mean net GHG emissions of switchgrass pathways to model inputs. The results include 1:1 displacement of the relevant fossil fuel product (gasoline or fossil LDPE). The edges of the tornado bars show the output mean for the simulations representing lowest (respectively highest) 10% of values for the selected input.

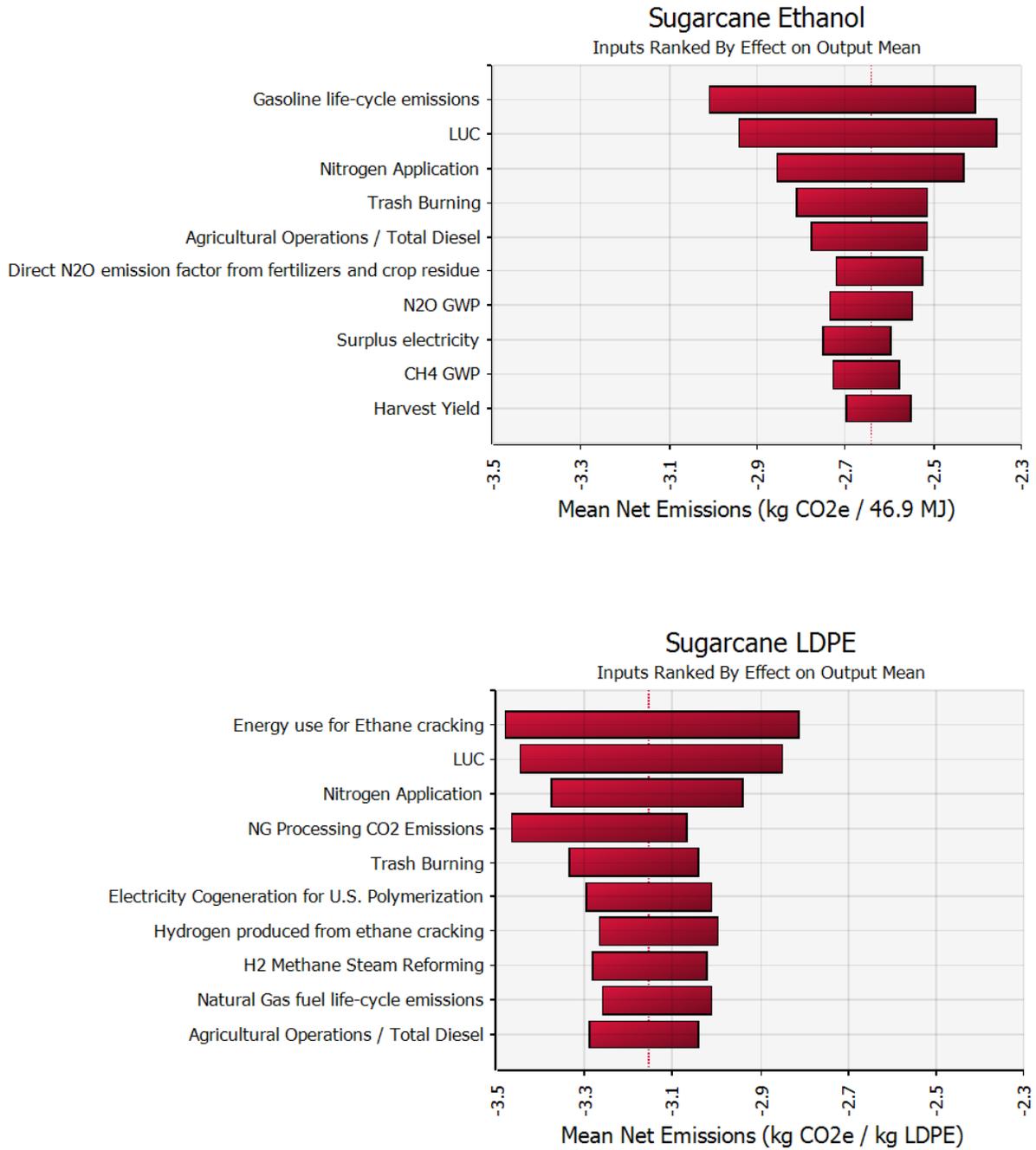


Figure A.5. Sensitivity of mean net GHG emissions of sugarcane pathways to model inputs. The results include 1:1 displacement of the relevant fossil fuel product (gasoline or fossil LDPE). The edges of the tornado bars show the output mean for the simulations representing lowest (respectively highest) 10% of values for the selected input.

Within the fossil LDPE pathway (disaggregated results not shown), uncertainty/variability on natural gas processing emissions, primary energy source for U.S. polymerization electricity cogeneration, the global warming potential of CH₄ and inputs for the steam cracking phase (total energy requirements, H₂ produced, and offset emissions from H₂ production) are all prominent contributors to overall uncertainty.

For corn and switchgrass pathways, modeled uncertainty in emissions from the bio-based pathways is larger than uncertainty in emissions from the displaced fossil fuel counterparts. For sugarcane, modeled uncertainty from ethanol production is lower, allowing uncertainty from the fossil fuel pathways to play a more prominent role. For all biomass pathways (especially corn and sugarcane), land-use change (LUC) emissions play a prominent role; this is in spite of employing a relatively narrow distribution that does not fully capture the range of literature estimates for LUC emissions. For corn pathways, most of the other important contributors to uncertainty relate to N₂O from fertilizer use (e.g. direct and indirect N₂O emission factors, N₂O GWP, nitrogen runoff and corn yield per hectare) and energy used for ethanol production. For switchgrass pathways, the most important inputs are those affecting the availability of surplus electricity: energy required for ethanol production, hydrolysis yield, ethanol yield, composition of switchgrass. Carbon intensity of displaced electricity is also an important contributor to uncertainty.

A.2.4 Sensitivity to Treatment of Electricity:

The treatment of electric grid emissions is an important parameter subject to a large degree of spatial and temporal variability. The large ranges employed capture much of this uncertainty, notably encompassing both estimates of ‘average’ and ‘marginal’ carbon intensity for the U.S. NERC regions as discussed above. For Brazilian electricity, however, there is a significant difference between average electricity (dominated by hydro power) and marginal generation, which is generally attributed to natural gas^{392,393}. Thus, for the sugarcane route only, an additional model run was performed using marginal (Brazilian) electricity emissions factors. Results are presented in Figure A.6

As is evident from the figure, switching to marginal electricity reduces the net emissions from the fuel pathway while increasing the emissions from the LDPE pathway; this is because the ethanol pathway is a net producer of electricity (due to surplus bagasse), while the LDPE pathway is a net consumer of electricity due to large electricity requirements further downstream (ethylene production and polymerization). Sugarcane ethanol fuel now achieves slightly greater GHG savings. Both pathways continue to meet EISA targets (50% GHG reduction relative to gasoline) with confidence levels in excess of 85% of model runs.

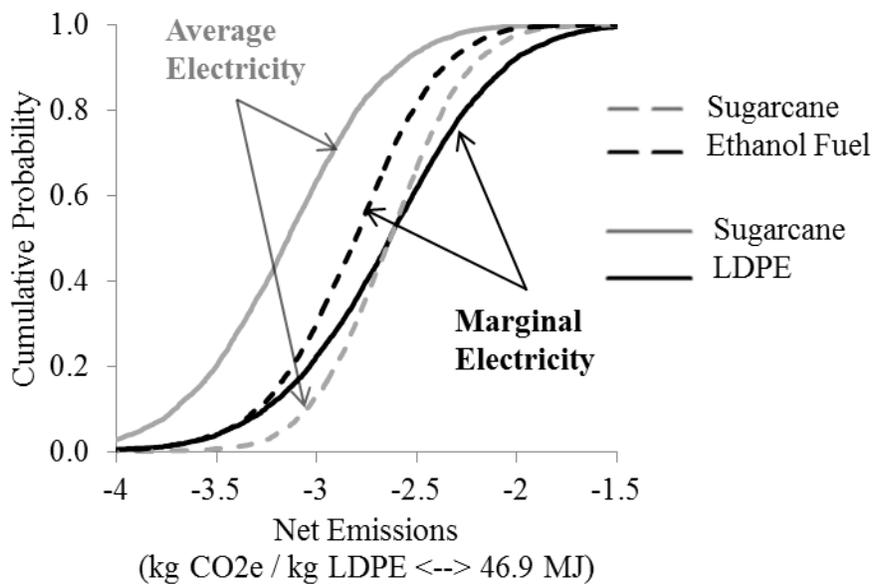


Figure A.6. Net emissions from sugarcane pathways using either average or marginal Brazilian electricity emissions factors. The figure shows the cumulative distribution function for net emissions from both chemical (LDPE) and fuel pathways, including savings from 1:1 displacement of the relevant fossil fuel product (gasoline or fossil LDPE). The functional unit is scaled so that equivalent volumes of ethanol are considered.

As discussed above, emission credits from the sale of surplus electricity are critical to both switchgrass pathways. An additional case is modeled with no credits for surplus electricity for the event that ethanol production facilities are unable to sell this product to the grid. Results for switchgrass pathways are shown in Figure A.7. Removing credits for surplus electricity makes little difference to the baseline model for sugarcane pathways.

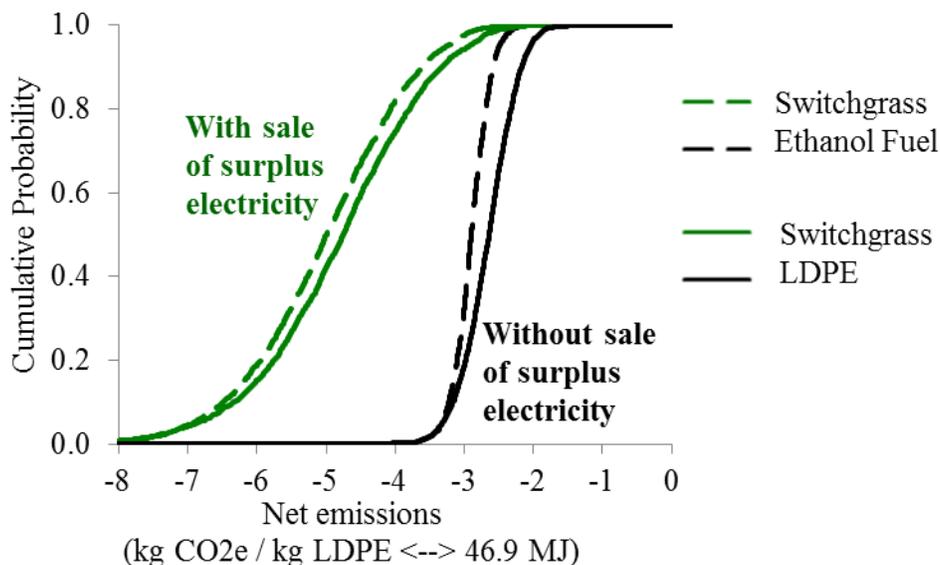


Figure A.7. Net emissions from switchgrass pathways both with and without credits for the sale of surplus electricity. The figure show the cumulative distribution function for net emissions from both chemical (LDPE) and fuel pathways, including savings from 1:1 displacement of the relevant fossil fuel product (gasoline or fossil LDPE). The functional unit is scaled so that equivalent volumes of ethanol are considered.

Inability to sell surplus electricity considerably increases the net emissions from switchgrass pathways while decreasing the modeled uncertainty. Although switchgrass ethanol fuel retains a high likelihood (>95% of model runs) of meeting the EISA target for cellulosic ethanol (60% reduction relative to gasoline), the LDPE pathway can only meet the same EISA target in 50% of model runs, a substantial drop from the base case. Without credits for surplus electricity, there is now substantial overlap in emissions between switchgrass and sugarcane pathways. Summary results for this section are presented in Table A.17.

Table A.17. Summary of net emissions (including 1:1 displacement of the baseline fossil fuel product) for alternate assumptions regarding emissions from electricity.

	Mean simulated net emissions (kg CO ₂ e/functional unit)		
	Base Case	Marginal Electricity	No sale of surplus electricity
Corn Ethanol	+0.33	–	–
Corn LDPE	+0.74	–	–
Sugarcane Ethanol	-2.6	-2.8	-2.6
Sugarcane LDPE	-3.2	-2.7	-3.1
Switchgrass Ethanol	-5.0	–	-2.9
Switchgrass LDPE	-4.7	–	-2.5

A.2.5 Sensitivity Treatment of Displaced Fossil Products

This analysis makes several important assumptions regarding displaced fossil products. First, fossil ethylene is assumed to be derived from natural gas ethane. Although ethane is the dominant feedstock in the U.S., heavier feedstocks like naphtha still account for close to 15 to 20% of domestic ethylene production.¹⁸⁵⁻¹⁸⁷ As naphtha crackers tend to display lower profit margins,^{237,394} heavier feedstocks would likely be displaced first by an increase in bioethylene production. To investigate this possibility, a model was developed to account for the emissions from naphtha-derived ethylene. Life cycle emissions from naphtha production are assumed to be equivalent to the reported emissions for gasoline production reported by Venkatesh *et al.*¹⁹⁸ Emissions from naphtha cracking were modeled in the same way as emissions from ethane cracking, using naphtha-specific estimates for energy requirements²¹⁷ and co-product volumes.²²¹

Naphtha-derived LDPE is found to be approximately 25% more GHG intensive than ethane-derived LDPE. Mean modeled emissions for Naphtha LDPE are 2.4 kg CO₂e / kg LDPE with a 90% confidence interval from 2.0-2.9 kg CO₂e / kg LDPE. Net emissions for each bio-based pathway assuming displacement for naphtha-derived LDPE for bio-LDPE pathways are presented in Figure A.8 (compare with Figure A.2). Under the assumption that naphtha-derived LDPE is displaced (rather than ethane-derived LDPE), bio-LDPE is marginally preferred over bio-ethanol fuel even for

U.S. pathways. The ability for each pathway to meet the relevant EISA GHG reduction target is not significantly affected.

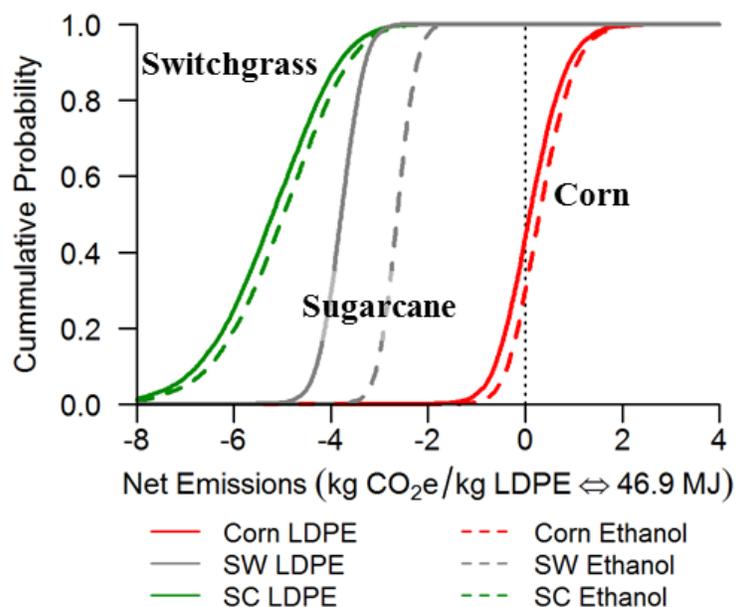


Figure A.8. Net emissions from examined bio-based pathways treating naphtha as the feedstock for fossil ethylene. The figure shows the cumulative distribution function for net emissions from both chemical (LDPE) and fuel use of bio-based ethanol, including any savings from 1:1 displacement of the relevant fossil fuel product (gasoline of naphtha-derived LDPE).

Another important assumption in this chapter is that GHG savings for bio-based pathways are calculated assuming 1:1 displacement of the corresponding fossil fuel product (gasoline or fossil LDPE). While 1:1 replacement is accurate on a physical basis, the resulting changes in market prices make 1:1 replacement unlikely across the entire market. Policies which encourage the use of biofuel or bio-based chemicals may cause a variety of market-mediated effects, some of which have already been accounted for by including emissions from indirect land-use change. Another important market-mediated effect involves the global market for fossil fuel products and has been termed the indirect fuel use effect (IFUE), see for example ref.²³⁶ Mandates like RFS2 decrease demand for fossil products and may result in a global change in demand as fossil prices drop, resulting in replacement of fossil products that is less than 1:1. On the other hand mandates like RFS2 increase the price of the final product mix in regulated sectors which could also result in a negative IFUE (for example, if people drive less in response to higher fuel prices). The increase in global demand for fossil products relative to the counterfactual of 1:1 replacement with bio-products is sometimes

called “rebound,” however to avoid confusion with the energy efficiency literature I prefer the terms “IFUE” (for fuel markets) or more generally “indirect demand change” (IDC) for fossil products. As an example, a +20% “indirect demand change” for LDPE indicates that introducing 1 unit of bio-LDPE into the market will lead to a net decrease of 0.8 units of fossil LDPE.

A limited number of studies have investigated the magnitude of IFUE, and were the subject of a recent critical review by Smeets *et al.*³²⁸. To capture the range presented, indirect demand change for gasoline (due to the introduction of bio-ethanol) is simulated with a uniform distribution ranging from -1% to 85% (i.e. introduction of 1 MJ of ethanol results in a market wide decrease in gasoline use ranging from 1.01 MJ to 0.25 MJ). The upper bound (85%) deliberately excludes cases presented in³²⁸, which relate to tax credits rather than an RFS2-style mandate. No studies were available to estimate indirect demand change in the fossil ethylene market, and so a fossil LDPE indirect demand change is simulated with a uniform distribution from 0% to 100%. Results are presented in Figure A.9 to Figure A.11. Inclusion of indirect demand change effects increases the modeled net emissions in all pathways. Nevertheless, sugarcane LDPE and both switchgrass pathways continue to meet EISA targets with a high degree of confidence. For reasons discussed below, indirect demand change has a larger effect in the fuels market (despite lower modeled indirect demand change percentages). As a result, bio-LDPE is now the preferred pathway for both U.S. and Brazilian pathways (Figure A.11).

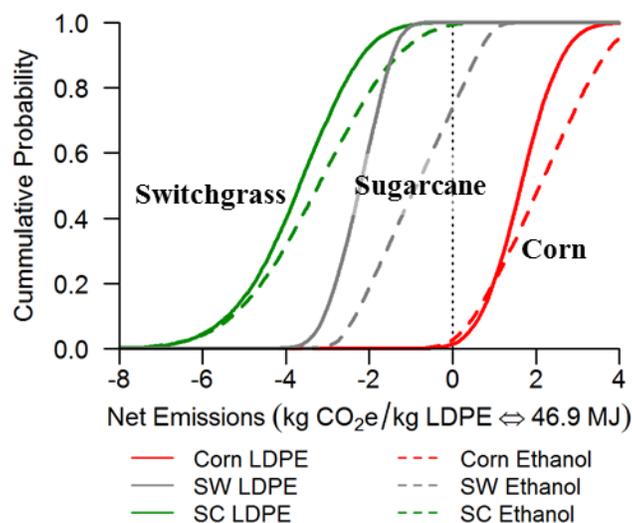


Figure A.9. Net emissions from examined bio-based pathways. The figure shows the cumulative distribution function for net emissions from both chemical (LDPE) and fuel use of bio-based ethanol, including savings displacement of the relevant fossil fuel product (gasoline or fossil LDPE), with market induced indirect demand change. The functional unit is scaled so that equivalent volumes of ethanol are considered.

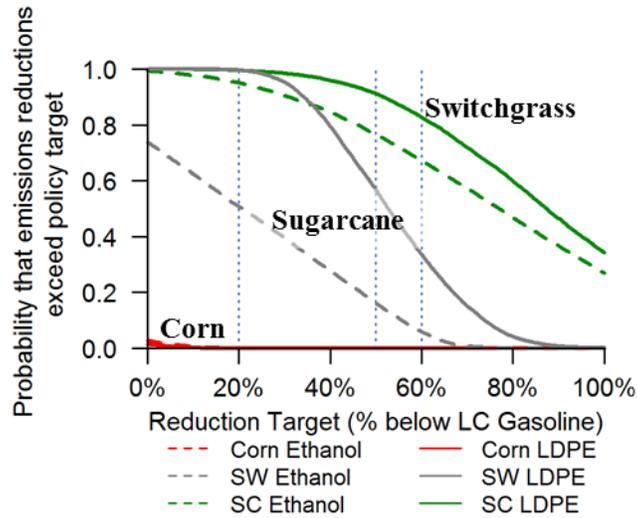


Figure A.10. Probability (proportion of model runs) that GHG emission from each bio-based pathway are below those of the fossil fuel counterpart (at 0%) or below some policy target. Fossil product displacement is modeled with uncertain market-induced indirect demand change. Policy targets are given as a percent reduction relative to simulated gasoline life cycle (LC) emissions. EISA targets (20% for corn biofuel, 50% for advanced biofuels and 60% for cellulosic biofuels) are shown with vertical blue lines.

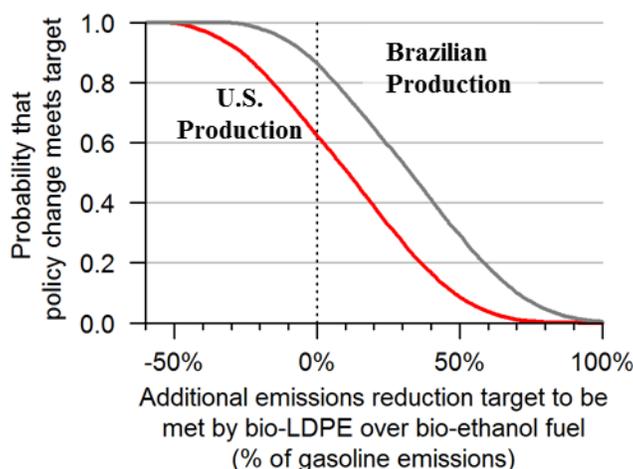


Figure A.11. Probability (proportion of model runs) that GHG savings from bio-LDPE are superior to those from bio-ethanol (at 0% on the x-axis) or in excess of some policy target. Positive values indicate that more stringent reductions can be met with bio-LDPE. Negative values represent needed relaxation in the target emissions reductions (as a % of gasoline emissions). Figure includes market-induced indirect demand change effects.

In Figure A.12 to Figure A.14, indirect demand change in the fossil product market (gasoline or fossil LDPE) is treated parametrically for each of the bio-based pathways considered.

Indirect demand change in the gasoline market has a higher impact than indirect demand change in the LDPE market; this is because gasoline has higher emissions per functional unit than fossil LDPE. For corn ethanol, substantial *negative* indirect demand change is required before RFS2 targets can be met; even with such indirect demand decreases, corn LDPE remains unable to meet the RFS2 20% reduction target, as modeled. For sugarcane ethanol pathways, modest gasoline indirect demand increases threaten RFS2 targets, while only relatively large indirect demand increases would cause net increase in emissions. For sugarcane LDPE and both switchgrass pathways, high levels of indirect demand change could interfere with RFS2 targets, but a net increase in emissions is almost never observed in the model (reflecting the high probability of negative emissions for these pathways, even excluding fossil product displacement).

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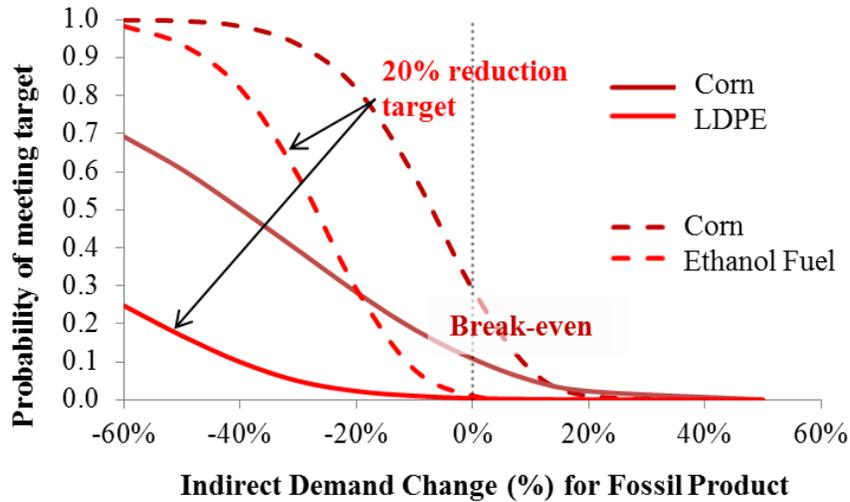


Figure A.12. Probability that corn ethanol and corn LDPE achieve net GHG emission reductions (“break-even”), or the RFS2 renewable biofuel reduction target (20% reduction compared to gasoline) as a function of market-induced indirect demand change in the fossil product market.

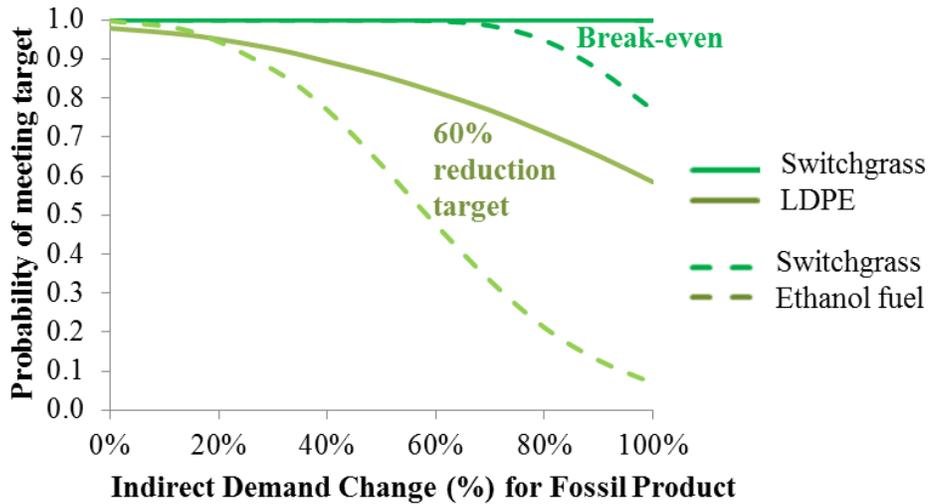


Figure A.13. Probability that switchgrass ethanol and switchgrass LDPE achieve net GHG emission reductions (“break-even”), or the RFS2 cellulosic biofuel reduction target (60% reduction compared to gasoline) as a function of market-induced indirect demand change in the fossil product market.

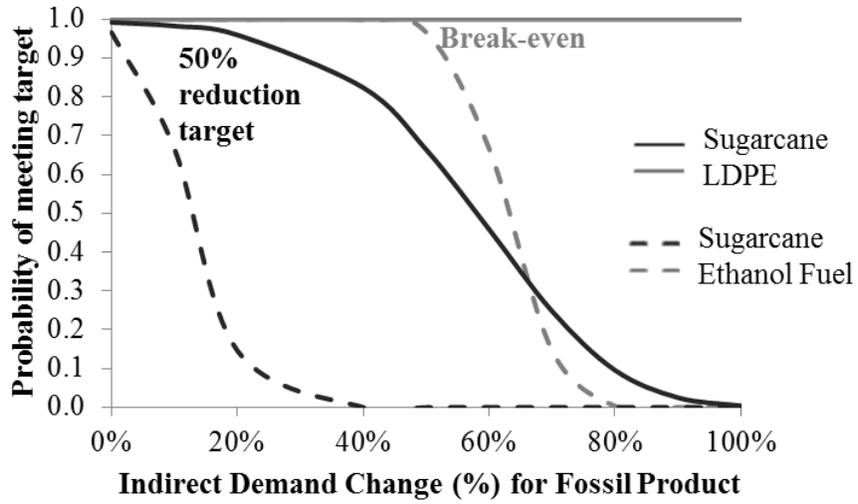


Figure A.14. Probability that sugarcane ethanol and sugarcane LDPE achieve net GHG emission reductions (“break-even”), or the RFS2 advanced biofuel reduction target (50% reduction compared to gasoline) as a function of market-induced indirect demand change in the fossil product market.

A.2.6 Sensitivity to Other Select Assumptions

Table A.18. Selected assumptions and their impact on main conclusions of the study:

Category	Assumption	Impact on Study Conclusions
General Assumptions		
Choice of product	LDPE chosen as the reference ethylene-based product	Low impact: stages taking place after the production of ethylene are only important for Brazilian production. Products with higher electricity requirements would reinforce the conclusion that Brazilian bioethylene is preferred to bio-ethanol. Products with lower electricity requirements would result in GHG savings for bioethylene that are similar to the savings from bio-ethanol fuel.
Point estimates	All pathways contain a small number of parameters for which uncertainty is not modeled	Underestimation of uncertainty. No model will ever capture all uncertainty. Nevertheless, calculated ranges presented here are likely to be representative of the modeled pathways.
Gasoline		
Baseline life cycle emissions	Life cycle emissions modeled as in Venkatesh <i>et al.</i> ¹⁹⁸ ; mean not scaled to match EPA reported value	Low Impact: the mean value employed here is 89 g CO ₂ e/MJ, compared to 93 g CO ₂ e/MJ reported by EPA. Calibrating gasoline emissions so that the mean matches the EPA reported value favors bio-ethanol fuel routes but does not overturn any qualitative conclusions.
Natural Gas LDPE		
Allocation	Production and processing products treated by mass allocation	Low impact: allocation by energy content would slightly decrease the emissions from fossil LDPE (increasing the net emissions from bio-LDPE)
Allocation	Hydrogen from steam cracking treated by system expansion.	Moderate impact: treating H ₂ as fuel slightly increases the emissions from fossil LDPE (decreasing net emissions from bio-LDPE). Treating H ₂ by mass allocation (the least favorable possible assumption) substantially increases the emissions from fossil LDPE such that bio-LDPE is preferred over fuel ethanol even for U.S (corn and switchgrass) routes.

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Allocation	Non-Hydrogen products from steam cracking treated by mass allocation	Low impact: non-hydrogen co-products are very minor compared to ethylene. Treatment by (HHV) energy allocation would slightly increase the emissions from fossil LDPE (decreasing net emissions from bio-LDPE).
Correlation between well workovers and estimated ultimate recovery	No correlation	Low impact: correlation would reduce variance, but contribution from workovers to final results is minimal
Lease fuel and plant fuel composition	Composed entirely of CO ₂ and CH ₄	Low Impact: In 2011, CO ₂ and CH ₄ together accounted for 87.6% of national natural gas content ²¹² . The remaining composition will be a mixture of inert gasses (like nitrogen, argon and helium) and higher hydrocarbons (like ethane, propane, butane and pentane). The latter will increase the (per unit volume) CO ₂ emissions while the former will reduce them.
Production site vented and flared gas	All flared	Under estimation of fossil LDPE emissions. Even if all gas were vented (an extreme scenario), emissions for fossil LDPE would rise only by about 10% and net emissions for bio-LDPE would fall by 5 percentage points (expressed as a percent of gasoline emissions).
Displacement of fossil LDPE	Bio-LDPE replaces ethane-based LDPE	Under estimation of fossil LDPE emissions: although ethane is the dominant feedstock for U.S. ethylene production, there is no guarantee that it will be on the margin (i.e., that this is the feedstock bio-LDPE will replace). Heavier feedstocks are generally reported to have higher emissions for ethylene production, which would therefore decrease net emissions from bio-LDPE products. This was discussed in section 1.4.4.
Displacement of fossil LDPE	Bio-LDPE replaces fossil LDPE on a 1:1 ratio	High impact: market forces make it unlikely that bio-LDPE would actually replace fossil LDPE on a 1:1 basis. The sign and magnitude of emission changes due to secondary market interactions is unclear. This was discussed in section 1.4.4.
<i>Switchgrass Pathways</i>		
Allocation	Surplus electricity treated by	Moderate impact: system expansion represents the most

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	system expansion	optimistic possible assumption for surplus electricity. The most pessimistic assumption (no credit for surplus electricity has already been discussed). Treating surplus electricity by energy content allocation lies in between these extremes.
<i>Sugarcane Pathways</i>		
Allocation	Surplus electricity treated by system expansion	Low impact: surplus electricity production is small

A.2.7 Cost Analysis

Production costs for bio-ethanol and bioethylene have been estimated by the International Renewable Energy Agency,¹⁸⁴ where mean and confidence intervals were provided, these data were used as the parameters (min, mode and max) for triangular distributions. The cost for fossil ethylene was estimated from historical data by subtracting ethane cracker margins from the retail price of ethylene as reported by multiple sources.²³⁷⁻²³⁹ The minimum and maximum values obtained from these sources for the period from January 2012 to July 2013 (the latest data available) were used to parameterize a uniform distribution.

Gasoline production costs are estimated as the sum of crude oil and refining costs. EIA provides monthly data on the components of the average U.S. gasoline price over time.²⁴⁰ The data does not separate refining costs from refiner margins. Instead, refiner margins were estimated using data from the International Energy Agency (IEA).²⁴¹ IEA data is available annually from 2004 to 2010 and quarterly for 2011. For each U.S. refinery type, the refiner margin is calculated as a percent of net product worth (also provided by IEA). For each available time period, the refinery margin percentage is simulated as a uniform distribution ranging over all U.S. refinery types. This percent markup is then converted back into a dollar value (restricted to positive values) using net product worth calculated from the EIA data (averaged across the IEA time periods).²⁴⁰ For each IEA time period, refiner costs are calculated by subtracting these refiner margins from the average gross refining contribution to retail gasoline prices reported by EIA for that period.²⁴⁰ Total refining cost is then simulated as a uniform distribution across the available time periods and fitted to a single continuous distribution to reduce computational intensity. Crude oil costs are simulated as a uniform distribution spanning the minimum and maximum monthly crude oil costs reported by EIA from January 2012 to January 2014.²⁴⁰ Finally crude oil and refining costs are assigned a correlation of 0.5 based on historical data.

Results of the cost analysis are presented in Figure A.15. Bioethylene (from any source) is substantially more expensive to produce than ethane-derived ethylene. In contrast, ethanol, particularly from sugarcane, may already be competitive with gasoline.

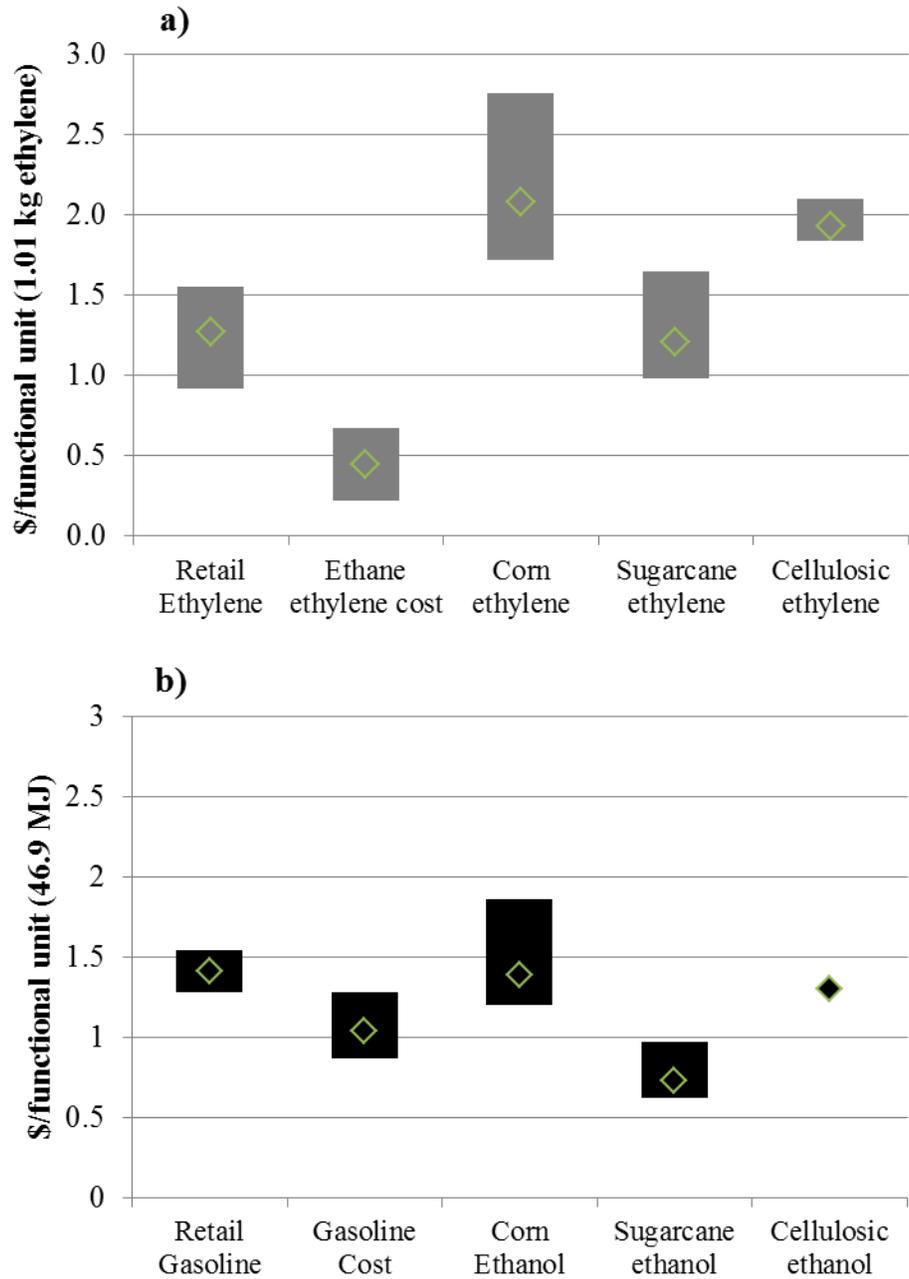


Figure A.15. Simulated costs per functional unit. Rectangles show the range of simulated costs and diamonds show the mean or best estimate for each feedstock. a) Retail price and feedstock specific cost of production for 1.01 kg ethylene. b) Retail price and feedstock specific cost per 46.9 MJ of fuel.

For each bio-based pathway net GHG savings are combined with cost estimates to simulate an implicit carbon price. Results are presented in Table A.19. No value is shown for corn pathways as no net GHG savings are achieved. While bio-ethanol appears to be a reasonable GHG

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mitigation strategy, bioethylene can only be justified (at current production costs) if substantial co-benefits are expected. Nevertheless, *private* investment into bioethylene is already taking place.^{11,12} Adopting a more flexible standard in place of RFS2 can only decrease the overall cost of compliance, particularly as market prices change and new production technologies evolve.

Table A.19. Implicit Carbon Price for bio-ethanol and bioethylene (90% confidence interval, \$/tonne CO₂e). Confidence interval is formed as a percent of model runs, and may not represent true probability.

	Corn	Sugarcane (\$/tonneCO ₂ e)	Switchgrass (\$/tonneCO ₂ e)
Bio-ethanol	N/A	-200 to 0	0 to 100
Bioethylene	N/A	150 to 400	200 to 550

Appendix B. Supporting Information for Chapter 3

B.1. Model and Data

B.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.¹⁴⁵ 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,¹⁹⁸ as well as natural gas extraction and processing, along with ethane and naphtha steam cracking (for the production of olefins and pygas).¹⁵⁴ Due to confidentiality requirements, the Franklin Associates report¹⁴⁵ suppresses details for the production of ethylene glycol, and so I model the energy demands for this step using the Ecoinvent database.³⁹⁵ For several unit processes, the Franklin Associates¹⁴⁵ include a category for ‘recovered energy.’ This represents exported steam, which I assumed displaces natural gas (accounting for natural gas boiler efficiency, as per section B.1.12). In the production of benzene for PS, a portion of the feedstock is burned for energy, which Franklin Associates¹⁴⁵ list as a mass quantity of “internal offgas.” For simplicity, I treat the direct emissions from internal offgas as methane (2.75 kg CO₂/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) (Chapter 2).¹⁵⁴ Table B.1 presents key parameters and distributions used in the fossil polymer model.

B.1.2 Land Use Change (LUC)

As explained in Posen *et al.* (2015) (Chapter 2): 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.”¹⁵⁴ Argonne National Laboratory’s GREET model²⁶⁷ includes a carbon calculator for land use change (CCLUB) tool. CCLUB models global land

changes induced by the U.S. biofuel mandate,⁴ as predicted by the Global Trade Analysis Project (GTAP) general equilibrium model.³⁹⁶ The present work 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 chapter 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.³⁹⁷ For corn, the updated 2013 modeling scenario is employed. The lower bound (1.8 g CO₂e/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 CO₂e/MJ ethanol) results from using the Winrock model for both domestic and international emissions. For switchgrass, the lower bound (-3.8 g CO₂e/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 CO₂e/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 CO₂e/MJ ethanol). This estimate is excluded as it is inconsistent with other existing estimates for cellulosic crops,⁸⁵ 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.³⁸⁰ 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 short ton for switchgrass). Further discussion of LUC modeling choices is available in sections 0 and B.2.6.

B.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)).²⁷⁹ Using 2014 data, total fertilizer application of each type is divided by total corn production in each state for the same year.²⁷⁹ 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.²⁶⁷

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.²²⁵ Using equation 11.6 of the IPCC guidelines, $Area_{(T)}$ is set to 1, $Area_{burnt(T)}$ 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-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.²²⁵ $Crop_{(T)}$ 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.²⁷⁹ 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.²⁷⁸ I 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 B.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)²⁸⁰ 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, I 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)²⁸⁰ quote a 2005 article calling the issue “unsettled” and suggesting that the range is “not narrowing, nor is a central tendency developing”³⁹⁸. 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),²⁸⁰ with mode (100 kg N/ha) set to where the authors indicate “a hint of an optimum.”²⁸⁰ Using the IPCC Guidelines⁹⁵ to calculate nitrogen in crop residue, as above, results in an estimate for N₂O emissions that is far higher than reported by other sources.^{167,259,267} Thus, I instead use an estimate for above and below ground nitrogen from GREET 2014 (0.54 g nitrogen / kg switchgrass)²⁶⁷ 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 (K₂O, P₂O₅, and herbicides), on farm energy use (diesel and electricity), and emissions from feedstock transportation are taken from GREET.²⁶⁷ Table B.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 CO₂ emissions from limestone (CaCO₃ application) are taken from the GREET model.²⁶⁷ Nitrous oxide (N₂O) 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.²²⁵ The combined effect of the different modes of N₂O production is a mean conversion factor (from N to N₂O-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 report²²⁵ (1.2% and 1.3% respectively) or in GREET (1.5%).²⁶⁷ Sections 0 and B.2.6 present results assuming a lower value of N₂O, 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 my resulting distributions are still low compared with top-down estimates of N₂O emissions from agriculture.³⁹⁹ Table B.4 presents key parameters and distributions related to agrochemicals and field emissions common to both feedstocks.

B.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. I consult multiple sources to estimate distributions for total process yield and for the mass of each co-product per unit of corn processed.^{262,263,267,400,401} Akiyama *et al.* (2003)²⁶³ report yield on the basis of corn oil, corn meal & feed, and glucose. I 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.^{400,401} I 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 database⁴⁰⁰) is treated as corn gluten feed. The resulting distributions are presented in Table B.5.

Four data sources are considered for the emissions from the wet milling process.^{244,262,263,400} Akiyama *et al.* (2003)²⁶³ provide CWM primary energy use by fuel type (residual oil, natural gas, coal, electricity, others) per kg product, allocated on a mass basis. I 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 CO₂e/kg dry corn processed.

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Kim and Dale (2008)²⁴⁴ 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 CO₂e), per kg PHB. The authors also present the emissions from corn entering the wet mill (965 g CO₂e/kg PHB) and their emissions factor for corn production (219 g CO₂e/kg PHB) from which I 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 B.12), and the authors' original estimates for chemical inputs, I arrive at a distribution centered on 0.32 kg CO₂e / kg dry corn processed.

Vink *et al.* (2015)²⁶² report total emissions from their CWM unit process (“dextrose production”) to be 0.29 kg CO₂e/kg PLA (using mass allocation). They also provide the yield of PLA (10.2 kg PLA/bu corn), which I use to convert CWM emissions to a per kg corn processed basis. The authors do not present their raw data, and so I am unable to harmonize this emissions estimate using our own emissions factor. I do, however, update the global warming potential using the following method. Vink *et al.* (2015)²⁶² use characterization factors from CML2001 (April 2013 update), which lists methane at 25 g CO₂e / g CH₄.⁴⁰² In a 2010 paper studying the same PLA production process,²⁶⁰ Vink *et al.* (2010)²⁶⁰ list raw emissions of methane and CO₂ separated by activity type (fuel production, fuel use, transport, process and biomass). I calculate the ratio of CH₄ to CO₂ from across the fuel production, fuel use, and production process stages (CH₄:CO₂ = 0.00478:1 on a mass basis). Assuming the same ratio of gases applies to the results from Vink *et al.* (2015),²⁶² I calculate a 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 CO₂e / kg dry corn processed.

Finally, the Agri-Footprint database, available in commercial SimaPro software provides emissions estimates for CO₂, CH₄ and N₂O from wet mill starch production (“Maize starch, from wet milling (starch drying) at plant/US Mass”).⁴⁰⁰ 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 CO₂e / kg dry corn processed.

Since corn wet milling is a relatively mature technology, I 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 2009,²⁸³ and add approximately 13 g CO₂e / kg glucose. Table B.5 presents key parameters and distributions related to corn wet milling.

B.1.5 Corn Co-product Treatment

The mass distribution of co-products from corn wet milling and corn dry milling are described in sections B.1.4 and B.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 B.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.²⁶⁷ 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% moisture) / 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 B.1.2 and B.1.3 above. Emissions from displaced urea are taken directly from GREET.²⁶⁷ Emissions for displaced soy oil and soybean meal are based on GREET, but with our own distribution for N₂O emissions from fertilizer and crop residue, as described in section B.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 I take an average across these models. Additional details are available in Table B.5.

B.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.^{403,404} Dilute acid pretreatment was selected for this study based on its near-term potential, and high data availability.^{259,261,267,283,284,405} Emissions from chemical and enzyme inputs are calculated alternately from MacLean and Spatari (2009)²⁸³, and from the GREET 2014 pretreatment module.^{267,405} Data in GREET is presented per tonne of sugar; I convert the data to emissions per tonne of feedstock input using a value of 0.53 kg sugar / kg dry switchgrass, which I calculate using the values for switchgrass composition and yield of sugars assumed in GREET (tables 1 and 4 of Adom *et al.* 2014⁴⁰⁵). The resulting estimates are centered on 53 g CO₂e/kg dry feedstock (based on MacLean and Spatari (2009)²⁸³) and 93 g CO₂e/kg dry feedstock (based on GREET^{267,405}); the latter is stochastic due to uncertainty in GWP for CH₄ and N₂O. 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 B.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.* 2014,⁴⁰⁵ 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).²⁸⁴ 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). I 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 B.6.

I 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).⁷⁴ 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).²⁸³ For PLA and PHB, only the mid-term yield model is considered. Table B.6 presents key parameters and distributions related to switchgrass scenarios.

B.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).²⁵¹ 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

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data on farm land allocated to PLA production (2,081 m²/ metric tonne PLA) and sugarcane yield (57 tonnes/ha year), from which I 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 tonne of sugar is co-produced with 463 kg of molasses.²⁵¹ They perform economic allocation based on the 2006 Thai selling prices of sugar and molasses (no citation given), which I retrieve from a USDA report.⁴⁰⁶ I calculate the allocation factor for sugar to be 89.6%, from which I calculate 13.2 kg sugarcane / kg PLA (before allocation). Finally, using data on sugar production, as reported by Groot and Boren (2010)²⁵¹ (9,653 kg sugarcane / tonne sugar), I estimate sugar input to be 1.37 kg / kg PLA.

For the actual PLA production step, Groot and Boren (2010)²⁵¹ provide data on GHG emissions from chemical production and supporting processes (lime, H₂SO₄, auxiliary chemicals and waste water treatment), which I use without modification (sum: 0.87 kg CO₂e/kg PLA). Using the authors' reported steam emissions (689 kg CO₂e/tonne PLA), together with their data source for boiler emissions,⁴⁰⁷ I 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, I start with emissions, reported by Groot and Boren (2010)²⁵¹ as 610 kg CO₂e/tonne PLA. Using figure 5 of that study, I estimate a change of 8.6 kg CO₂e/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), I extrapolate that the authors' employed an electricity emissions factor of 0.72 kg CO₂e/ kWh. From this, I calculate process electricity requirements to be 846 kWh electricity/tonne PLA. Applying our own emissions factors for electricity and natural gas, I estimate a distribution for PLA production (unit process) centered on 2.3 kg CO₂e/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).²⁶² 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, I 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 CO₂e / kg PLA), lactide production (0.54 kg CO₂e/kg PLA) and polymer production (0.20 kg CO₂e/kg PLA). These values are updated to reflect the GWP of methane used in this chapter, as described in section B.1.4. The resulting distribution for PLA production (unit process) is centered around 2.0 kg CO₂e/kg PLA (for scenarios without internal energy generation from fermentation residues).

Corn Cases 3 and 4 are based on Vink *et al.* (2015)²⁶² for lactic acid production (as in case 2), together with data from Sakai *et al.* (2004)²⁶⁴ 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, I model case 4, using the polymerization energy requirements of Sakai *et al.* (2004),²⁶⁴ assuming that 100% of the energy is provided by steam heat. Table B.8 presents key parameters and distributions related to PLA production cases.

B.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).²⁴⁷ 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)²⁴⁷ 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).²⁶³ Therefore, in the present study, I assume 0.36 kg PHB / kg sugar, which is in line with the other cases reviewed here.

Harding *et al.* (2007)²⁴⁷ 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 CO₂e/kg PHB) of their reported process GHG emissions. I 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 CO₂e/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).²⁶³ The authors report primary energy for steam and electricity, as well as energy intensity of steam and electricity production, which I use to calculate direct energy use (6.88 MJ electricity and 4.11 kg steam), to which I apply our own emissions factors. The authors also provide emissions from NH₃ production, cooling water, sodium dodecylsulfate (SDS) production, and NaOCl production (amounting to 0.23 kg CO₂e / kg PHB). I exclude their estimates of fermentation emissions (which are biogenic in origin), and emissions from glucose production (which I account for separately). My resulting distribution is centered on 2.9 kg CO₂e/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).²⁶³ The authors report primary energy for steam and electricity, as well as energy intensity of steam and electricity production, which I use to calculate direct energy use (4.48 MJ electricity and 3.96 kg steam), to which I apply our own emissions factors. The authors also provide emissions from NH₃ production, cooling water, SDS production, and NaOCl production (amounting to 0.20 kg CO₂e / kg PHB). As for case 2, I exclude their estimates of fermentation emissions and emissions from glucose production. My resulting distribution is centered on 2.2 kg CO₂e/kg PHB (for scenarios without internal energy generation from fermentation residues).

Case 4

Case 4 is based on Kim and Dale (2008).²⁴⁴ 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 B.1.4, I estimate that the net process yield is 4.4 kg corn / kg PHB for the

Kim and Dale (2008) study.²⁴⁴ 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 supporting information.

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 I apply our own emissions factors. Additional emissions from water, potassium hydroxide and ammonia production (amounting to 0.25 kg CO₂e/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. My resulting distribution (for the corn-based pathway) is centered on 3.2 kg CO₂e/kg PHB.

Case 5

Case 5 is based on Gerngross (1999).²⁴⁶ 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). I apply our own emissions factors to the steam and electricity generation. I treat inorganic salts as their primary constituent, ammonia, with an emissions factor (1.68 kg CO₂e/kg NH₃) taken from Akiyama *et al.* (2003).²⁶³ The resulting distribution is centered on 5.8 kg CO₂e/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 B.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 B.7 presents key parameters and distributions related to PHB production cases.

B.1.9 Bioethylene Production

Bioethylene is produced via the dehydration of bioethanol. Bioethylene production from ethanol is modeled as in Posen *et al.* (2015) (Chapter 2),¹⁵⁴ based on Kochar *et al.* (1981),¹⁸⁰ Haro *et al.* (2013),⁴⁰⁸ and Geisler *et al.* (2005)²²⁷. 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.²⁸¹ I 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.²⁸² Reported co-product yields violate mass balance, and so I adjust these downward (dynamically) as follows. I 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 glucose⁷⁴). Thus, the theoretical maximum yield of ethanol is 0.568 kg ethanol / kg starch (1.76 kg starch / kg ethanol). I assume that corn oil and DDG are always produced in the same ratio (0.53:15.73) as reported by Mueller and Kwik (2013),²⁸¹ in quantities set to restore mass balance on the corn feedstock, assuming 100% product yield from the dry mill. I 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) (Chapter 2),¹⁵⁴ based on Mullins *et al.* (2011).⁷⁴ These include energy requirements for pretreatment. Starting with sugars available after pretreatment and saccharification (section B.1.6), ethanol yield is modeled as in Spatari and MacLean (2010)²⁶¹, again following the 2 scenarios (near-term/lower yields and mid-

term/higher yields) laid out by those authors. Table B.9 presents key parameters and distributions related to bioethylene production cases. I assume that switchgrass ethanol will be transported by truck from the Southeast to the Gulf Coast.

B.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 B.1.7, B.1.8 and B.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, I 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, I 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 B.1.6.

In the base case, I 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,^{74,262,263} respectively. I use these yields to calculate quantities of unfermented monomeric sugars, which I combine with quantities of unhydrolyzed 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 B.2.6. Table B.6 presents key parameters and distributions related to switchgrass scenarios; energy densities for switchgrass components are listed in Table B.14.

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I 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, I 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.^{305,306,308} For steam and electricity generation, I 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%⁴⁰⁹ to 96%⁴¹⁰ (modeled as a uniform distribution). When internal energy is used, I 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, I assume the power:heat ratio cannot exceed 1:3 (i.e. no more than 25% of the available energy may be extracted as electricity).⁴¹¹ 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, I 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.

B.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 CO₂ / kg PLA), PHB (2.0 kg CO₂ / kg PHB) and bioethylene (3.1 kg CO₂ / 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. I model disposal of conventional polymers (including bioethylene-based polymers) following the U.S. Environmental Protection Agency (EPA) Waste Reduction Model (WARM).²⁶⁸ Conventional polymers and PLA are assumed to be inert under landfill conditions. Thus, landfilling is assumed to generate emissions of 0.04 metric tonnes (Mt) CO₂e / short ton plastic (0.044 kg CO₂e/kg plastic), related only to landfill machinery and transportation of waste to the landfill.²⁶⁸

For the incineration option, I assume combustion proceeds with 100% efficiency; CO₂ emissions are calculated based on the chemical composition of each polymer. Yu and Chen (2008)⁴¹² provide the energy content of PHB. The energy contents of all other polymers are taken from the EPA WARM documentation.²⁶⁸ The incineration facility is assumed to be equipped with energy recovery capabilities, generating electricity at a net efficiency of 17.8%.²⁶⁸ I 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 CO₂e / short ton plastic (0.033 kg CO₂e/kg plastic).²⁶⁸

Recycling is modeled following the EPA WARM model.²⁶⁸ 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 CO₂e / short ton plastic (0.22 kg CO₂e/kg plastic). Recycling process emissions amount to 0.35 Mt CO₂e/ short ton HDPE (0.39 kg CO₂e/kg HDPE), and 0.77 Mt CO₂e/ short ton PET (0.85 kg CO₂e/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.^{413,414} Thus, for all other polymers, I 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, I assume that process emissions (for transportation and fuel to turn the compost pile) amount to 0.04 Mt CO₂e/ short ton plastic (0.44 kg CO₂e/kg plastic).²⁶⁸ I further assume that 90% of the carbon content of the plastic is lost as CO₂, resulting from 44% loss during composting, and only 18% of the remaining carbon being sequestered in soil.²⁴⁴ 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 I 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, I 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, I use data relating to the anaerobic biodegradation of a PHB co-polymer (Poly(3-hydroxybutyrate-co-3-hydroxyoctanoate))^{269,270} to estimate generation of CO₂ and CH₄ 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).²⁶⁹ Following Levis and Barlaz (2011),²⁷⁰ I calculate the methane fraction of released carbon to be 56.3%, using the Buswell equation, cited in Parkin and Owen (1986).⁴¹⁵ The remainder of the mineralized carbon is assumed to be generated as CO₂. I model oxidation of uncollected methane as a triangular distribution (min: 10%, mode: 10%, max: 40%) based on Levis and Barlaz (2011).²⁷⁰ For landfills with a gas collection system installed, I 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.²⁶⁸ All collected methane is assumed to be combusted with 100% efficiency. For landfills with energy recovery in place, I assume an electricity generation efficiency of 29.2%.²⁶⁸ Finally, the proportion of landfills with gas collection, and the proportion of landfills with energy recovery are modeled following Levis and Barlaz (2011).²⁷⁰ I 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 B.11 and Table B.10.

B.1.12 Fuels and Electricity

As in Posen *et al.* (2015) (Chapter 2),¹⁵⁴ emissions from grid electricity are modeled at the level of individual North American Reliability Corporation (NERC) regions,²⁰⁸ employing distributions that span the range of available literature estimates.^{267,272-275} Consistent with existing production,^{230,260} 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.¹²⁸ I 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.²⁷⁶ 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).³⁶⁵

Emissions from other conventional fuels are discussed in the main text. For this chapter, the distribution for emissions from natural gas is modified from the original source²⁶⁶ as follows. The @RiskTM 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)²⁶⁶ for upstream emissions. Instead, a Pearson V distribution provides a close fit to the original authors' recommended

distribution. Further, the present work considers large industrial facilities that would likely receive natural gas directly from transmission lines, and so I remove emissions from natural gas distribution, as fit to the parameters for distribution emissions provided in Tong *et al.*²⁶⁶ Finally, I model combustion as per the original source for Tong *et al.*^{95,201,266}

When energy requirements are cited in terms of steam energy, I assume that steam is generated from natural gas combustion. When a data source presents only the mass of steam required, I assume it is at atmospheric pressure, with an energy content of 2.68 MJ/kg steam. Following Abrahams *et al.* (2015),²⁶⁵ 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.^{305,306,308} Table B.12 presents key parameters and distributions related to fuels and electricity.

B.1.13 Model Parameters

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

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Table B.1. Summary of key parameters for fossil polymer production

Parameter	Value or Distribution	Units	Source and notes
<i>Upstream processes</i>			
Crude oil extraction	Pearson5 (7.1, 1.7, 0.049) (mean: 0.33, CI ^a : 0.18-0.65)	kg CO ₂ e / kg crude oil	Fitted to underlying model from ¹⁹⁸
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 (Approx: Pearson5 (14.5, 2.11, 0.098))	kg CO ₂ e / kg wet gas	Approximate fit; actual model as described in ¹⁵⁴
Natural gas processing	mean: 0.074, CI ^a : 0.013, 0.367 (Approx: Pearson5 (3.25, 0.28, -0.0237))	kg CO ₂ e / kg processed gas	
<i>Ethylene glycol inputs</i>			
Ethylene oxide	0.710	kg ethylene oxide / kg ethylene glycol	Calculated from stoichiometry
Electricity	0.391	kWh / kg ethylene glycol	ref ³⁹⁵
<i>Other unit processes</i>			
Energy requirements (by fuel type)	Various	Various	ref ¹⁴⁵

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

(a) 95% confidence interval (CI)

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Table B.2. Summary of key parameters for corn agriculture

Parameter	Value or Distribution	Units	Source and notes
<i>Corn</i>			
LUC emissions	Uniform (18,159)	g CO ₂ e/ kg dry corn	Based on the GREET CCLUB model ²⁶⁷
Crop yield	Extreme value min (161, 13.9) (mean: 153, CI ^a : 110,180)	bu / acre	Own analysis of USDA data ²⁷⁹ ; used to calculate N in crop residue, and fuel use/bu
Nitrogen applied	Exponential (0.0391, 0.353) (mean: 0.392, CI ^a : 0.35, 0.50)	kg N / bu	Own analysis of USDA data ²⁷⁹
Phosphate applied	Triangular (0.093, 0.093, 0.23)	kg P ₂ O ₅ / bu	
Potash applied	Uniform (0.029, 0.25)	kg K ₂ O / bu	
CaCO ₃ applied	1150	g CaCO ₃ / bu	
Herbicides applied	7	g / bu	ref ²⁶⁷
Insecticides applied	0.06	g / bu	
Nitrogen in crop residues	approx: Normal (9.88, 3.83)	g N / kg dry corn	Based on ²²⁵ ; actual distribution is described in section B.1.3.
Gasoline used	1.9 (250)	gallons / acre (MJ HHV / acre)	ref ²⁷⁸
Diesel used	5.2 (750)	gallons / acre (MJ HHV / acre)	
LPG used	1.7 (160)	gallons / acre (MJ HHV / acre)	
Natural gas used	0.2 (230)	MCF / acre (MJ HHV / acre)	
Electricity used	30.4	kWh / acre	
Feedstock transportation	410 0.706 0.007	g CO ₂ / bu g CH ₄ / bu g N ₂ O / bu	ref ²⁶⁷

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)

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Table B.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 ²⁶⁷
Crop yield	Weibull (2.8, 17.4, -2.69, [3.0,25.6]) (mean: 12.8, CI ^a : 4, 23.4)	Mg dry matter / ha	Based on ²⁸⁰
Nitrogen applied	Triangular (0, 100, 180)	kg N / ha	
Nitrogen in crop residue	0.54	g N / kg dry SW	ref ²⁶⁷
P ₂ O ₅ applied	114 (0.251)	g / short ton dry SW (g / kg dry SW)	ref ²⁶⁷
K ₂ O applied	227 (0.125)	g / short ton dry SW (g / kg dry SW)	
Herbicides applied	31.8 (0.0351)	g / short ton dry SW (g / kg dry SW)	
Diesel used	18700 (0.218)	Btu/short ton dry SW (MJ HHV / kg dry SW)	
Electricity used	14500 (0.0169)	Btu/short ton dry SW (MJ electricity / kg dry SW)	
Feedstock transportation	13700	g CO ₂ / short ton dry SW	
	23.8	g CH ₄ / short ton dry SW	
	0.205	g N ₂ O / short ton dry SW	
	(15.1) (0.0262) (2.3 E-4)	(g CO ₂ / kg dry SW) (g CH ₄ / kg dry SW) (g N ₂ O / 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)

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Table B.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 ²⁶⁷
CaCO ₃ Production	0.0137 ^a	kg CO ₂ e / kg CaCO ₃	
K ₂ O Production	0.661 ^a	kg CO ₂ e / kg K ₂ O	
P ₂ O ₅ Production	1.53 ^a	kg CO ₂ e / kg P ₂ O 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 ₂ O from synthetic fertilizer and crop residue	Triangular (0.003, 0.01, 0.03)	kg N ₂ O-N/kg N applied	ref ²²⁵
Volatilization from synthetic fertilizer	Triangular (0.03, 0.1, 0.3)	(kg NH ₃ -N + kg NO _x -N) / kg N	
Indirect N ₂ O from volatized N	Triangular (0.002, 0.01, 0.05)	kg N ₂ O-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 ₂ O from runoff	Triangular (0.0005, 0.0075, 0.025)	kg N ₂ O-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.

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Table B.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: ²⁶³ , upper bound: ²⁶⁷ , modal cluster: ^{262,400,401}
Corn gluten feed yield	Uniform (0.21, 0.29)	kg / kg dry corn processed	Lower bound: ²⁶³ , upper bound: ²⁶⁷
Corn oil yield	Uniform (0.033, 0.054)	kg / kg dry corn processed	Lower bound: ²⁶² , upper bound: ²⁶⁷
Total process yield	Uniform (98.7, 99.6) %	% of dry corn processed	Lower bound: ²⁶³ , upper bound: ⁴⁰¹
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 ^{244,262,263,400} , as described in section B.1.4.
<i>Emissions credit for displaced products</i>			For the system expansion scenario only. Displacement rates are discussed in section B.1.5
Soy oil	0.74 ^a	kg CO ₂ e / kg soy oil	Calculated based on ²⁶⁷
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 N₂O emission factors.

Table B.6. Summary of key parameters common to all switchgrass scenarios

Parameter	Value or Distribution	Units	Source and notes
<i>Switchgrass Composition</i>			
Glucan (cellulose) content	Triangular (31, 34.4, 37.2)	%	ref ⁷⁴
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
<i>Pre-treatment and Saccharification</i>			
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 ²⁸³ ; upper bound calculated based on ^{267,405}
Pre-treatment electricity required	Uniform (0.15, 0.18)	MJ electricity / kg feedstock processed	Bounds calculated based on ²⁸⁴ and ²⁶⁷ , 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)	ref ²⁶¹ . Used for PHB, PLA and mid-term bioethylene
Near-term yield of glucose from glucan	Normal (0.675, 0.038)	% (molar conversion)	ref ²⁶¹ . Only used for near-term bioethylene scenario
Near-term yield of sugars from hemicellulose	Normal (0.635, 0.0097)	% (molar conversion)	
<i>Internal energy use</i>			
Biomass boiler	Triangular (68, 70, 74.5)	% (HHV)	Lower: ³⁰⁵ , mode: ³⁰⁶ , upper: ³⁰⁷
CHP electric generator efficiency	Uniform (85,96)	%	Lower: ⁴⁰⁹ , upper: ⁴¹⁰
Maximum CHP heat:power ratio	1:3	Ratio	ref ⁴¹¹ (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.

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Table B.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
<i>PHB Case 1</i>			
PHB Yield	0.36	kg PHB/kg sugar	Calculated based on ²⁴⁷
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	
<i>PHB Case 2</i>			
PHB Yield	0.37	kg PHB/kg sugar	Calculated based on ²⁶³
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	
<i>PHB Case 3</i>			
PHB Yield	0.3	kg PHB/kg sugar	Calculated based on ²⁶³
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	
<i>PHB Case 4</i>			
PHB Yield	0.35	kg PHB/kg sugar	Calculated based on ²⁴⁴
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	
<i>PHB Case 5</i>			

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PHB Yield	0.3	kg PHB/kg sugar	ref ²⁴⁶
Chemical production emissions	0.25	kg CO ₂ e/kg PHB	Calculated based on ²⁴⁶ , with an emission factor from ²⁶³
Electricity required	5.32	kWh/kg PHB	ref ²⁴⁶
Steam required	2.78	kg / kg PHB	
<i>Full distribution</i>			
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)

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Table B.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
<i>PLA Case 1</i>			
PLA Yield	0.72	kg PLA/kg sugar	Calculated based on ²⁵¹
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	
<i>PLA Cases 2-4</i>			
PLA Yield	0.64	kg PLA/kg sugar	Calculated based on ^{260,262}
Lactic acid production emissions	1.04 0.0050	kg CO ₂ / kg PLA kg CH ₄ / kg PLA	
<i>PLA Case 2</i>			
Lactide production and polymerization emissions	0.66 0.0032	kg CO ₂ / kg PLA kg CH ₄ / kg PLA	Calculated based on ^{260,262}
<i>PLA Case 3</i>			
Lactide production and polymerization electricity required	1.71	kWh/kg PLA	ref ²⁶⁴
<i>PLA Case 4</i>			
Lactide production and polymerization steam required	6.16	MJ / kg PLA	Based on ²⁶⁴

Distributions are written as: Uniform (min, max)

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Table B.9. Summary of key parameters for bioethylene pathways

Parameter	Value or Distribution	Units	Source and notes
<i>Corn bioethanol</i>			
Electricity use	Normal (0.75, 0.23) (Normal (0.90, 0.28))	kWh / gal EtOH (MJ / kg EtOH)	Mean: ²⁸¹ , Stdev based on ²⁸²
Fuel use	Normal (23862, 2798) (Normal (8.4, 0.99))	Btu LHV / gal EtOH (MJ / kg EtOH)	
Ethanol yield	Normal (2.8, 0.018) (Normal (0.39, 0.017))	gal EtOH / bu corn (kg EtOH / kg dry corn)	
Transportation distance	Uniform (1000, 1800)	km	Approximate distance from existing corn ethanol refineries ²³⁰ to gulf states ethylene infrastructure ²³¹ , as per ¹⁵⁴
Truck fuel consumption	0.0203	L diesel / t-km	ref ²²⁹
<i>Corn co-products</i>			
Co-product ratio from corn ethanol production	29.7	kg DDGS / kg corn oil	Calculated from ²⁸¹ Actual quantities determined based on mass balance per section B.1.9.
Emissions credit for displaced soybean meal	0.31 ^a	kg CO ₂ e / kg soybean meal	Calculated based on ²⁶⁷ ; displacement rates are discussed in section B.1.5.
Emissions credit for displaced urea	1.32 ^a	kg CO ₂ e / kg urea	
<i>Switchgrass bioethanol</i>			
Total production energy	Uniform (0.44, 0.72) (Uniform (12,19))	MJ / MJ EtOH LHV (MJ / kg EtOH)	ref ⁷⁴
Percent of energy as electricity (remainder as heat)	10%	%	
Midterm ethanol yield (all sugars)	0.95	Fraction of theoretical	ref ²⁶¹
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)	Triangular (0, 0, 0.855)	Fraction of theoretical	

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sugars)			
Transportation distance	Uniform (1000, 1800)	km	Approximate distance from projected switchgrass ethanol facilities ¹²⁸ to gulf states ethylene infrastructure ²³¹ , as per ¹⁵⁴
Truck fuel consumption	0.0203	L diesel / t-km	ref ²²⁹
<i>Ethanol dehydration to ethylene</i>			
Ethylene yield	Uniform (1.70, 1.74)	kg ethanol / kg ethylene	Lower: ⁴⁰⁸ , upper: ¹⁸⁰
Fuel used	Lognormal (1.67, 0.611)	MJ LHV /kg ethylene	ref ¹⁵⁴ based on ^{180,227}
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 N₂O emission factors.

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Table B.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	ref ²⁶⁸
Landfilling (PHB only)			
Mineralization	Triangular (41.1, 42.0, 52.5)	%	ref ²⁶⁹
Fraction of mineralized carbon to methane (rest to CO ₂)	56.25%	Fraction of mineralized carbon in PHB	Based on ^{270,415} , treated as PHB
Landfills with LFG collection	Triangular (60, 69, 84)	% of all landfills	ref ²⁷⁰
Landfills with energy recovery	Triangular (40, 50, 66)	% of landfills with LFG collection	ref ²⁷⁰
LFG collection efficiency	Triangular (59.2, 64.8, 78.8)	% of generated methane	Based on ²⁶⁸
Oxidation of uncollected methane (to CO ₂)	Triangular (10, 10, 40)	% of generated methane	ref ²⁷⁰
Efficiency of LFG to electricity	29.2%	% (assumed HHV)	ref ²⁶⁸
Composting			
Reduced carbon sequestration	89.9%	% of carbon in PHB or PLA	Based on ²⁴⁴ ; all carbon is lost as CO ₂
Transportation and equipment operation	0.044	kg CO ₂ e/kg waste	ref ²⁶⁸
Recycling			
Net recycling efficiency	0.86 (HDPE) 0.89 (PET) Uniform (0.86, 0.89) (Others)	kg virgin product displaced / kg waste recycled	ref ²⁶⁸
Process emissions	0.35 (HDPE) 0.77 (PET) Uniform (0.35, 0.77) (Others)	kg CO ₂ e / kg waste	ref ²⁶⁸
Transportation emissions	0.22	kg CO ₂ e / kg waste	ref ²⁶⁸
Incineration with energy recovery			
Efficiency of electricity generation	17.8%	%	ref ²⁶⁸
Transportation emissions	0.033	kg CO ₂ e/kg waste	ref ²⁶⁸

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

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

Plastic	Carbon content based on stoichiometry (kg CO₂ / kg plastic)	Energy content (MJ / kg plastic)	Source for energy content
HDPE	3.1	46.5	ref ²⁶⁸
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	

Table B.12. Boiler efficiencies, and emission factors for fuels and electricity.

Parameter	Value	Units	Source and notes
<i>Fuel Emissions</i>			
Gasoline life cycle emissions	Log-logistic [†] (2.2, 0.2, 80)	g CO ₂ e/MJ (LHV)	ref ¹⁹⁸
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)	ref ²⁰⁶
Natural gas: all upstream emissions (including distribution)	Pearson5 (7.66, 54.9, -0.306, [0, ∞]) Pearson5 (4.14, 0.232, 0.179, [0, ∞])	g CO ₂ / MJ (LHV) g CH ₄ / MJ (LHV)	Approximate fit to results from ²⁶⁶
Natural gas distribution	Triangular (0.047, 0.06, 0.073)	g CH ₄ / MJ (LHV)	Approximate fit to results from ²⁶⁶
Natural gas combustion emissions	Triangular (54.3, 56.1, 58.3) Triangular (3E-4, 1E-4, 3E-3) Triangular (3E-5, 1E-4, 3E-4)	g CO ₂ / MJ (LHV) g CH ₄ / MJ (LHV) g N ₂ O / MJ (LHV)	ref ⁹⁵ (original source for ²⁶⁶).
<i>Boiler efficiencies</i>			
Natural gas boiler	Triangular (70%, 80%, 94%)	% (HHV)	ref ²⁶⁵
Biomass boiler	Triangular (68%, 70%, 74.5%)	% (HHV)	Lower: ³⁰⁵ , mode: ³⁰⁶ , upper: ³⁰⁷
<i>Electricity Emissions</i>			
U.S. average electricity	Uniform (163, 208) ^a	g CO ₂ e/MJ	Lower bound: ²⁰² , upper bound: ²⁷⁷
MRO electricity	Uniform (197, 313) ^a	g CO ₂ e/MJ	Lower bound: ²⁰² ; upper bound: ²⁷³
TRE electricity (encompasses SERC as well)	Uniform (164, 220) ^a	g CO ₂ e/MJ	Lower bound from ²⁰² for TRE. Upper bound from ²⁷² .

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 B.13. Global warming potentials.

Parameter	Value	Units	Source
<i>Global warming potentials</i>			
CH ₄ GWP	Normal (36, 8.5)	g CO ₂ e / g CH ₄	refs ^{204,205}
N ₂ O GWP	Normal (298, 52.5)	g CO ₂ e / g N ₂ O	

Table B.14. Energy and mass densities used throughout this chapter

<u>Liquids</u>			
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
<u>Gasses</u>			
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
<u>Solids</u>		<u>Solids</u>	
Item	HHV Energy Density (MJ/kg)	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^{202,267}(b) Calculated from³⁰⁵(c) ref³⁹¹(d) ref⁴¹⁶(e) ref⁴⁰⁰

B.2. Additional Results and Sensitivity Analysis

B.2.1 Numerical GHG emission Results For Upstream Operations (Agriculture and Corn Wet Milling)

Table B.15. Modeled greenhouse gas emissions (mean and 95% confidence interval) from corn production, excluding carbon uptake credit (kg CO₂e / 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 B.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 CO₂e / 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 B.17. Modeled greenhouse gas emissions (mean and 95% confidence interval) from switchgrass production, excluding carbon uptake credit (kg CO₂e / 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)

B.2.2 Numerical GHG Emission Results for Cradle-to-Gate Polymer Production**Pathways****Table B.18. Modeled greenhouse gas emissions (mean and 95% confidence interval) from fossil polymer production with conventional energy, under different input assumptions (kg CO₂e / 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
Hydrogen from steam cracking treated by mass allocation	PVC	2.25	2.01	2.54
	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	

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Table B.19. Modeled greenhouse gas emissions (mean and 95% confidence interval) from corn-based PHB polymer production (kg CO₂e / 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

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Table B.20. Modeled greenhouse gas emissions (mean and 95% confidence interval) from switchgrass-based PHB polymer production (kg CO₂e / 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

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	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 (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

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Table B.21. Modeled greenhouse gas emissions (mean and 95% confidence interval) from corn-based PLA polymer production (kg CO₂e / 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 B.22. Modeled greenhouse gas emissions (mean and 95% confidence interval) from switchgrass-based PLA polymer production, case 1 (kg CO₂e / 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

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Table B.23. Modeled greenhouse gas emissions (mean and 95% confidence interval) from polymers produced using corn bioethylene (kg CO₂e / 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

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Table B.24. Modeled greenhouse gas emissions (mean and 95% confidence interval) from polymers produced using switchgrass bioethylene with near-term yield (kg CO₂e / 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

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Table B.25. Modeled greenhouse gas emissions (mean and 95% confidence interval) from polymers produced using switchgrass bioethylene with mid-term yield (kg CO₂e / 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

B.2.3 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 B.26 shows a breakdown of these differences for corn PLA, and Table B.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) (Chapter 2),¹⁵⁴ and follows a similar model structure. Emissions from corn bioethylene are lower in the present chapter 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) (Chapter 2)¹⁵⁴ also estimated emissions from production of bio-LDPE in Brazil, using sugarcane as a feedstock (mean: -1.3 kg CO₂e / kg LDPE), which is similar to results from the more optimistic switchgrass bio-LDPE scenarios in the present chapter. Likewise, results from the more optimistic switchgrass bio-HDPE scenarios in the present chapter are in the same range as emissions previously reported for Braskem's bio-HDPE production using Brazilian sugarcane (-2.15 kg CO₂e / kg HDPE).⁴¹⁷ Braskem is currently among the largest producers of bioethylene based plastics.¹⁸⁴

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Table B.26. Comparison of life cycle corn PLA emissions between this study (mean results) and original data sources. All values in kg CO₂e/kg PLA. The column heading F&P stands for fermentation and polymerization. The column heading CO₂ credit refers to the CO₂ 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 CO₂/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
	<i>Corn production</i>	<i>Wet milling</i>	<i>Co-product credit</i>				
Groot <i>et al.</i> (2010)²⁵¹	0.1 (sugarcane, not corn)			2.2	-1.8	0.502	Groot <i>et al.</i> (2010) ²⁵¹ 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 <i>et al.</i> (2015)²⁶² (MA)	0.25	0.29	-	1.9	-1.8	0.62	Vink <i>et al.</i> (2015) ²⁶² 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 <i>et al.</i> (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 <i>et al.</i> 2015) uses mass allocation, which is more favorable to PLA than system expansion.
Sakai <i>et al.</i>	-	-	-	-	-	-	Cases 3 and 4 are also based on Vink <i>et al.</i> (2015) ²⁶² , but use Sakai <i>et al.</i> (2004) ²⁶⁴ for polymerization energy requirements. Sakai <i>et al.</i>

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<i>(2004)</i> ²⁶⁴							<i>(2004)</i> ²⁶⁴ 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 B.27. Comparison of life cycle corn PHB emissions between this study (mean results) and original data sources. All values in kg CO₂e/kg PHB (or PHA). The column heading F&R stands for fermentation and recovery. The column heading CO₂ credit refers to the CO₂ 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
	<i>Corn production</i>	<i>Wet milling</i>	<i>Co-product credit</i>				
<i>Harding et al. (2007)</i> ²⁴⁷	-	-	-	-	?	1.96 or 2.6	<i>Harding et al. (2007)</i> ²⁴⁷ 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	
<i>Akiyama et al. (2003)</i> ²⁶³ case 9 (MA)	0.4	1.0	-	1.87	-2.8	0.48	<i>Akiyama et al. (2003)</i> ²⁶³ 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 ₂ O emissions rate. <i>Akiyama et al. (2003)</i> 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. <i>Akiyama et al. (2003)</i> 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	
<i>Akiyama et al. (2003)</i> ²⁶³ case 10 (MA)	0.5	1.2	-	2.31	-2.7	1.39	

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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)²⁴⁴ (SE)	0.97	0.06	-0.45	0.33	-2.05	-2.3	Kim and Dale (2008) ²⁴⁴ 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 I 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. My 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 I 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)²⁴⁶	-	-	-	-	-	-	Gerngross (1999) ²⁴⁶ does not report GHG emissions
This study, case 5 (SE)	2.5	1.6	-0.9	5.7	-2.05	6.9	

B.2.4 Uncertainty Importance Analysis

Figure B.1 to Figure B.7 present top contributors to uncertainty for select bio-polymer production pathways. The main text includes a discussion of key observations.

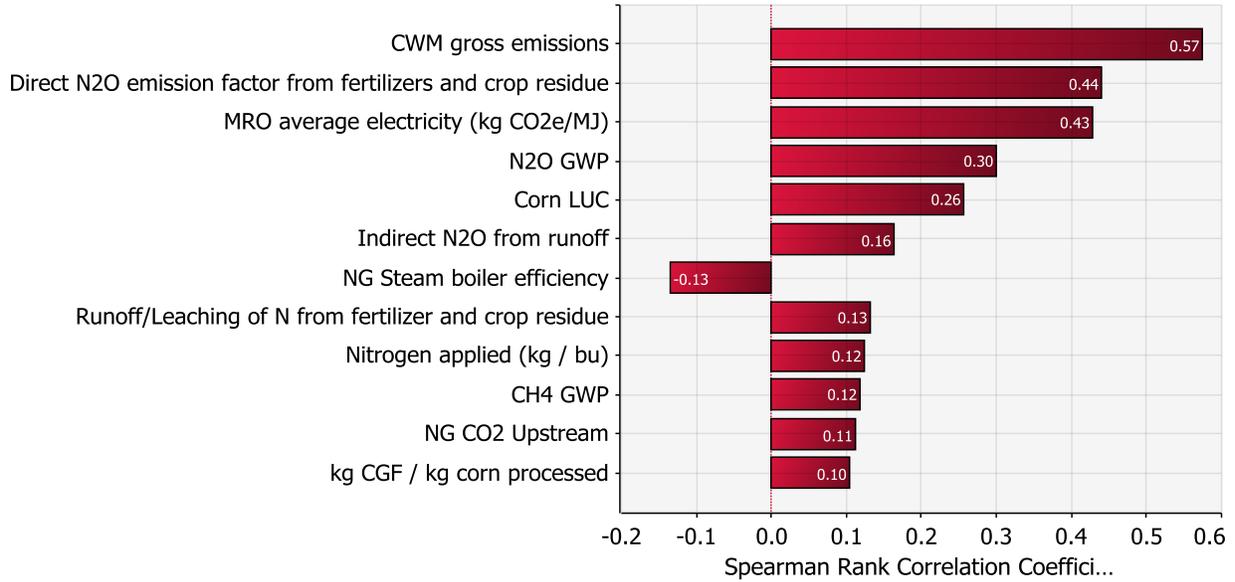


Figure B.1. Spearman rank correlation coefficient for top contributors to uncertainty in the life cycle GHG emissions for corn PHB (case 2, system expansion)

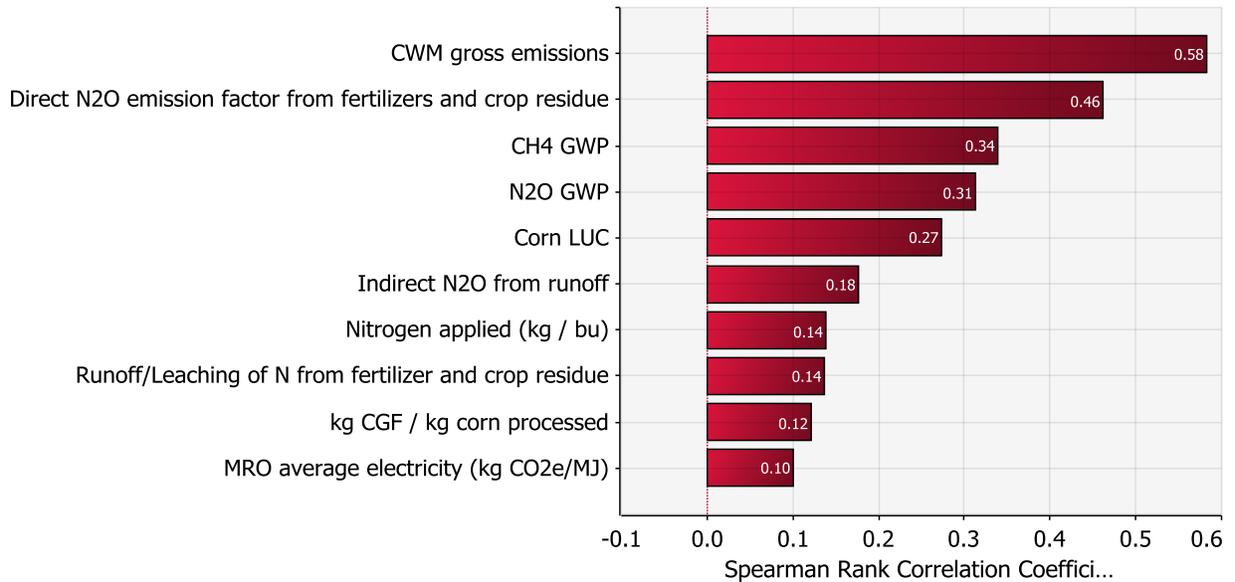


Figure B.2. Spearman rank correlation coefficient for top contributors to uncertainty in the life cycle GHG emissions for corn PLA (case 2, system expansion)

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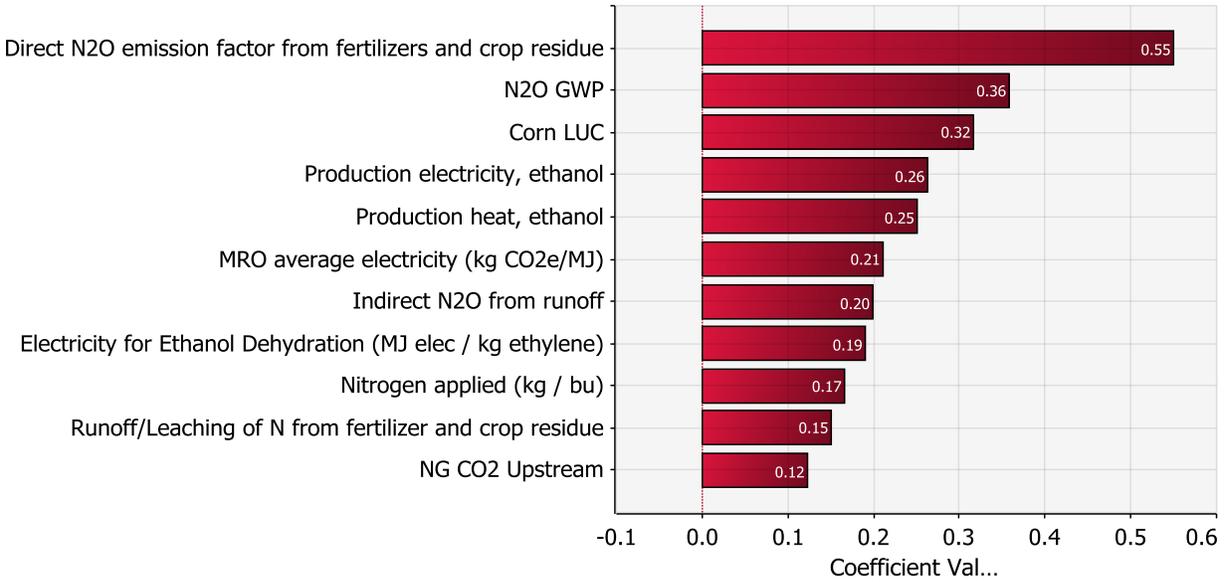


Figure B.3. Spearman rank correlation coefficient for top contributors to uncertainty in the life cycle GHG emissions for corn ethylene (system expansion)

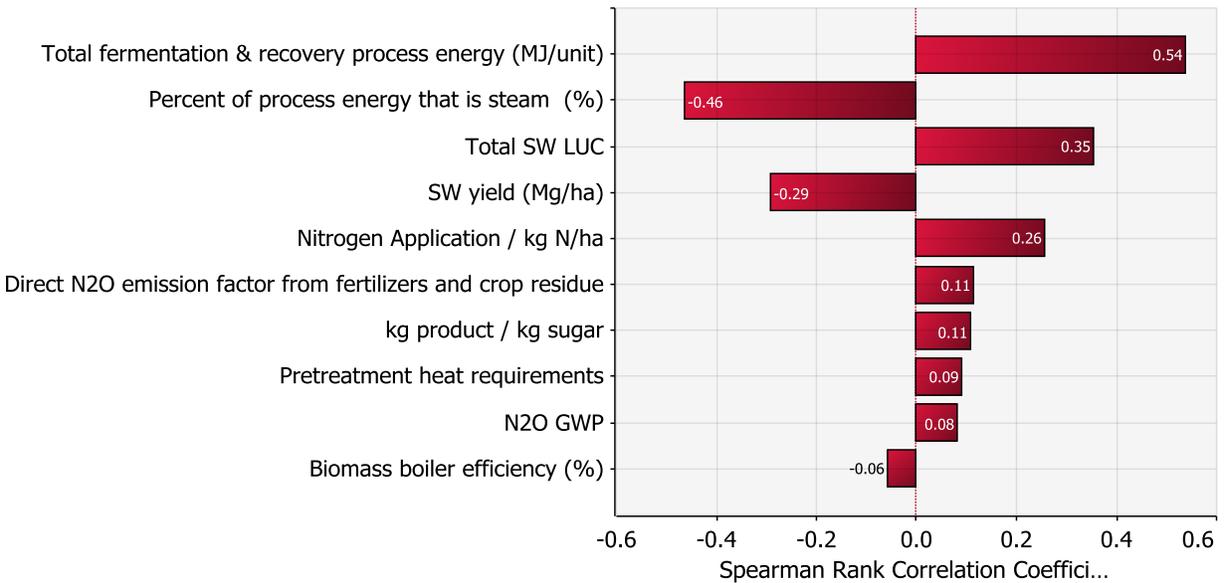


Figure B.4. Spearman rank correlation coefficient for top contributors to uncertainty in the life cycle GHG emissions for switchgrass PHB (full distribution, using fermentation residues for steam and electricity, and including a system expansion credit for surplus electricity)

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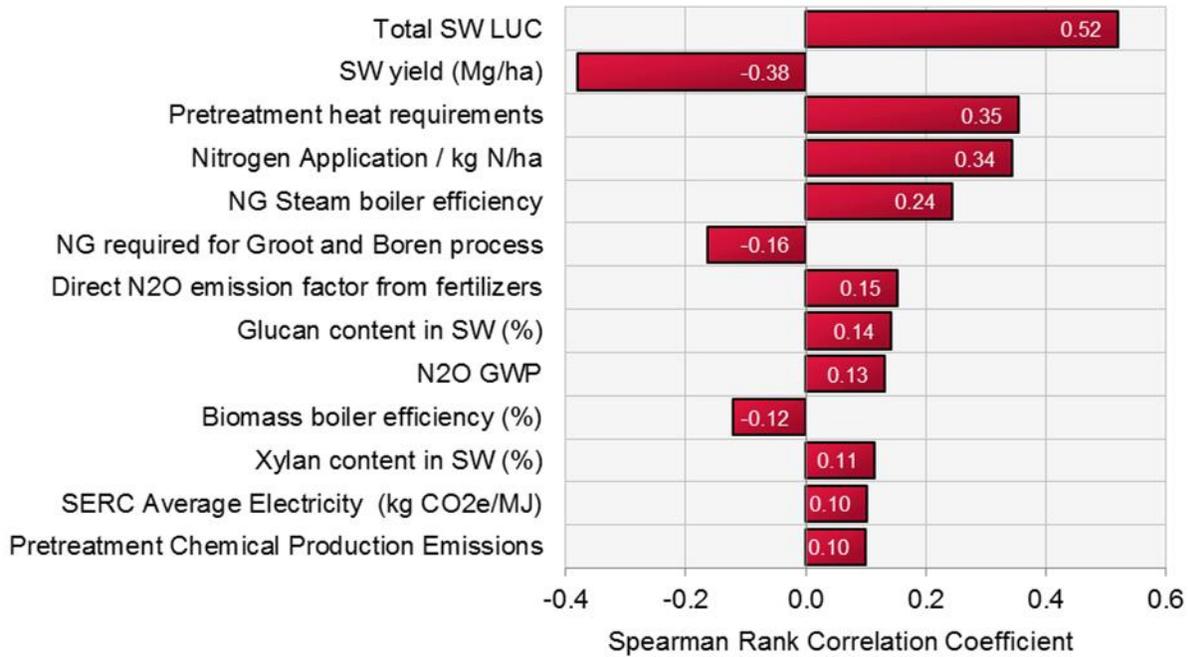


Figure B.5. Spearman rank correlation coefficient for top contributors to uncertainty in the life cycle GHG emissions for switchgrass PLA (case 1, using fermentation residues for steam and electricity, and including a system expansion credit for surplus electricity)

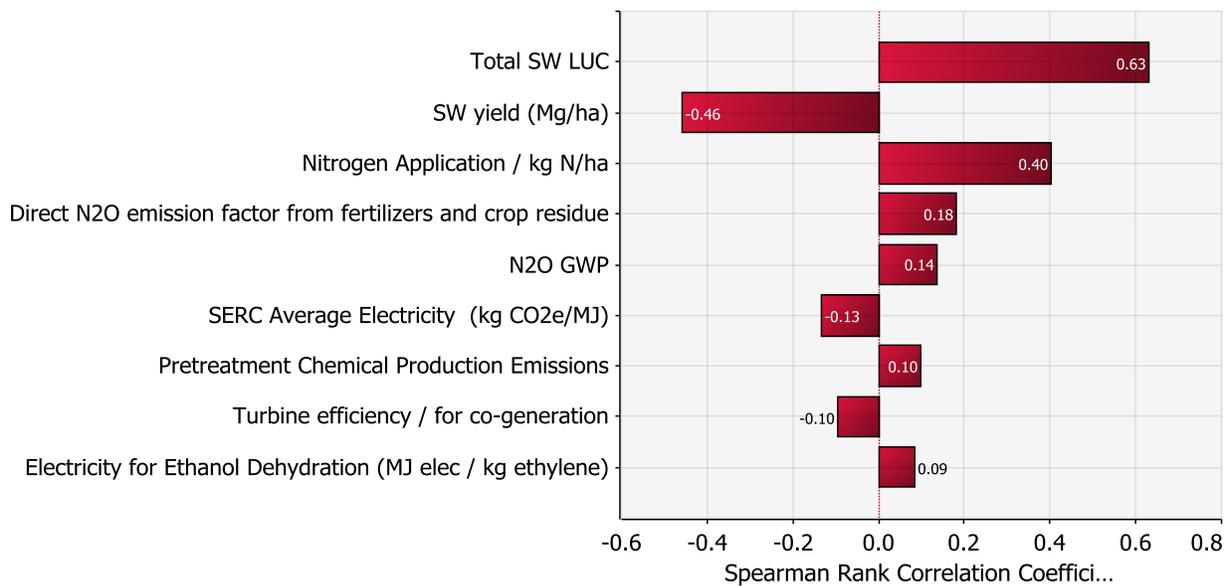


Figure B.6. Spearman rank correlation coefficient for top contributors to uncertainty in the life cycle GHG emissions for switchgrass ethylene (near-term yield, using fermentation residues for steam and electricity, and including a system expansion credit for surplus electricity)

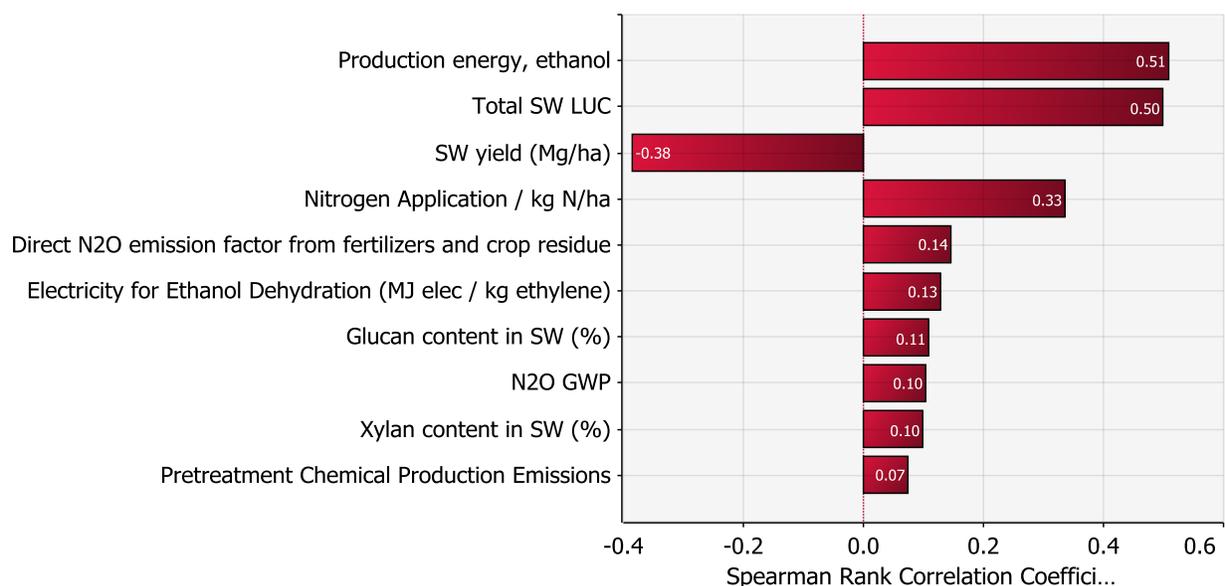


Figure B.7. Spearman rank correlation coefficient for top contributors to uncertainty in the life cycle GHG emissions for switchgrass ethylene (mid-term yield, using fermentation residues for steam and electricity, and including a system expansion credit for surplus electricity)

B.2.5 Numerical Results for GHG Savings from Corn Bioplastics, with Additional Scenarios

The following tables (Table B.28 to Table B.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 B.28 shows baseline results, corresponding to Figure 3.7 of the main text. As discussed in section B.1.3, this chapter uses a N₂O emissions factors for applied nitrogen in agriculture that is higher than the default value from the IPCC guidelines.²²⁵ Thus, Table B.29 presents results assuming a lower (deterministic) N₂O emissions factor of 1.325% for all applied nitrogen,

calculated using the IPCC methodology.²²⁵ Finally, to account for deep uncertainty in emissions from land use change (LUC), this section includes results from 3 alternate LUC scenarios. Table B.30 presents results assuming there are no LUC emissions – this serves as a lower bound. Table B.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).²⁸⁵ The distribution I employ is lognormal with mean = 24.4 and stdev = 7.5; this fits the 95% confidence interval reported by Plevin *et al.* (2015).²⁸⁵ Finally, Table B.32 presents results for a ‘high LUC’ scenario, of 1 kg CO₂e / kg dry corn, which corresponds approximately to 100 g CO₂e / MJ ethanol.

Table B.28. 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 baseline results, corresponding to Figure 3.7 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%

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Table B.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 N₂O 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 ₂ O 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 ₂ O 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%
Corn Ethylene (system expansion) (low N ₂ O emissions)	PVC	0.64	0.24	1.06	100%
	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%

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Table B.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%

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Table B.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)²⁸⁵

Bio-plastic	Fossil Plastic	Mean	2.5%	97.5%	P(>0)
Corn PHB (optimistic, case 2, system expansion) (LUC from Plevin <i>et al.</i> 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 <i>et al.</i> 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 <i>et al.</i> 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 B.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 CO₂e / 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%

B.2.6 Numerical Results for GHG Savings from Switchgrass Bioplastics, with Additional Scenarios

The following tables (Table B.33 to Table B.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 B.33 shows baseline results, corresponding to Figure 3.7 of the main text. Table B.34 shows results assuming that fermentation residues are only used to generate steam for the fermentation and recovery process. Table B.35 shows results assuming there is no use of fermentation residues. As discussed in section B.1.3, this chapter uses a N₂O emissions factors for applied nitrogen in agriculture that is higher than the default value from the IPCC guidelines.²²⁵ Thus, Table B.36 presents results assuming a lower (deterministic) N₂O emissions

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factor of 1.325% for all applied nitrogen, calculated from the IPCC methodology.²²⁵ To account for deep uncertainty in emissions from land use change (LUC), this section includes results from 2 alternate LUC scenarios. Table B.37 presents results assuming there are no LUC emissions – this serves as a lower bound. Table B.38 presents results using a high estimate for LUC emissions (670 g CO₂e / kg dry switchgrass), based on the Winrock scenario from the GREET CCLUB model,²⁶⁷ as discussed in section B.1.2. As explained in section B.1.10, the baseline model assumes that all switchgrass is either transformed into product, or available for energy recovery (as fermentation residues). Table B.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.^{267,405}

As explained in section B.1.3, using the IPCC guidelines⁹⁵ to calculate nitrogen in switchgrass crop residue, results in an estimate for N₂O emissions that is far higher than reported by other sources.^{167,259,267} Thus, the baseline model used an estimate for above and below ground nitrogen from GREET 2014 (0.54 g nitrogen / kg switchgrass).²⁶⁷ Table B.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:⁹⁵

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

Where:

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

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

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

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

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

These variables are all defined in the IPCC source document.⁹⁵ I 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)
- $Frac_{remove} = 0$
- $R_{BG-BIO} =$ 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 B.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).²⁵⁹ Finally, Table B.42 presents results for a scenario in which switchgrass crop yield and applied nitrogen fertilizer are perfectly correlated (correlation coefficient of 1)

Table B.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 3.7 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%

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Table B.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%

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Table B.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%
Switchgrass ethylene plastics (near-term ethanol yield, none)	PVC	0.83	0.16	1.32	99%
	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%
Switchgrass ethylene plastics (mid-term ethanol yield, none)	PS	-0.56	-1.44	0.04	3.8%
	PVC	-0.87	-2.23	0.07	3.8%
	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%

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Table B.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 N₂O 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 N₂O)	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 N₂O)	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%
Switchgrass ethylene plastics (near-term ethanol yield, S, E, EC) (Low N₂O)	PVC	2.02	1.42	2.58	100%
	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%
Switchgrass ethylene plastics (mid-term ethanol yield, S, E, EC) (Low N₂O)	PVC	1.69	0.71	2.51	100%
	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%

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Table B.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%
Switchgrass ethylene plastics (near-term ethanol yield, S, E, EC) (No LUC)	PVC	2.14	1.48	2.67	100%
	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%
Switchgrass ethylene plastics (mid-term ethanol yield, S, E, EC) (No LUC)	PVC	1.95	0.74	2.63	99%
	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%

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Table B.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.²⁶⁷

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%
Switchgrass ethylene plastics (near-term ethanol yield, S, E, EC) (High LUC)	PVC	0.75	0.08	1.27	98%
	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%
Switchgrass ethylene plastics (mid-term ethanol yield, S, E, EC) (High LUC)	PVC	-0.92	-2.18	-0.26	0%
	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%

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Table B.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%
Switchgrass ethylene plastics (near-term ethanol yield, S, E, EC) (Lignin only for energy recovery)	PVC	1.64	0.97	2.17	100%
	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%
Switchgrass ethylene plastics (mid-term ethanol yield, S, E, EC) (Lignin only for energy recovery)	PVC	0.86	-0.44	1.73	94%
	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%

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Table B.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.²²⁵

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%
Switchgrass ethylene plastics (near-term ethanol yield, S, E, EC) (High crop residue)	PVC	1.64	0.82	2.31	100%
	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%
Switchgrass ethylene plastics (mid-term ethanol yield, S, E, EC) (High crop residue)	PVC	0.91	-0.63	2.00	91%
	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 B.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).²⁵⁹

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%
Switchgrass ethylene plastics (near-term ethanol yield, S, E, EC) (High crop yield)	PVC	2.05	1.51	2.60	100%
	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%
Switchgrass ethylene plastics (mid-term ethanol yield, S, E, EC) (High crop yield)	PVC	1.77	0.98	2.53	100%
	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%

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Table B.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%

B.2.7 Sensitivity to Displacement Rates

The comparative analysis presented in Figure 3.7 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 B.8 to Figure B.11 consider a range of displacement rates for each of the main PLA and PHB scenarios presented in Figure 3.7 of the main text. I 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 3.7 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 B.8 (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 B.9 (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 B.10 and Figure B.11 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.

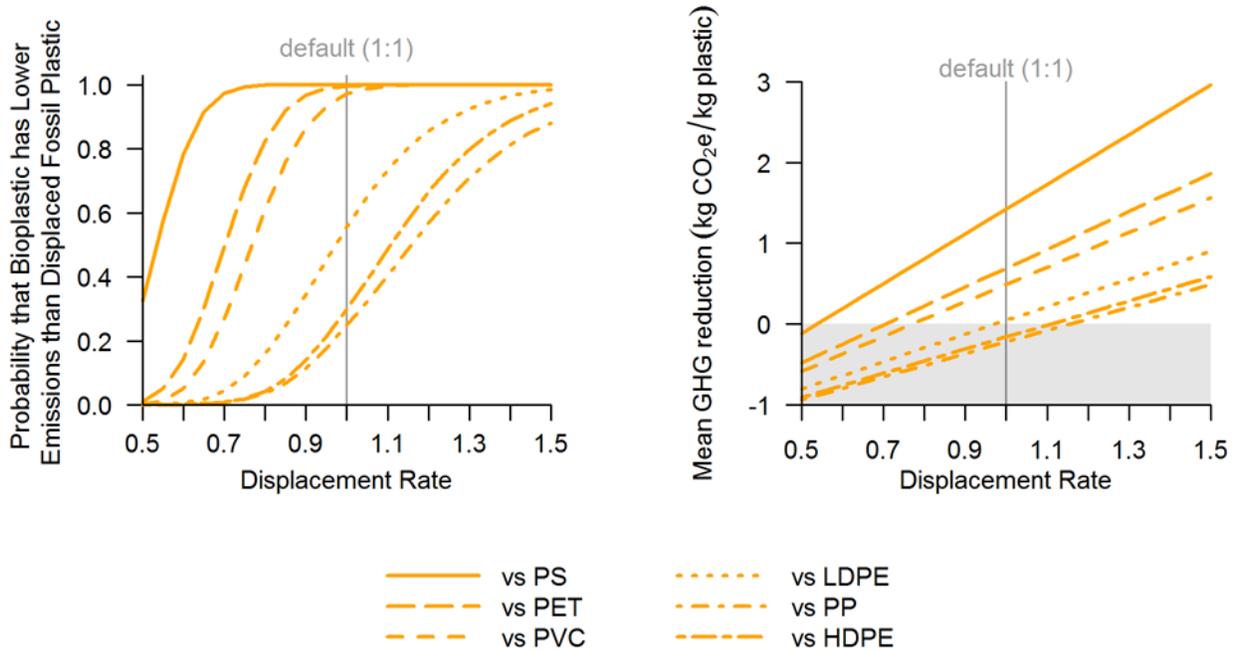


Figure B.8. Sensitivity of cradle-to-gate net emissions from corn PLA (baseline case 2, system expansion) to fossil plastic displacement rate. The x-axis in each figure corresponds to the quantity of fossil plastic displaced by 1 mass unit of PLA. The left figure shows the probability that 1 kg corn 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.

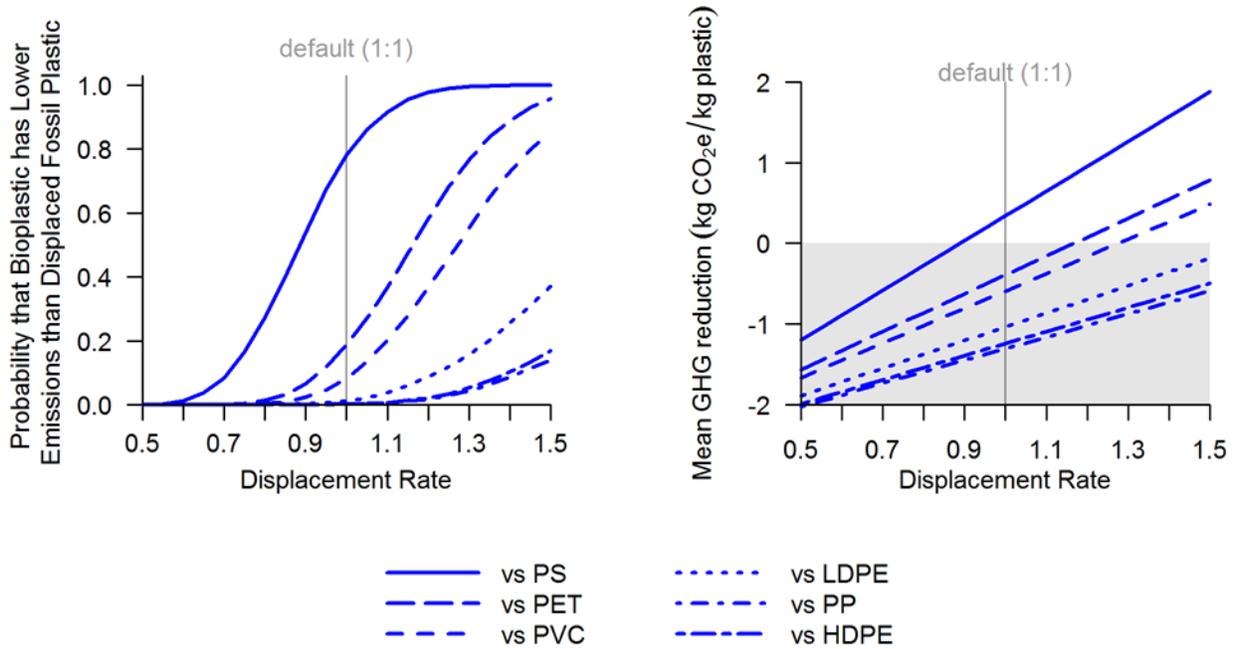


Figure B.9. Sensitivity of cradle-to-gate net emissions from corn PHB (optimistic, case 2, system expansion) to fossil plastic displacement rate. The x-axis in each figure corresponds to the quantity of fossil plastic displaced by 1 mass unit of PHB. The left figure shows the probability that 1 kg corn 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.

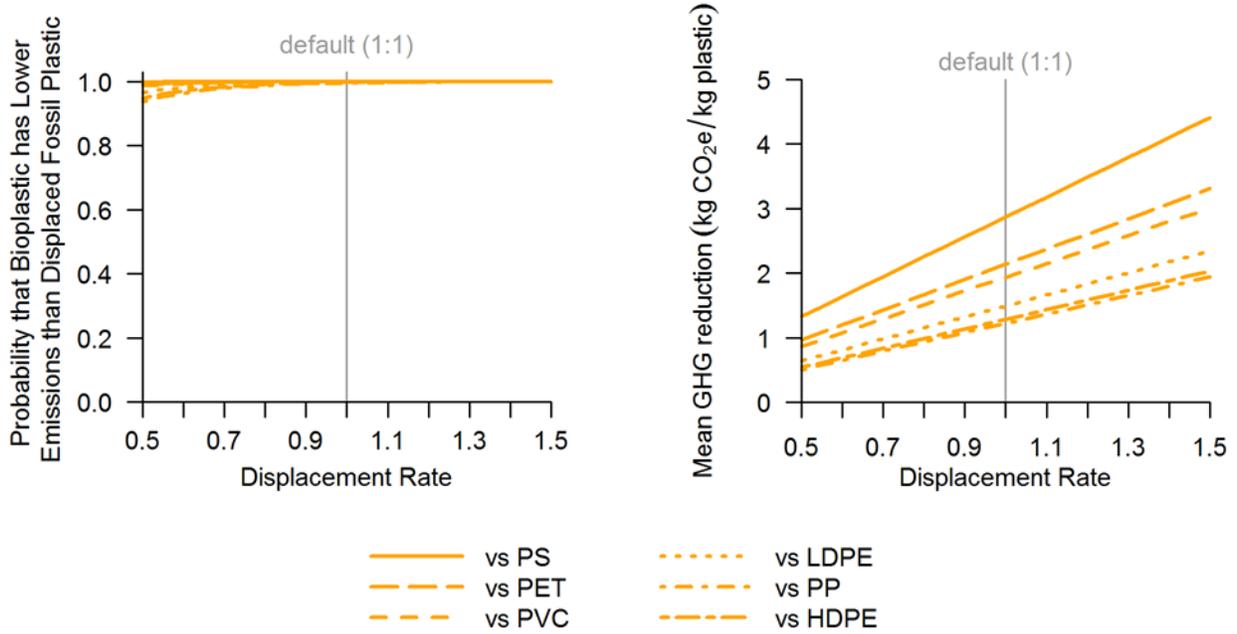


Figure B.10. Sensitivity of cradle-to-gate net emissions from switchgrass PLA (case 1, S, E, EC) to fossil plastic displacement rate. The x-axis in each figure corresponds to the quantity of fossil plastic displaced by 1 mass unit of PLA. The left figure shows the probability that 1 kg corn PLA has lower 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.

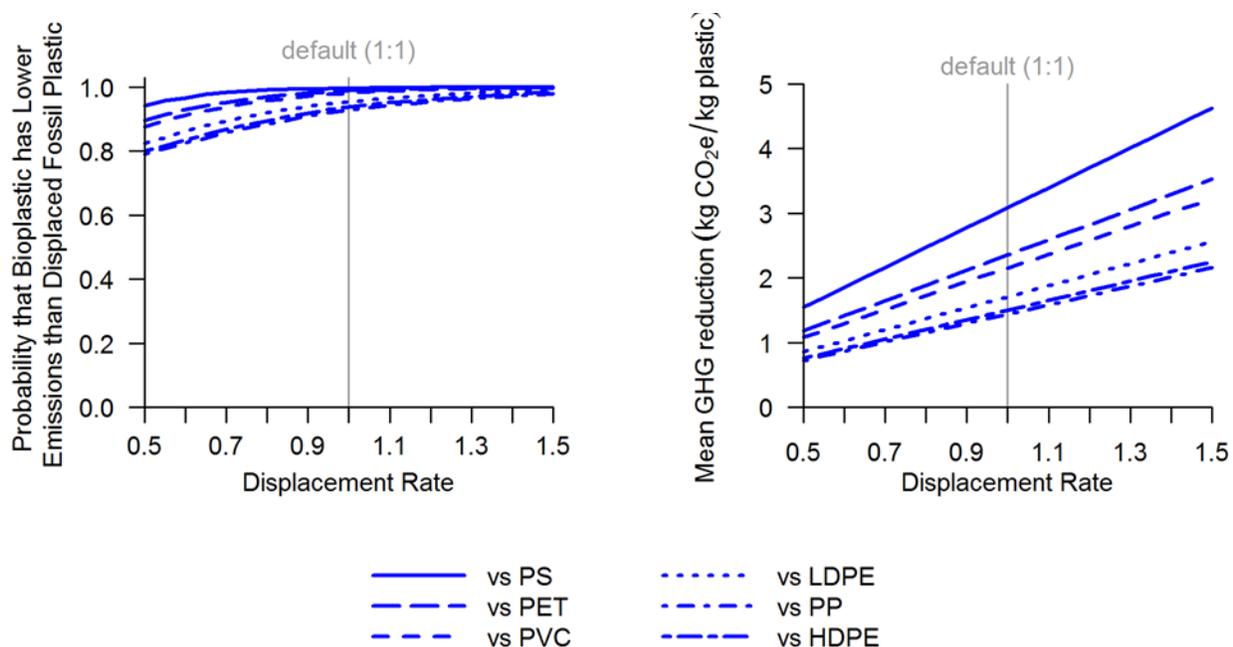


Figure B.11. Sensitivity of cradle-to-gate net emissions from switchgrass PHB (full distribution, S, E, EC) to fossil plastic displacement rate. The x-axis in each figure corresponds to the quantity of fossil plastic displaced by 1 mass unit of PHB. The left figure shows the probability that 1 kg corn 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.

B.2.8 Sensitivity to Omitted Stages

As noted in the main text, my model excludes emissions from downstream processing and transportation. Table B.43 explores the sensitivity of the main bio-based plastic pathways (those presented in Figure 3.7 of the main chapter) 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, I assume that road transportation is carried out with a diesel powered single unit truck (0.0203 L diesel/t-km,²²⁹ resulting in mean emissions of 0.072 g CO₂e/kg-km), ship transportation is carried out via ocean freighter (0.00493 L residual fuel oil/t-km,²³² resulting in mean emissions of 0.019 g CO₂e/kg-km), process heat is provided

by natural gas (mean: 64 g CO₂e/MJ HHV as parametrized in Table B.12), and process electricity is generated with the U.S. average emissions factor (mean: 0.19 g CO₂e/MJ, per Table B.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.²³³ Very few entries in the table are within these ranges.

Table B.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

Appendix B

	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	-	-

Appendix C. Supporting Information for Chapter 4

C.1. Methods

The main text (section 4.3) provides an overview of the model employed in Chapter 4. Table C.1 presents key parameters for the modeling of renewable energy pathways in this chapter, corresponding to section 4.3.2. Table C.2 summarizes the key parameters used for cost estimation, corresponding to section 4.3.3

Appendix C

Table C.1. Key parameters for the modeling of renewable energy pathways

Parameter	Value or Distribution ^a	Units	Source and notes
Renewable natural gas			
RNG processing efficiency	Triangular (91, 94.4, 97)	%	ref ³⁰⁴
Emissions from combustion of LFG in a reciprocating engine	54.6 0.423 0.000822	g CO ₂ / MJ LHV g CH ₄ / MJ LHV g N ₂ O / MJ LHV	Calculated from ²⁶⁷
Fugitive emissions	0.02	MJ fugitive CH ₄ / MJ RNG product	ref ²⁶⁷
Offset flaring emissions	56.1 0.0299 0.00104	g CO ₂ / MJ LHV flared g CH ₄ / MJ LHV flared g N ₂ O / MJ LHV flared	Calculated from ²⁶⁷ (Applies to LFG burned in reciprocating engine, fugitive emissions, and RNG product)
Natural gas transmission	Lognormal (1.62, 1.65, 0.18) Lognormal (0.015, 0.0079, 0.075)	g CO ₂ / MJ (LHV) g CH ₄ / MJ (LHV)	Approximate fit to results from ²⁶⁶
Natural gas combustion emissions	Triangular (54.3, 56.1, 58.3) Triangular (3E-4, 1E-4, 3E-3) Triangular (3E-5, 1E-4, 3E-4)	g CO ₂ / MJ (LHV) g CH ₄ / MJ (LHV) g N ₂ O / MJ (LHV)	ref ⁹⁵ (original source for ²⁶⁶).
Natural gas heating value ratio	1.108	MJ HHV / MJ LHV	Calculated from ²⁶⁷
Renewable electricity emissions			
Wind power (before line losses)	Log-logistic (1.47, 8.94, 2.91) (mean: 12.4, stdev: 9.3)	g CO _{2e} / kWh	Fit to “harmonized by all” from ³⁰³ ; Must be adjusted for ~6% line losses.
Biomass energy content			
Switchgrass	18.1	MJ HHV / kg	Calculated from ²⁶⁷
Boiler efficiencies			
Natural gas boiler	Triangular (70%, 80%, 94%)	% (HHV)	ref ²⁶⁵ (also used for other fossil fuels)
Biomass boiler	Triangular (68%, 70%, 74.5%)	% (HHV)	Lower: ³⁰⁵ , mode: ³⁰⁶ , upper: ³⁰⁷

a) Distributions are written as: Triangular (lower, mode, upper), Log-logistic (location, scale, shape), Lognormal (mean of the lognormal distribution, standard deviation of the lognormal distribution, shift).

Table C.2. Summary of key parameters for cost estimation

Product	Value or Distribution ^a	Units	Source and notes
Plastics			
PLA	2.82	2015 USD / kg	Calculated based on ³⁰⁹⁻³¹¹
PHA (treated as PHB)	5.94	2015 USD / kg	
HDPE	1.78	2015 USD / kg	
LDPE	See HDPE	2015 USD / kg	
PP	1.63	2015 USD / kg	
PS	2.08	2015 USD / kg	
PVC	1.48	2015 USD / kg	
PET	2.23	2015 USD / kg	
Feedstocks			
Fossil ethylene	Uniform (0.35, 0.65)	2015 USD / lb	Based on ³¹²
Corn bioethylene	Triangular (1780, 2180, 2925)	2015 USD / lb	Based on ¹⁸⁴
Electricity			
Wind power	Triangular (35, 66, 111)	\$ / MWh	ref ³¹⁵
US wholesale electricity	Log-logistic (13.7, 31.0, 4.2) (mean: 48, CI ^b : 27, 87)	\$ / MWh	ref ³¹⁶
Fuels			
RNG	Exponential (2.05, 5.19) (mean: 7.2, CI ^b : 5.2, 12.8)	\$ / MMBtu	Based on ³¹³
Natural Gas	Extreme value (4.32, 0.53) (mean: 4.6, CI ^b : 3.6, 6.3)	\$ / MCF	ref ³¹⁴
Residual Fuel Oil	Uniform (1.09, 2.61)	\$ / gallon	
Coal	Uniform (67.8, 70.7)	\$ / short ton	
Distillate / Diesel	Triangular (1.6, 3.2, 3.4)	\$ / gallon	

a) Distributions are written as: Uniform (lower, upper), Triangular (lower, mode, upper), Log-logistic (location, scale, shape), Exponential (mean, shift), Extreme value (location, shape)

b) 95% confidence interval (CI)

C.2. Additional Results

C.2.1 Other Low-Carbon Energy Sources

For the low-carbon energy pathways, direct combustion of biomass or wind power (through increased electrification), could also replace on-site fuels (instead of using RNG). Table C.3 presents these scenarios for each fossil-based polymer. Switchgrass combustion produces similar results to RNG use, but with slightly higher uncertainty. Increased use of wind power further reduces emissions relative to RNG use.

Table C.3. Emissions factors (mean and 95% confidence intervals) for fossil-based plastics produced using different energy sources.

	Emissions factor with conventional energy (kg CO₂e/kg plastic)	Emissions factor with wind and RNG (kg CO₂e/kg plastic)	Emissions factor with wind and switchgrass combustion (kg CO₂e/kg plastic)	Emissions factor with wind and electrification of heat (kg CO₂e/kg plastic)
High Density Polyethylene (HDPE)	1.48 (1.02, 1.96)	0.59 (0.19, 1.01)	0.58 (0.18, 1.06)	0.35 (0.01, 0.72)
Low Density Polyethylene (LDPE)	1.75 (1.27, 2.25)	0.65 (0.23, 1.10)	0.64 (0.2, 1.2)	0.35 (0, 0.74)
Linear Low Density Polyethylene (LLDPE)	1.48 (1.01, 1.97)	0.64 (0.24, 1.06)	0.64 (0.23, 1.12)	0.41 (0.06, 0.78)
Polypropylene (PP)	1.54 (1.14, 1.96)	0.84 (0.5, 1.21)	0.83 (0.49, 1.23)	0.65 (0.36, 0.99)
Polyethylene (PET)	2.39 (2.18, 2.65)	1.04 (0.83, 1.29)	1.03 (0.79, 1.37)	0.81 (0.67, 1.04)
Polystyrene (PS)	3.12 (2.78, 3.54)	1.64 (1.28, 2.05)	1.63 (1.21, 2.22)	1.24 (1, 1.58)
Polyvinyl Chloride (PVC)	2.19 (1.92, 2.49)	0.63 (0.36, 0.92)	0.62 (0.3, 1.07)	0.31 (0.14, 0.52)

C.2.2 Results for Individual Plastics

Figure C.1. presents the difference in life cycle GHG emissions that result from switching from fossil-based polymers with conventional energy to fossil-based polymers with low-carbon energy, or to different bio-based polymers (assuming 1:1 mass substitution). In addition to the PLA and bioethylene scenarios discussed in the main text, the figure also includes results for poly-3-hydroxybutyrate (PHB). The results for PHB presented here use only the lowest emission PHB scenarios, which rely on PHB case 2 from Posen *et al.* (2016) (Chapter 3)¹⁴⁴ for corn scenarios, or PHB case 1 from Posen *et al.* (2016) (Chapter 3)¹⁴⁴ for switchgrass scenarios; those scenarios are based respectively on Akiyama *et al.* (2003)²⁶³ and Harding *et al.* (2007).²⁴⁷ Since PHB is both more expensive, and has higher GHG emissions than other bioplastics, I did not include it in the feedstock substitution scenarios presented in the main text.

The results in Figure C.1 assume optimistic end of life scenarios for bio-based polymers: PHB is composted, while bioethylene plastics and PLA are landfilled and act as a carbon sink. Each bar shows mean GHG savings for the different emission reduction strategies, applied to a different baseline plastic. For example, the red bar in panel a) shows that switching to wind and RNG across the chemical industry for PET would reduce GHG emissions by a mean of 1.4 kg CO₂e/kg PET. The next 3 bars show the change in emissions when 1 kg of each corn-based bioplastic (PLA, PHB, or PET made with bioethylene) replaces 1 kg PET, and so on. These results reinforce the message of the main text, showing that low carbon energy results in greater GHG reductions than near-term (corn-based) feedstock substitution, for every individual fossil plastic considered. The figure also shows that advanced feedstock substitution scenarios can result in greater GHG reductions than energy substitution, though only for a subset of pathways (i.e. PLA substituting for any plastic, or bioethylene used for polyethylene plastics). Table C.4 to Table C.6 show numerical results corresponding to Figure C.1. Table C.4 also shows an additional case where low carbon energy is applied only to the final plastic polymerization stage, and not across the entire chemical industry.

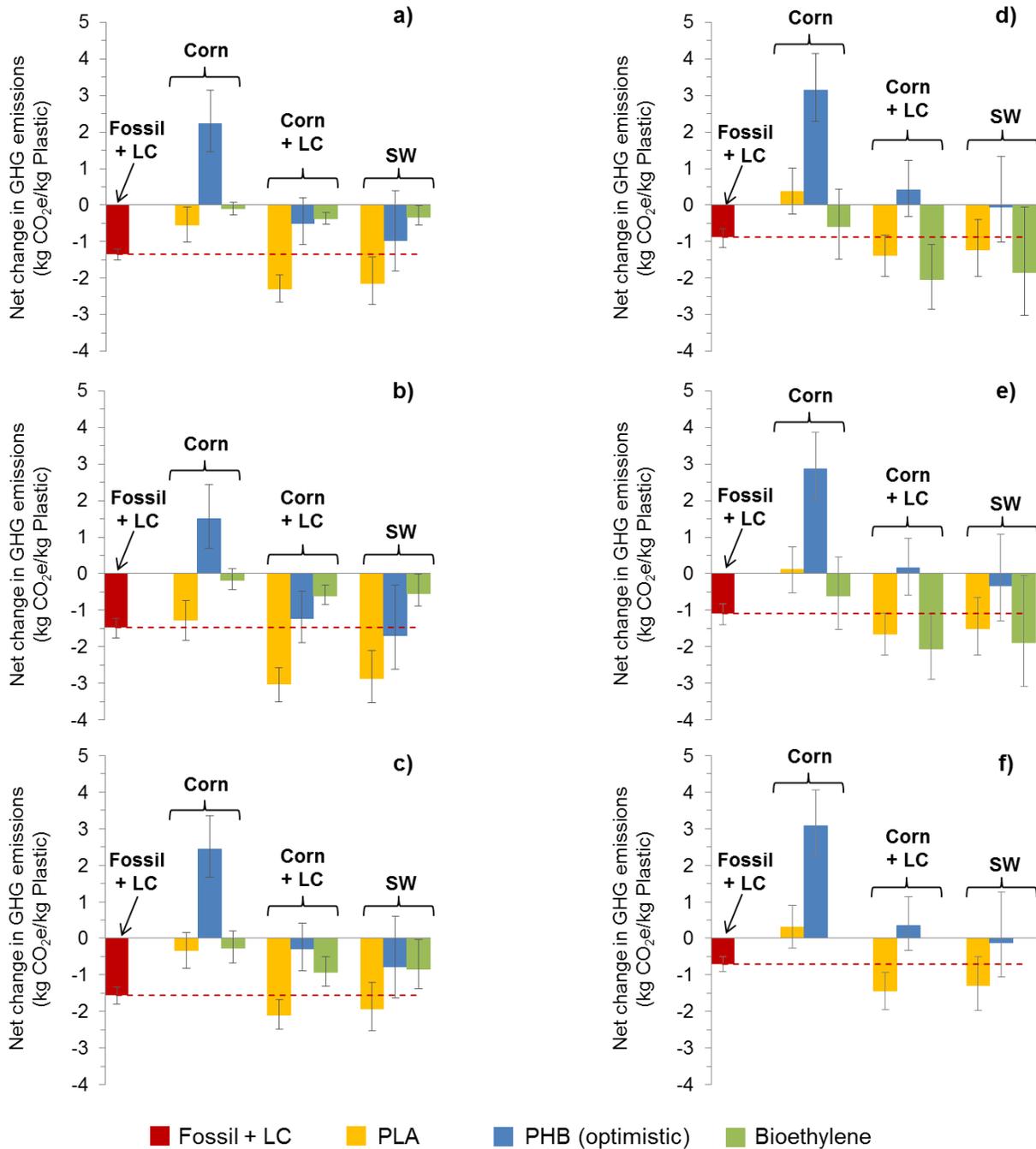


Figure C.1. Life cycle comparison of emission reduction strategies for a) PET, b) PS, c) PVC, d) HDPE, e) LDPE, f) PP. Results for LLDPE are not shown, but are similar to those for HDPE. Negative values represent emission reductions. Fossil + LC refers to the use of low carbon energy in the production of the conventional polymer. Corn refers to corn-based biopolymers produced with conventional energy. Corn + LC refers to corn-based biopolymers produced with low carbon energy. SW refers to switchgrass-based biopolymers. The values in this figure result from subtracting modeled emissions for each conventional polymer from the life cycle emissions for each alternate polymer. The dotted line matches the LC fossil scenario and is included for

reference only. Wind and RNG are the low-carbon energy sources. For PHB, only the most optimistic scenarios are shown (case 1 and 2 from Posen *et al.*¹⁴⁴ (Chapter 3), for corn and switchgrass pathways, respectively). The graph shows mean results; error bars span 95% of simulations.

Table C.4. Comparison of emission reduction strategies, using corn-grain for bio-based polymers (with conventional energy). Negative numbers indicate the alternate plastic has lower cradle-to-gate GHG emissions than the conventional plastic (kg CO₂e / kg plastic). For each bioplastic, the table also shows the probability that this plastic has lower GHG emissions than the conventional plastic produced with low carbon energy (P<LC). Case numbers are as described in Chapter 3 and described above. This table presents results corresponding to Figure C.1, assuming PHB is composted and other plastics are landfilled.

Conventional Plastic	Alternate polymer	Mean	2.5%	97.5%	P<LC
PET	Low carbon energy (full supply chain)	-1.35	-1.51	-1.20	-
	Low carbon energy (polymerization only)	-0.73	-0.81	-0.66	-
	PLA	-0.53	-1.00	-0.02	0%
	PHB (optimistic, case 2)	2.27	1.47	3.18	0%
	bio-PET (made with bioethylene)	-0.11	-0.28	0.08	0%
PS	Low carbon energy (full supply chain)	-1.48	-1.76	-1.23	-
	Low carbon energy (polymerization only)	-0.12	-0.13	-0.10	-
	PLA	-1.27	-1.81	-0.71	22%
	PHB (optimistic, case 2)	1.54	0.69	2.49	0%
	bio-PS (made with bioethylene)	-0.17	-0.45	0.13	0%
PVC	Low carbon energy (full supply chain)	-1.55	-1.80	-1.34	-
	Low carbon energy (polymerization only)	-0.25	-0.29	-0.22	-
	PLA	-0.33	-0.82	0.20	0%
	PHB (optimistic, case 2)	2.48	1.67	3.40	0%
	bio-PVC (made with bioethylene)	-0.27	-0.69	0.20	0%
HDPE	Low carbon energy (full supply chain)	-0.88	-1.16	-0.65	-
	Low carbon energy (polymerization only)	-0.28	-0.32	-0.25	-
	PLA	0.38	-0.26	1.03	0%
	PHB (optimistic, case 2)	3.19	2.27	4.19	0%
	bio-HDPE (made with bioethylene)	-0.59	-1.52	0.44	27%
LDPE	Low carbon energy (full supply chain)	-1.09	-1.40	-0.83	-
	Low carbon energy (polymerization only)	-0.48	-0.55	-0.41	-
	PLA	0.11	-0.54	0.77	0%
	PHB (optimistic, case 2)	2.92	1.99	3.93	0%
	bio-LDPE (made with bioethylene)	-0.60	-1.54	0.45	15%
PP	Low carbon energy (full supply chain)	-0.70	-0.92	-0.51	-
	Low carbon energy (polymerization only)	-0.21	-0.24	-0.19	-
	PLA	0.32	-0.27	0.93	0%
	PHB (optimistic, case 2)	3.12	2.24	4.10	0%

Table C.5. Comparison of emission reduction strategies, using corn-grain for bio-based polymers (with wind and RNG satisfying energy needs for biomass processing). Negative numbers indicate the alternate plastic has lower cradle-to-gate GHG emissions than the conventional plastic (kg CO₂e / kg plastic). For each bioplastic, the table also shows the probability that this plastic has lower GHG emissions than the conventional plastic produced with low carbon energy (P<LC). Case numbers are as described in chapter and summarized above. This table presents results corresponding to Figure C.1, assuming PHB is composted and other plastics are landfilled.

Conventional Plastic	Alternate polymer	Mean	2.5%	97.5%	P<LC
PET	Low carbon energy (full supply chain)	-1.35	-1.51	-1.20	-
	PLA	-2.30	-2.65	-1.90	100%
	PHB (optimistic, case 2)	-0.49	-1.07	0.28	0%
	bio-PET (made with bioethylene)	-0.37	-0.52	-0.20	0%
PS	Low carbon energy (full supply chain)	-1.48	-1.76	-1.23	-
	PLA	-3.03	-3.50	-2.56	100%
	PHB (optimistic, case 2)	-1.22	-1.87	-0.41	22%
	bio-PS (made with bioethylene)	-0.60	-0.84	-0.32	0%
PVC	Low carbon energy (full supply chain)	-1.55	-1.80	-1.34	-
	PLA	-2.09	-2.49	-1.67	100%
	PHB (optimistic, case 2)	-0.29	-0.89	0.50	0%
	bio-PVC (made with bioethylene)	-0.93	-1.30	-0.50	0%
HDPE	Low carbon energy (full supply chain)	-0.88	-1.16	-0.65	-
	PLA	-1.38	-1.94	-0.82	98%
	PHB (optimistic, case 2)	0.42	-0.32	1.30	0%
	bio-HDPE (made with bioethylene)	-2.03	-2.84	-1.08	99%
LDPE	Low carbon energy (full supply chain)	-1.09	-1.40	-0.83	-
	PLA	-1.65	-2.23	-1.08	99%
	PHB (optimistic, case 2)	0.15	-0.59	1.03	0%
	bio-LDPE (made with bioethylene)	-2.07	-2.89	-1.10	98%
PP	Low carbon energy (full supply chain)	-0.70	-0.92	-0.51	-
	PLA	-1.44	-1.96	-0.93	100%
	PHB (optimistic, case 2)	0.36	-0.33	1.21	0%

Table C.6. Comparison of emission reduction strategies, using switchgrass for bio-based polymers. Negative numbers indicate the alternate plastic has lower cradle-to-gate GHG emissions than the conventional plastic (kg CO₂e / kg plastic). For each bioplastic, the table also shows the probability that this plastic has lower GHG emissions than the conventional plastic produced with low carbon energy (P<LC). Case numbers are as described in Chapter 3 and described above. This table presents results corresponding to Figure C.1, assuming PHB is composted and other plastics are landfilled. All switchgrass pathways include cogeneration of steam and electricity, but with no emissions credits for surplus energy.

Conventional Plastic	Alternate polymer	Mean	2.5%	97.5%	P<LC
PET	Low carbon energy (full supply chain)	-1.35	-1.51	-1.20	-
	PLA	-2.14	-2.72	-1.43	98%
	PHB (optimistic, case 1)	-0.97	-1.82	0.35	24%
	bio-PET (bioethylene, mid term yield)	-0.34	-0.55	-0.02	0%
PS	Low carbon energy (full supply chain)	-1.48	-1.76	-1.23	-
	PLA	-2.87	-3.53	-2.12	100%
	PHB (optimistic, case 1)	-1.70	-2.62	-0.36	70%
	bio-PS (bioethylene, mid term yield)	-0.55	-0.90	-0.03	0%
PVC	Low carbon energy (full supply chain)	-1.55	-1.80	-1.34	-
	PLA	-1.94	-2.55	-1.21	98%
	PHB (optimistic, case 1)	-0.77	-1.64	0.56	4%
	bio-PVC (bioethylene, mid term yield)	-0.85	-1.39	-0.04	1%
HDPE	Low carbon energy (full supply chain)	-0.88	-1.16	-0.65	-
	PLA	-1.23	-1.97	-0.42	98%
	PHB (optimistic, case 1)	-0.06	-1.03	1.31	4%
	bio-HDPE (bioethylene, mid term yield)	-1.85	-3.04	-0.09	91%
LDPE	Low carbon energy (full supply chain)	-1.09	-1.40	-0.83	-
	PLA	-1.50	-2.25	-0.68	98%
	PHB (optimistic, case 1)	-0.32	-1.31	1.04	7%
	bio-LDPE (bioethylene, mid term yield)	-1.88	-3.09	-0.09	88%
PP	Low carbon energy (full supply chain)	-0.70	-0.92	-0.51	-
	PLA	-1.29	-1.98	-0.51	99%
	PHB (optimistic, case 1)	-0.12	-1.06	1.22	13%

C.2.3 Additional Energy Substitution Scenarios: Allocation and Scope of Substitution

Table C.7 shows additional scenarios for the production of conventional plastics with low carbon energy. The hydrogen co-produced during the olefin production process (steam cracking) can also be combusted for energy or subject to mass allocation, instead of being treated by system expansion. Additionally, it is possible that resin manufacturers have control only over the final polymerization process, but may not be able to introduce low-carbon energy across the supply

chain. In all three additional cases, the emissions from conventional polymers would be substantially higher than in the energy substitution presented in the main chapter.

Table C.7. Cradle-to-grave greenhouse gas emissions (mean and 95% confidence interval) from fossil polymer, produced with renewable energy (RNG for heat requirements and wind power for electricity), under different input assumptions (kg CO₂e / kg plastic)

Scenario	Plastic	Mean	2.5%	97.5%
Base-Case (Renewable energy across the entire chemical supply chain; hydrogen from steam cracking treated by system expansion)	HDPE	0.59	0.19	1.01
	LDPE	0.65	0.23	1.10
	LLDPE	0.64	0.24	1.06
	PP	0.84	0.50	1.21
	PET	1.04	0.83	1.29
	PS (GPPS)	1.64	1.28	2.05
	HIPS	1.63	1.27	2.04
	PVC	0.63	0.36	0.92
Hydrogen combusted (Renewable energy across the entire chemical supply chain; hydrogen from steam cracking combusted for energy)	HDPE	1.23	0.95	1.61
	LDPE	1.31	0.99	1.70
	LLDPE	1.29	1.01	1.67
	PP	1.38	1.12	1.71
	PET	1.15	0.95	1.40
	PS (GPPS)	1.96	1.63	2.35
	HIPS	1.96	1.63	2.35
	PVC	0.93	0.69	1.20
Hydrogen mass allocation (Renewable energy across the entire chemical supply chain; hydrogen from steam cracking combusted treated by mass allocation)	HDPE	1.33	1.00	1.72
	LDPE	1.40	1.04	1.83
	LLDPE	1.39	1.06	1.78
	PP	1.45	1.16	1.80
	PET	1.17	0.96	1.43
	PS (GPPS)	2.01	1.65	2.41
	HIPS	2.01	1.65	2.42
	PVC	0.97	0.70	1.26
Renewable energy for polymerization only (All other unit processes powered by conventional energy; hydrogen from steam cracking treated by system expansion)	HDPE	1.19	0.73	1.68
	LDPE	1.26	0.79	1.77
	LLDPE	1.25	0.79	1.74
	PP	1.32	0.93	1.75
	PET	1.65	1.46	1.89
	PS (GPPS)	3.00	2.67	3.42
	HIPS	2.97	2.63	3.39
	PVC	1.93	1.67	2.23

Appendix D. Supporting Information for Chapter 5

D.1. Regression Analysis

D.1.1 Main Models

Partial adjustment and adaptive expectations models are standard in the economics literature. In brief the partial adjustment model assumes that refiner behavior is dictated by an unobserved ‘target’ production function, but that production decisions are sticky across time periods (i.e. current production is a weighted combination of last period’s production and current target production). The adaptive expectations model assumes that refiners make production decisions in function of (unobserved) expected prices; these expected prices adjust when shocks occur, but are likewise sticky (i.e. the future expected price is a weighted combination of last period’s expected price and last period’s observed price). Derivations for the basic functional forms of these models can be found in most standard econometrics textbooks (e.g. Dougherty 2007, chapter twelve⁴¹⁸).

Quantitatively, the main adaptive expectations model presented in section 5.3.2 is described by equation (D.1):

$$\log(\beta_{it}) = a_0 + a_1 \sum_{j=0}^k \lambda * (1 - \lambda)^j \log\left(\frac{p_{g(t-j)}}{p_{o(t-j)}}\right) + a_2 \sum_{j=0}^k \lambda * (1 - \lambda)^j \log\left(\frac{p_{d(t-j)}}{p_{o(t-j)}}\right) \quad (D.1)$$

$$+ a_3 t + a_4 * M, \quad i \in (g, d)$$

where β_{gt} and β_{dt} are respectively the gasoline share and distillate share of total refinery output in time period t ; p_{gt} and p_{dt} are the price of gasoline and diesel by refiners in time period t ; p_{ot} is the refiner crude oil acquisition cost in time period t ; t represents a deterministic time trend and M represents a set of dummy variables corresponding to each month of the year. The resulting coefficients a_1 and a_2 represent the product yield with respect to the normalized gasoline diesel prices respectively; λ represents the speed at which expectations adapt ($\lambda = 0$ means future expectations do not respond to current prices; $\lambda = 1$ means future expectations are exactly equal to current prices); k is a parameter representing the number of lags included in the model. In theory, the model requires an infinite number of lagged variables. In practice, k must only be

sufficiently large such that the remaining error is relatively small. In this case, I set $k=10$, representing lagged variables going back 10 months. The model is solved by non-linear least squares.

Similarly, the main partial adjustment model presented in section 5.3.2 is described by the following equation :

$$\begin{aligned} \log(\beta_{it}) = & a_0 * \lambda + a_1 * \lambda * \log\left(\frac{p_{gt}}{p_{ot}}\right) + a_2 * \lambda * \log\left(\frac{p_{dt}}{p_{ot}}\right) + (1 - \lambda) * \log(\beta_{i(t-1)}) \\ & + a_3 * t + a_4 * M, \quad i \in (g, d) \end{aligned} \quad (D.2)$$

where all variables are the same as in the adaptive expectations model, except that now λ represents the speed of production adjustment ($\lambda = 0$ means there is no adjustment, and current yields are based only on previous yields; $\lambda = 1$ means adjustment is instantaneous, and yields always match the hidden ‘target’ levels). In principle, the partial adjustment model can also be estimated using the same equation as the adaptive expectations model by first repeatedly substituting the lagged regression equation in place of the lagged dependent variable. The models require different assumptions about their error terms; for additional detail, the reader is referred to (e.g. Dougherty 2001, chapter thirteen⁴¹⁸).

The ‘lagged prices’ model is related to the above models (in the form of equation (D.3)), but without imposing the same restrictions on how the regression coefficients for different time periods are related. Essentially, this model allows current yields to be a function of both current and past prices. The effective elasticity reported in section 5.3.2 corresponds to the sum of the coefficients for current and lagged prices. Since prices are strongly correlated across observations, individual coefficients are relatively unstable (large standard errors); the sum of the coefficients on current and lagged prices is, however far more stable. Thus, the model is estimated using the following functional form:

$$\log(\beta_{it}) = a_0 + a_1 \log\left(\frac{p_{gt}}{p_{ot}}\right) + \sum_{j=1}^k a_{1j} \left(\log\left(\frac{p_{g(t-j)}}{p_{o(t-j)}}\right) - \log\left(\frac{p_{gt}}{p_{ot}}\right) \right) + a_2 \log\left(\frac{p_{gt}}{p_{ot}}\right) + \sum_{j=1}^k a_{2j} \left(\log\left(\frac{p_{d(t-j)}}{p_{o(t-j)}}\right) - \log\left(\frac{p_{dt}}{p_{ot}}\right) \right) + a_3 * t + a_4 * M, \quad (D.3)$$

$i \in (g, d)$

where a_1 represents the sum of product yield elasticities relative to current and past gasoline prices; a_{1j} represents the yield elasticity relative to the gasoline price lagged j periods; a_2 represents the sum of product yield elasticities relative to current and past diesel prices; a_{2j} represents the yield elasticity relative to the price of diesel lagged j periods; k represents the number of lagged prices included in the model. For the model presented in section 5.3.2, I set $k=3$, meaning that the model uses prices going back for a total of 3 months. Coefficients a_1 and a_2 can be interpreted as the product yield elasticity relative to a permanent price change (i.e. an equal increase in both current and lagged prices), such as may be induced by biofuel policies.

Despite already including a lag structure, the lagged prices and adaptive expectations models each exhibit autocorrelation in the error terms, as determined via a Durbin-Watson d -test (Table D.1). In contrast, the Durbin h -test (for models with lagged dependent variables) does not reject the null hypothesis of no autocorrelation within the partial adjustment model. To ensure model robustness, the main chapter also presents results for each of the three models assuming AR(1) type autocorrelation, by performing the standard model manipulation described in Dougherty (2007)⁴¹⁸ section 13.3. Since the results are stable across all 6 specifications, the autocorrelation structure was not probed further.

Table D.1. Tests for autocorrelation in the error terms among the main regression models presented above.

Model	Dependent variable: distillate yield	Dependent variable: gasoline yield
Lagged prices ^a	0.68**	0.76**
Partial adjustment ^b	-0.52	-0.28
Adaptive expectations ^a	0.71**	0.78**

**reject null hypothesis of no autocorrelation at the 1% level

a) Table reports Durbin-Watson d -statistic

b) Table reports Durbin h -statistic (for use in models with lagged dependent variable)

D.1.2 Additional Models and Results

In the lagged prices model described above, there is a large degree of flexibility concerning how many lags to include. Table D.2 shows results from the lagged prices model for differing numbers of lags. The elasticity estimates are fairly stable across differing numbers of lags, especially after the first month or two of lags are included. The model with 0 lags is equivalent to the simple model laid out in equations (5.1) and (5.2).

Table D.2. Elasticity of diesel and gasoline yields from crude oil with respect to the ratio of diesel and gasoline prices to the acquisition cost of crude oil for the lagged prices model, with differing numbers of lags. Standard errors are shown in parentheses. Results are based on nationally aggregated, monthly, U.S. data.

Lagged Prices Model – number of lags	Distillate yield		Gasoline yield	
	Elasticity with respect to distillate price ratio	Elasticity with respect to gasoline price ratio	Elasticity with respect to distillate price ratio	Elasticity with respect to gasoline price ratio
0	0.321*** (0.0292)	-0.266*** (0.0218)	-0.178*** (0.0159)	0.144*** (0.0119)
1	0.367*** (0.0289)	-0.306*** (0.0215)	-0.203*** (0.0160)	0.164*** (0.0120)
2	0.384*** (0.0305)	-0.324*** (0.0264)	-0.211*** (0.0170)	0.165*** (0.0126)
3	0.401*** (0.0315)	-0.341*** (0.0230)	-0.218*** (0.0178)	0.170*** (0.0130)
4	0.409*** (0.0329)	-0.355*** (0.0238)	-0.219*** (0.0188)	0.172*** (0.0136)
5	0.407*** (0.0340)	-0.365*** (0.0246)	-0.221*** (0.0195)	0.178*** (0.0141)
6	0.399*** (0.0348)	-0.376*** (0.0249)	-0.217*** (0.0202)	0.178*** (0.0145)
12	0.369*** (0.0418)	-0.417*** (0.0296)	-0.211*** (0.0251)	0.179*** (0.0177)

***p<0.001

I also test the stability of estimated elasticities to the inclusion of different model controls. In the interest of brevity, Table D.3 reports only the results of these alternate models for the partial adjustment functional form. In general, the model results are robust to these minor changes in functional form. One partial exception is that the gasoline yield elasticities become substantially smaller when month controls are omitted.

Table D.3. Elasticity of diesel and gasoline yields from crude oil with respect to diesel and gasoline prices for different variants of the partial adjustment model. Standard errors are shown in parentheses. Results are based on nationally aggregated, monthly, U.S. data.

Model variant	Distillate yield		Gasoline yield	
	Elasticity with respect to distillate price or price ratio	Elasticity with respect to gasoline price or price ratio	Elasticity with respect to distillate price or price ratio	Elasticity with respect to gasoline price or price ratio
Original	0.485*** (0.0614)	-0.404*** (0.0471)	-0.243*** (0.0305)	0.201*** (0.0233)
Prices instead of price ratios ^a	0.507*** (0.0626)	-0.547*** (0.0739)	-0.244*** (0.0317)	0.260*** (0.0377)
No month dummies	0.470*** (0.0482)	-0.382*** (0.00364)	-0.088 (0.058)	0.070 (0.043)
Year dummies instead of time trend	0.449 ^b	-0.349 ^b	-0.208 ^b	0.189 ^b
Controlling for prices of other products ^c	0.597*** (0.150)	-0.391*** (0.0443)	-0.194* (0.0799)	0.197*** (0.0234)

***p<0.001, **p<0.01, *p<0.05

- a) All other models use the ratio of gasoline and diesel prices to the price of input crude oil. This model simply uses direct (nominal) gasoline and diesel prices instead.
- b) Model would not converge when running under non-linear least squares. An equivalent model was run using ordinary least squares, from which the relevant elasticities can be calculated. This model form does not allow standard errors to be calculated directly, but all underlying model coefficients had very small standard errors (p-values below 10⁻⁹).
- c) Independent variables include the logarithm of the prices of jet fuel, propane and residual fuel oil, expressed as a ratio to the price input of crude oil. Coefficients each of these other prices were not significant at the 5% level.

Additionally, I run each of the main models presented above using annual data. Each lag now represents a much longer period (1 year instead of 1 month), and so the lagged prices model includes only a single lag. Month dummies no longer have any meaning and so are excluded from the annual regression models. Table D.4 presents results from each of the main models using annual data. Elasticity estimates are generally slightly higher than those in the monthly model, though with higher standard errors as a result of the smaller number of data points.

Table D.4. Elasticity of diesel and gasoline yields from crude oil with respect to the ratio of diesel and gasoline prices to the acquisition cost of crude oil (based on nationally aggregated, annual, U.S. data). Standard errors are shown in parentheses.

Model	Distillate yield		Gasoline yield	
	Elasticity with respect to distillate price ratio	Elasticity with respect to gasoline price ratio	Elasticity with respect to distillate price ratio	Elasticity with respect to gasoline price ratio
Basic model (no lags)	0.0350** (0.110)	-0.309*** (0.0752)	-0.222*** (0.0492)	0.168*** (0.0338)
Lagged prices (1 lag)	0.378** (0.122)	-0.483*** (0.0855)	-0.268*** (0.0656)	0.212*** (0.0497)
Partial adjustment	0.817* (0.291)	-0.642** (0.202)	-0.361** (0.100)	0.256** (0.0665)
Adaptive Expectations	0.866 (0.476)	-0.904* (0.398)	-0.357** (0.0984)	0.257*** (0.0584)
Lagged prices AR(1)	0.470** (0.129)	-0.392*** (0.0949)	-0.301** (0.0779)	0.228*** (0.0537)
Partial adjustment AR(1)	0.694* (0.285)	-0.604** (0.201)	-0.350** (0.115)	0.251** (0.075)
Adaptive Expectations AR(1)	0.555* (0.204)	-0.413* (0.154)	-0.405** (0.112)	0.290*** (0.071)

***p<0.001, **p<0.01, *p<0.05

Finally, I run a series of models using data at the level of U.S. Petroleum Administration Defense District (PADD),⁴¹⁹ rather than the nationally aggregated results presented above. Table D.5 shows yield elasticity estimates separately for each PADD, using the basic partial adjustment model. The table also includes the original (national) model, shown for reference. The regression coefficients for each PADD have the intuitive sign, and are nearly all significant at the 1% level or less. The table also shows a total atmospheric distillation capacity, cracking capacity (sum of thermal cracking, catalytic cracking and hydrocracking, expressed as a percent of atmospheric distillation capacity), and average refinery size for each region for 2004, which is the median year of the sample period from 1993-2016. Though far from definitive, cracking capacity and refinery size both appear to be correlated with higher absolute elasticities. In future work, this PADD-level data can be combined as part of a more integrated panel-data regression analysis to explore this question further.

Table D.5. Elasticity of diesel and gasoline yields from crude oil with respect to the ratio of diesel and gasoline prices to the acquisition cost of crude oil (based on U.S. PADD-level, monthly, U.S. data). Regression results are based on the standard partial adjustment model. Standard errors are shown in parentheses. The table also shows atmospheric distillation capacity (measured in million barrels per stream day) and cracking capacity (as a percent of atmospheric distillation capacity), and average refinery size (thousand barrels per stream day per refinery) for the year 2004 (median year in the sample from 1993-2016).

Region	Elasticity of Distillate yield with respect to:		Elasticity of Gasoline yield with respect to:		2004 Total Capacity (mbpsd)	2004 Cracking capacity (%)	2004 Average refinery size (10 ³ bpsd per refinery)
	<i>Distillate price ratio</i>	<i>Gasoline price ratio</i>	<i>Distillate price ratio</i>	<i>Gasoline price ratio</i>			
U.S.	0.485*** (0.0614)	-0.404*** (0.0471)	-0.243*** (0.0305)	0.201*** (0.0233)	17.8	57%	119
PADD 1 (East Coast)	0.29** (0.088)	-0.35*** (0.073)	-0.17*** (0.044)	0.18*** (0.037)	1.9	46%	115
PADD 2 (Midwest)	0.37*** (0.053)	-0.38*** (0.045)	-0.30*** (0.046)	0.26*** (0.038)	3.7	48%	143
PADD 3 (Gulf Coast)	0.74*** (0.13)	-0.66*** (0.11)	-0.26*** (0.039)	0.27*** (0.034)	8.3	62%	150
PADD 4 (Rocky Mountain)	0.090^ (0.048)	-0.11** (0.037)	-0.11** (0.037)	0.072* (0.029)	0.6	41%	38
PADD 5 (West Coast)	0.25*** (0.051)	-0.13*** (0.032)	-0.15** (0.052)	0.08* (0.034)	3.3	62%	92

***p<0.001, **p<0.01, *p<0.05 ^p<0.10

D.2. Additional Details for Main Model

D.2.1 PRELIM Parameter Selection

In sections 5.3.1 and 5.4.2, the chapter presents results from running the PRELIM model multiple times with different crude oils and different refinery configurations. PRELIM requires the user to specify multiple parameters in addition to the crude oil assay and the refinery configuration. The results presented in the main chapter use the following options:

- Naphtha catalytic reformer option: SR Naphtha (i.e. only short-run naphtha is sent to the catalytic reformer)
- FCC hydrotreater option: enabled (i.e. the fluid catalytic cracker hydrotreater is turned on).
- Electricity source: natural gas fired power plant
- Global warming potential (GWP): 2013 IPCC AR5 (100 years). Note: instead of using the default values in PRELIM, I modify the GWP input to reflect climate-carbon

feedbacks; thus CH₄ has a GWP of 36 kg CO_{2e}/kg CH₄ and N₂O has a GWP of 298 kg CO_{2e}/kg N₂O.

- Asphalt production: 10% (where 0% represents minimizing asphalt production and 100% represents maximizing asphalt production)
- LPG production: On (i.e. allow liquefied petroleum gases to be produced as final products)
- Petrochemical feedstock production: On (i.e. allow petrochemical feedstocks to be produced as final products)

D.2.2 Additional Model Parameters

As stated in the main chapter, baseline upstream GHG emissions (crude oil extraction and refining) are from Venkatesh *et al.* (2011).¹⁹⁸ Using the mean and confidence interval reported for upstream gasoline emissions I fit a lognormal distribution to emissions from crude oil extraction and normal distribution to refining emissions. I then convert from the original units (emissions per unit energy) to the required units (emissions per unit volume) using the same conversion factor for gasoline (1.16 mmbtu/gal) as in the model spreadsheet provided by Venkatesh *et al.* (2011).¹⁹⁸

For the partial equilibrium model, both the emission standards and carbon taxes require that the regular assume specific global warming intensities (GWIs) for different fuels. I assume the same values as in Rajagopal and Plevin (2013),³³⁰ summarized in Table D.6. Table D.7 summarizes initial product yields, combustion emissions, and assumed energy densities. Initial yields of diesel and gasoline are the same as in Rajagopal and Plevin (2013).³³⁰ Relative yields of other products are based on United Nations data.³⁵¹ Combustion emissions are from the IPCC.⁹⁵ Energy densities are from EIA.^{352,353}

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Table D.6. Global warming intensity values assumed by the regulator; based on Rajagopal and Plevin (2013)³³⁰

Fuel Pathway or Product	Rating (g CO₂e/MJ)
Gasoline	89.2
Diesel	93.4
Other oil products	79.2
Corn ethanol (process only)	62.5
Cane ethanol (process only)	25
Corn ethanol ILUC	25
Cane ethanol ILUC	25

Table D.7. Initial (2007) global volumetric yields, combustion emissions and energy densities of petroleum products

Product	Initial global yield (%)	Combustion emissions (kg CO₂/GJ); parameters for triangular distribution			Energy Density (GJ/ barrel)
		<i>Min</i>	<i>Mode</i>	<i>Max</i>	
Gasoline	25.0%	67.5	69.3	73	5.4
Diesel	28.0%	72.6	74.1	74.8	6.0
Jet fuels	6.9%	69.7	71.5	74.4	6.0
Kerosene	0.25%	70.8	71.9	73.7	6.0
Residual fuel	14.4%	75.5	77.4	78.8	6.6
Liquefied Petroleum Gases (LPG)	5.7%	61.6	63.1	65.6	3.8
Fuel coke	2.1%	82.9	97.5	111.5	6.3
Refinery fuel gas	4.4%	48.2	57.6	69	6.3
Asphalt	2.6%	73	80.7	89.9	7.0
Petrochem feedstocks	7.4%	69.3	73.3	76.3	5.3
Aviation gasoline	0.06%	67.5	70	73	5.4
Miscellaneous lubricants	2.1%	72.2	73.3	74.4	6.1
Waxes	1.1%	71.9	73.3	75.2	6.4
	0.15%	72.2	73.3	74.4	5.8

D.3. Additional Results

D.3.1 Main Model

Figure D.1 and Figure D.2 show respectively the breakdown in GHG emissions from different policies, and the change in prices of major petroleum product prices predicted by the model when only refineries in the home region adjust their product slate in response to market prices. As expected, these figures show qualitatively similar results to the globally flexible refiner case (Figure 5.10 and Figure 5.11), though with reduced magnitude.

Figure D.3 and Figure D.4 show the frequency distribution for the change in oil consumption in the home region and in the world respectively, for both fixed refinery yields, and for the case when all refineries exhibit the same price response as those in the U.S. The fixed refinery yield case from Figure D.3 differs substantially from the results in Rajagopal and Plevin (2013)³³⁰ as the present results correct a mistake in the original code. Comparing the green and red boxes in the two figures shows that refiner flexibility has only a very small impact on the total quantity of oil consumed at either region scale.

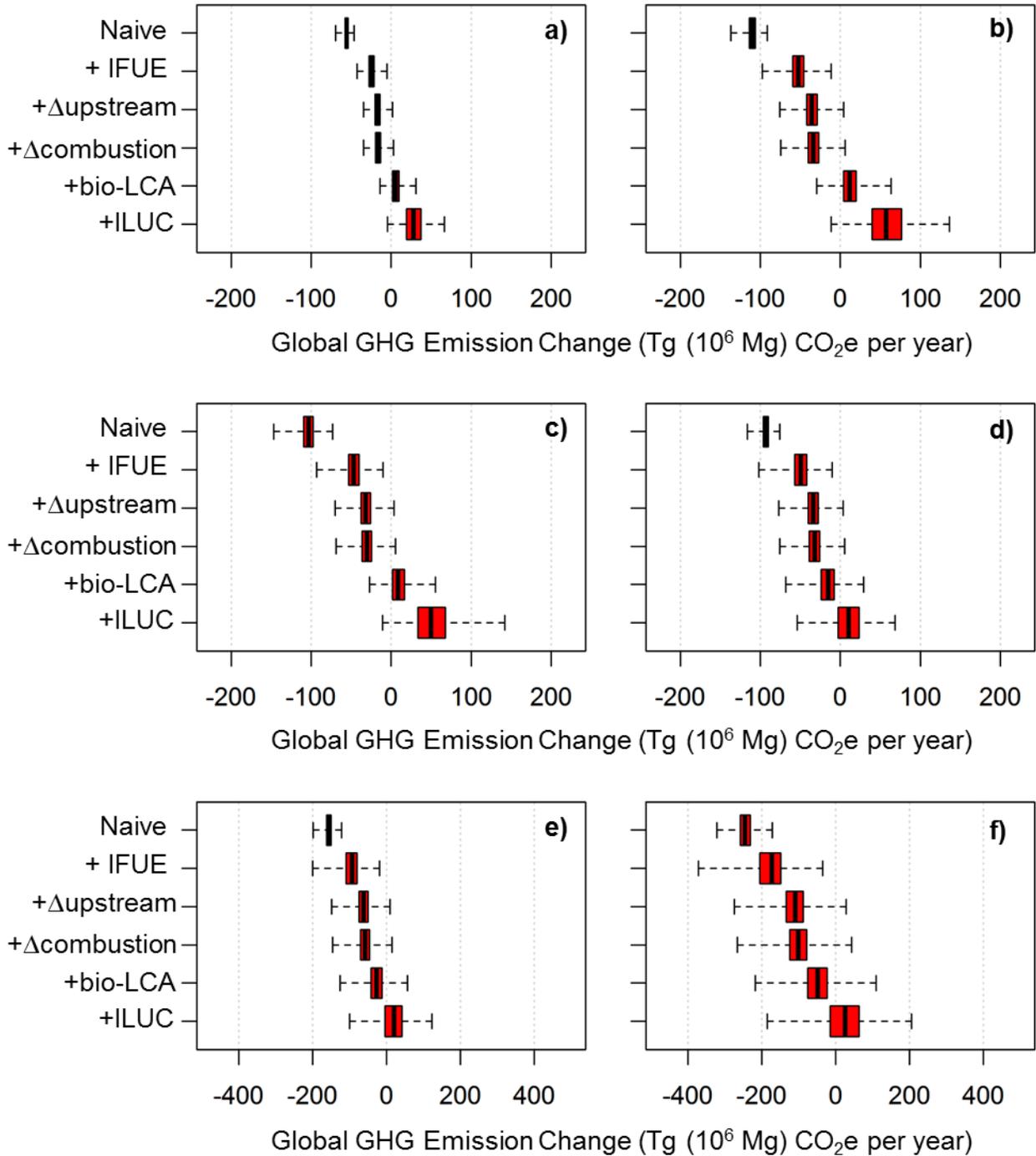


Figure D.1. Breakdown of emission changes from different policies, assuming only refineries in the home region adjust their product slate: a) 10% share mandate, b) 15% share mandate, c) 5% emission standard without ILUC, d) 5% emission standard with ILUC, e) 10% emission standard without ILUC, f) 10% emission standard with ILUC. Note the change in scale for the final 2 panels (e and f). The boxplots in each panel are built additively: “Naïve” represents the change in fossil fuel emissions, assuming biofuels are carbon neutral and displace gasoline perfectly without any market rebound. The next row adds the market

rebound / indirect fuel use effect (IFUE), assuming no change in carbon intensity within the petroleum industry. The next line adds the additional upstream emissions (crude oil extraction and refining) predicted due to the change in product yields. The next line adds the change in combustion emissions resulting from the shift in refinery yields. The final 2 rows represent emissions from biofuels, first excluding ILUC, and then including all emission sources.

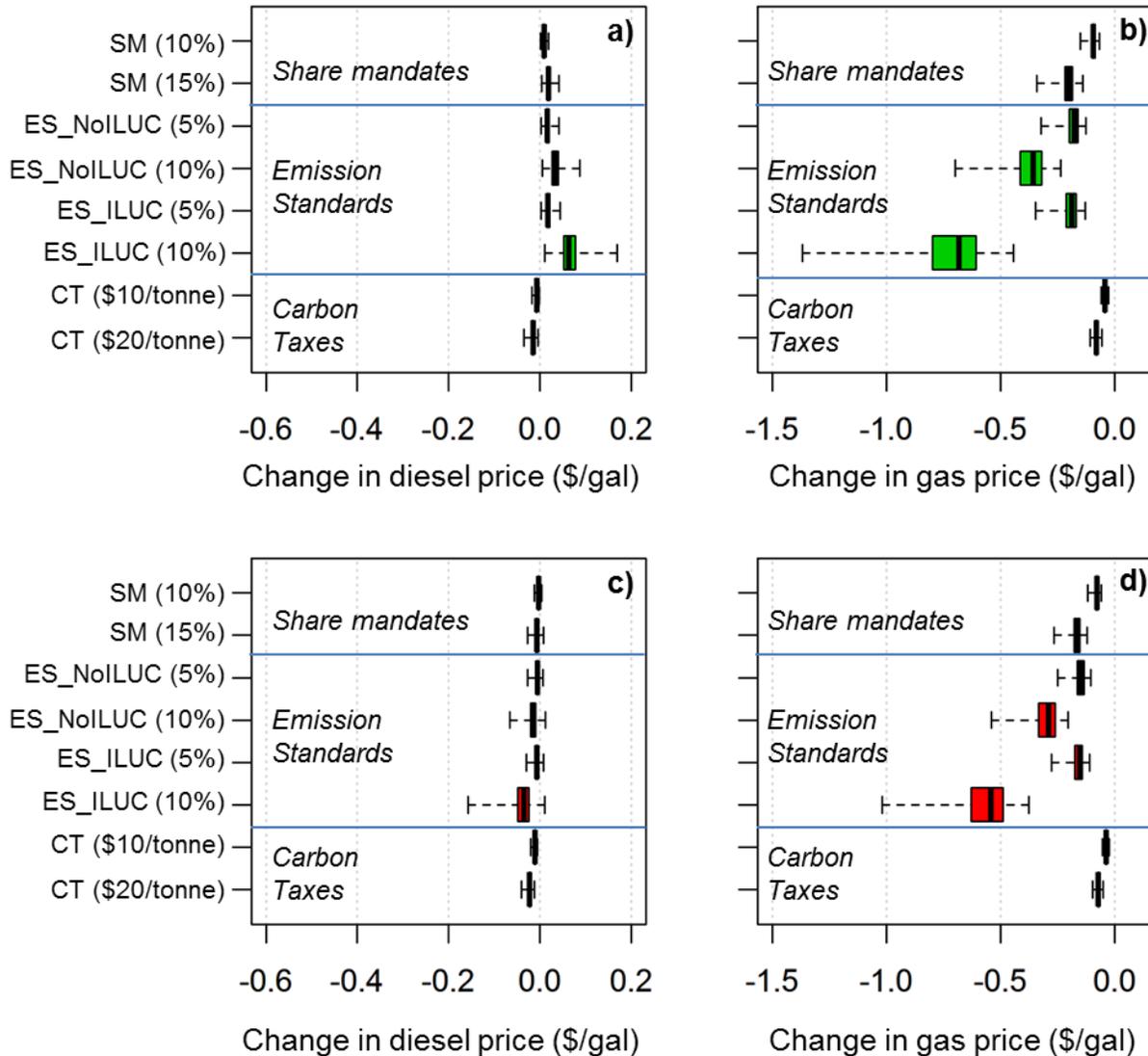


Figure D.2. Frequency distribution for change in diesel and gasoline prices induced by the different policies, with fixed refinery yields (panels a and b), or where refineries in only the home region adjust their product slate in response to market prices. (panels c and d). Policies include: SM = share mandate, ES = emission standard either with or without ILUC. CT = carbon tax. The box represents the interquartile range, the vertical line represents the median, and the whiskers show the extreme values of the simulation.

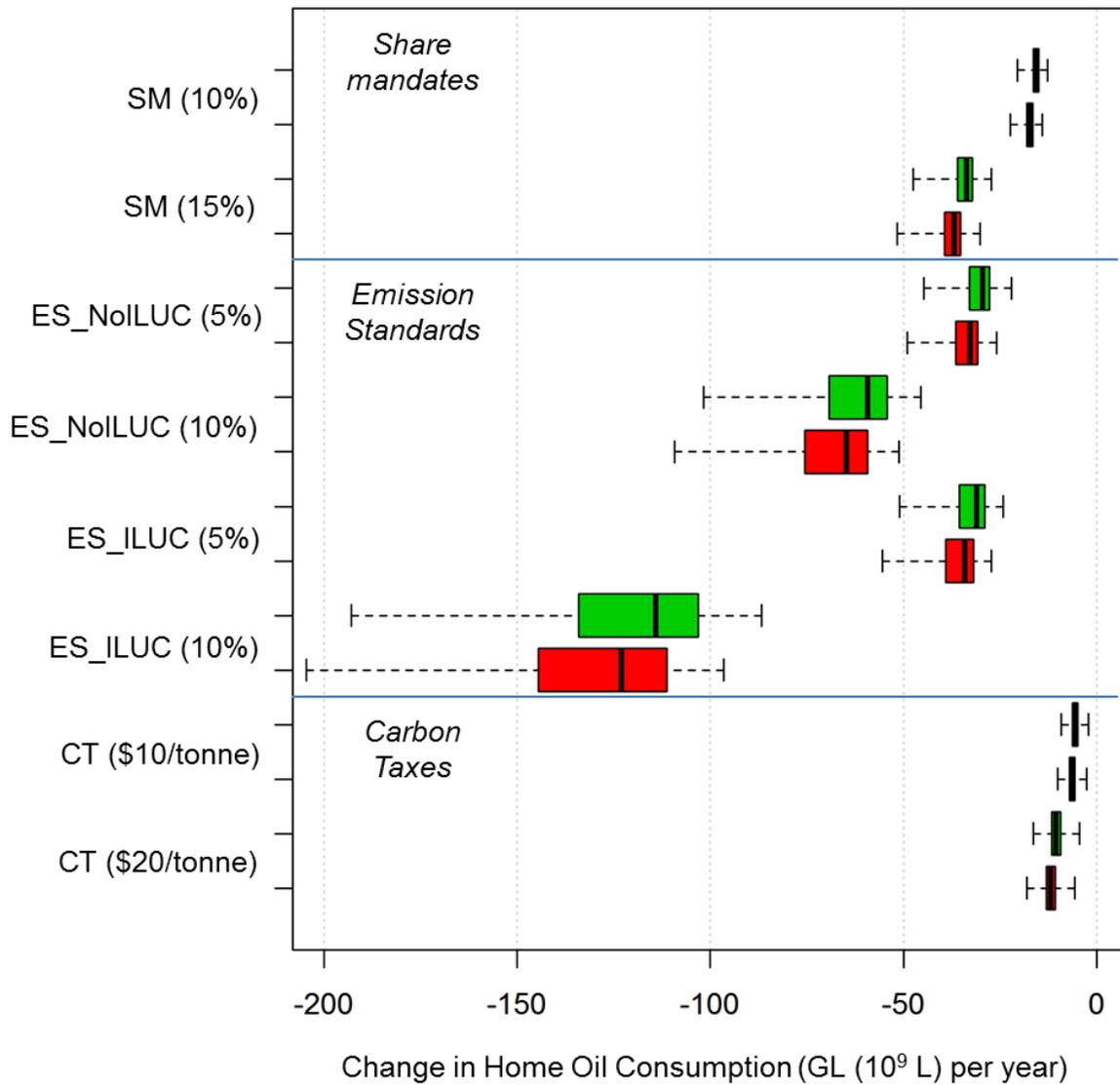


Figure D.3. Frequency distribution for the change in oil consumption in the home region brought about by different policies, with globally flexible refineries. SM = share mandate, ES = emission standard either with or without ILUC. CT = carbon tax. The box represents the interquartile range, the vertical line represents the median, and the whiskers show the extreme values of the simulation. Green boxes (the top member of each pair) represent the results when refinery yields are fixed. Red boxes represent results when all refineries exhibit the same price response as US refineries. Figure design based on Rajagopal and Plevin (2013).³³⁰

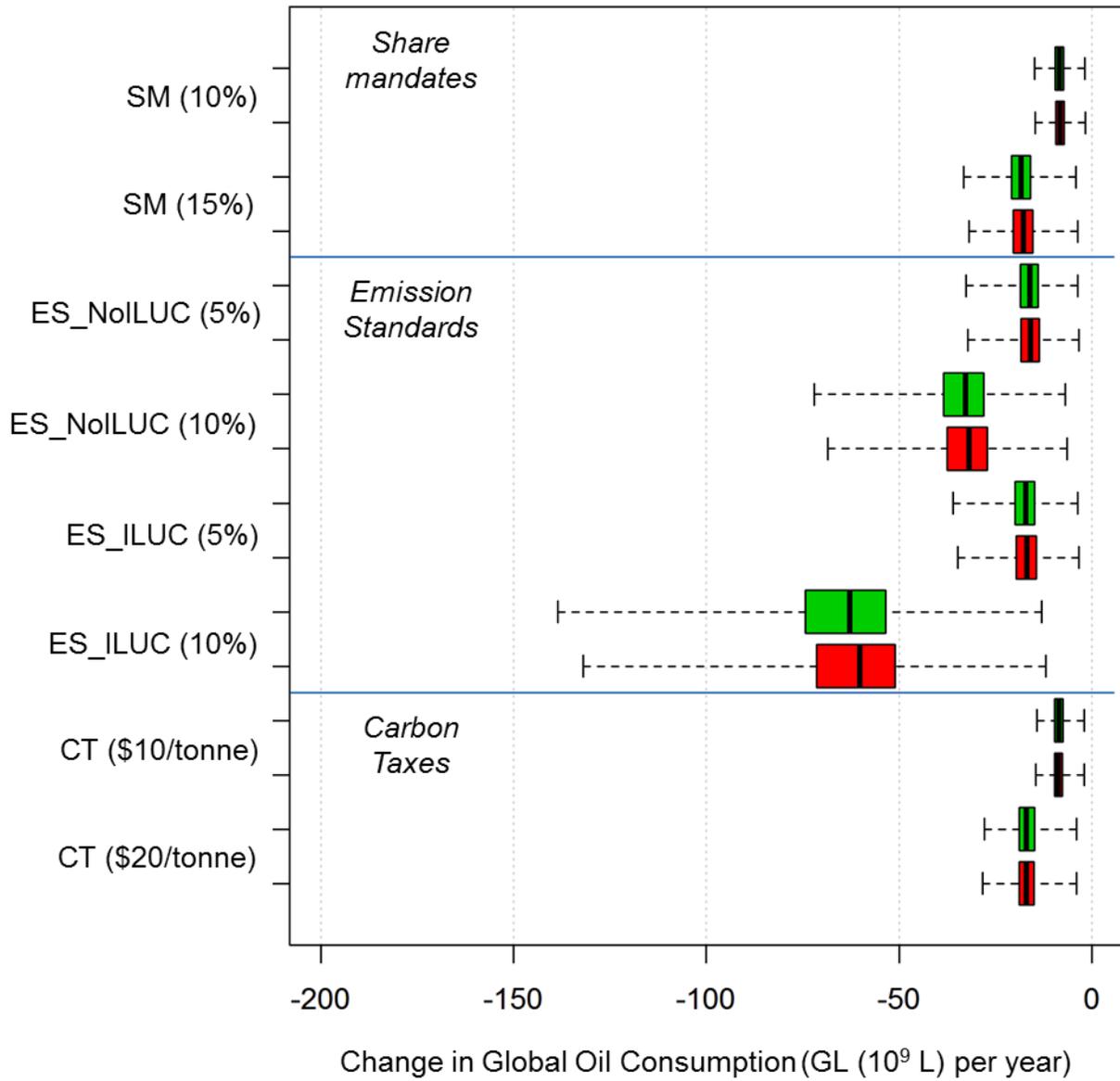


Figure D.4. Frequency distribution for the change in global oil consumption, brought about by different policies in the home region, with globally flexible refineries. SM = share mandate, ES = emission standard either with or without ILUC. CT = carbon tax. The box represents the interquartile range, the vertical line represents the median, and the whiskers show the extreme values of the simulation. Green boxes (the top member of each pair) represent the results when refinery yields are fixed. Red boxes represent results when all refineries exhibit the same price response as US refineries. Figure design based on Rajagopal and Plevin (2013).³³⁰

Appendix D

D.3.2 Supplement to Preliminary Analysis: Product Covariance Matrices**Table D.8. Covariance between yields of different petroleum products using national monthly data from EIA³⁴²**

	Gasoline	Distillate	Jet Fuel	Petroleum Coke	Still Gas	Residual Fuel Oil	Liquefied Refinery Gases	Asphalt	Petrochemical Naphtha	Lubricants	Miscellaneous	Special Naphthas	Kerosene	Aviation Gasoline	Waxes
Gasoline	1.46	-1.31	0.09	-0.07	-0.02	0.25	-0.69	0.05	0.05	0	-0.03	0.02	0.12	0	0
Distillate	-1.31	8.66	-0.51	1	-0.14	-2.23	-1	-1.35	-0.05	-0.14	0.22	-0.15	-0.35	-0.08	-0.1
Jet Fuel	0.09	-0.51	0.24	-0.06	-0.02	0.11	-0.04	0.02	0.02	0.02	-0.02	0.02	0.05	0	0.01
Petroleum Coke	-0.07	1	-0.06	0.17	-0.02	-0.31	-0.13	-0.16	0.01	-0.02	0.03	-0.02	-0.04	-0.01	-0.01
Still Gas	-0.02	-0.14	-0.02	-0.02	0.02	0.04	0.06	0.03	0	0	0	0	0	0	0
Residual Fuel Oil	0.25	-2.23	0.11	-0.31	0.04	0.88	0.08	0.25	-0.03	0.04	-0.06	0.04	0.11	0.02	0.03
Liquefied Refinery Gases	-0.69	-1	-0.04	-0.13	0.06	0.08	1.15	0.3	-0.01	0.02	-0.02	0.01	-0.06	0.01	0.01
Asphalt	0.05	-1.35	0.02	-0.16	0.03	0.25	0.3	0.43	0	0.02	-0.04	0.02	0.03	0.02	0.01
Petrochemical Naphtha	0.05	-0.05	0.02	0.01	0	-0.03	-0.01	0	0.05	0	0	0	0.01	0	0
Lubricants	0	-0.14	0.02	-0.02	0	0.04	0.02	0.02	0	0.01	0	0	0.01	0	0
Miscellaneous	-0.03	0.22	-0.02	0.03	0	-0.06	-0.02	-0.04	0	0	0.01	0	-0.01	0	0
Special Naphthas	0.02	-0.15	0.02	-0.02	0	0.04	0.01	0.02	0	0	0	0.01	0.01	0	0
Kerosene	0.12	-0.35	0.05	-0.04	0	0.11	-0.06	0.03	0.01	0.01	-0.01	0.01	0.04	0	0
Aviation Gasoline	0	-0.08	0	-0.01	0	0.02	0.01	0.02	0	0	0	0	0	0	0
Waxes	0	-0.1	0.01	-0.01	0	0.03	0.01	0.01	0	0	0	0	0	0	0

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Table D.9. Covariance between gasoline yield and yield of different petroleum products across crude oils, each for a fixed refinery configuration from PRELIM; results based on PRELIM

	Gasoline	Diesel	Jet Fuel	Fuel Oil	Coke or High Carbon Resid	Heavy Ends	Refinery Fuel Gas	Liquefied Petroleum Gases	Petrochemical Feedstocks	Asphalt
Prelim0	76.5	3.1	29.1	-7.7	0.0	-107.0	0.0	4.0	2.0	0.0
Prelim1	54.7	6.5	22.1	0.0	0.0	-86.5	0.0	3.0	1.5	-1.3
Prelim2	116.0	-52.3	35.7	0.0	0.0	-104.6	0.0	4.5	2.4	-1.8
Prelim3	74.9	-12.2	29.3	0.0	0.0	-95.9	0.0	3.6	1.9	-1.6
Prelim4	11.6	-4.9	-3.0	0.0	-3.6	-0.5	-0.1	0.3	0.2	-0.1
Prelim5	52.2	-52.6	17.5	0.0	-13.9	0.0	-1.2	-1.3	0.0	-0.7
Prelim6	22.7	-18.8	7.7	0.0	-8.8	-1.2	-0.5	-0.7	0.0	-0.4
Prelim7	17.9	-14.8	7.5	0.0	-7.7	-1.4	-0.8	0.2	-0.4	-0.5
Prelim8	57.5	-66.0	15.0	0.0	-7.3	0.0	-0.3	1.3	0.3	-0.6
Prelim9	27.9	-30.1	12.5	0.0	-8.1	-1.3	-0.7	0.6	-0.2	-0.6

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Table D.10. Covariance between gasoline yield and yield of different petroleum products across different refinery configurations, each for a fixed crude oil; results based on PRELIM

	Gasoline	Diesel	Jet Fuel	Fuel Oil	Coke or High Carbon Resid	Heavy Ends	Refinery Fuel Gas	Liquefied Petroleum Gases	Petro-chemical Feed-stocks	Asphalt
Bakken_Various_Sources	40.8	17.8	-1.4	-18.7	1.7	-44.0	0.0	1.9	1.2	0.7
North_Sea Dansk Blend_Statoil	89.4	43.5	-2.6	-21.7	11.3	-135.5	0.7	8.8	4.7	1.6
Nigeria_Agbami_Statoil	11.1	4.4	-0.7	-9.7	0.6	-6.7	0.0	0.5	0.4	0.1
Forties_Statoil_	24.5	6.3	-0.9	-8.2	3.5	-29.1	0.0	2.2	1.2	0.3
Canada_Hibernia_Statoil	60.2	29.7	-2.8	-22.5	7.9	-81.0	0.0	4.8	2.7	1.1
Ekofisk_Statoil	45.8	23.2	-2.1	-18.8	5.6	-60.1	0.0	3.5	2.0	0.8
Azeri_Light_Statoil	70.0	36.1	-3.5	-30.4	6.2	-86.7	0.0	4.5	2.7	1.2
Angola_Girassol_Statoil	52.8	20.2	-2.3	-15.2	9.9	-74.5	0.0	5.4	2.9	0.8
West_texas sour_Statiev	33.8	10.9	-0.9	-9.7	6.9	-46.4	0.0	3.2	1.8	0.5
West_texas intermediate_Statiev	42.2	22.4	-2.0	-16.9	4.5	-55.4	0.0	2.9	1.8	0.7
Venezuela_Tia Juana_Statiev	126.5	16.0	-2.6	-17.6	46.0	-196.6	2.6	16.4	8.0	1.5
Russian_Export Blend_Statiev	46.2	18.9	-1.6	-10.7	11.4	-72.9	0.0	5.3	2.7	0.7
MAYA_Statiev	64.3	32.7	-3.2	-6.2	39.3	-146.8	3.3	10.4	5.5	0.8
Louisiana_light sweet_Statiev	45.3	23.7	-2.2	-18.2	3.8	-57.6	0.0	2.7	1.7	0.8
Kuwait_Export_Statiev	49.1	22.2	-1.3	-11.5	15.9	-84.1	0.2	5.8	3.1	0.7
Isthmus_Statiev	37.5	14.9	-1.1	-8.7	10.3	-60.0	0.1	4.2	2.2	0.6
Ecuador_Oriente_Statiev	41.5	19.5	-1.9	-7.5	16.4	-77.8	0.5	5.7	3.0	0.6
Congo_Emeraude_Statiev	92.3	37.4	-3.5	-7.7	34.0	-177.9	3.6	14.0	6.9	0.9
Colombia_Cano Limon_Statiev	57.5	30.6	-2.7	-13.0	12.3	-95.5	0.5	6.2	3.3	0.8
Arab_Heavy_Statiev	57.0	25.3	-1.9	-10.3	21.2	-104.3	0.7	7.5	3.9	0.8
Arab_Medium_Statiev	48.9	21.1	-1.5	-10.0	16.5	-84.9	0.1	6.0	3.1	0.7
Arab_Light_Statiev	40.2	17.8	-1.4	-10.5	9.6	-62.9	0.0	4.3	2.3	0.6
Angola_Cabinda_Statiev	62.0	32.9	-2.1	-15.8	12.4	-100.7	1.1	6.0	3.3	0.9
Merey_O&G	185.4	14.4	-6.3	-20.0	43.5	-248.3	9.9	12.3	7.4	1.7

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Marine_Qatar_O&G	71.9	17.8	-1.7	-10.0	18.8	-111.2	0.0	9.1	4.5	0.7
Kirkuk_O&G	28.9	7.6	-0.9	-8.9	8.7	-40.6	0.0	3.0	1.7	0.5
Burgan_(Wafra)_O&G	83.5	8.2	-2.4	-15.4	26.1	-115.1	-0.2	9.4	4.9	1.0
Basrah_Heavy_O&G	79.8	24.8	-1.8	-11.2	36.7	-143.4	0.0	9.3	4.8	1.0
Wilmington_CA_Knovel	110.9	48.7	-4.7	-10.8	24.8	-200.5	5.5	17.5	7.8	0.8
Midway-Sunset_Knovel	111.1	53.5	-6.5	-8.5	26.4	-202.9	2.3	16.3	7.8	0.7
Hamaca_Venezuela_Knovel	33.3	14.3	-1.9	-12.9	11.9	-50.9	0.0	3.5	2.0	0.6
Belridge_Knovel	160.8	61.3	-6.4	-19.8	36.2	-276.9	8.8	24.1	10.9	1.1
Thunderhorse_Exxon	55.7	29.4	-2.3	-10.3	5.0	-87.2	0.3	5.7	3.0	0.7
Russia_Sokol_Exxon	41.6	22.7	-2.0	-12.1	4.9	-61.4	0.0	3.6	2.0	0.7
Nigera_Quaib_Exxon	16.4	9.0	-1.0	-3.5	3.2	-27.6	0.0	2.2	1.1	0.2
Nigera_Erha_Exxon	35.8	16.9	-1.8	-10.4	4.1	-50.4	0.0	3.3	1.8	0.6
Nigera_Bonga_Exxon	12.8	6.1	-0.9	-1.6	2.6	-21.8	0.0	1.8	0.9	0.1
Canada_Hibernia_Exxon	60.6	33.2	-2.0	-10.6	9.1	-101.6	0.7	6.5	3.4	0.8
Brent_Exxon	47.3	25.5	-1.8	-11.4	7.9	-75.7	0.4	4.6	2.5	0.7
Azeri_light_Exxon	104.6	47.6	-3.7	-20.6	11.5	-154.2	1.4	7.5	4.4	1.7
Alaskan_North Slope_Exxon	46.4	17.3	-1.4	-8.5	14.1	-77.6	0.2	6.0	3.1	0.6
Angola_Girassol_Exxon	62.2	24.9	-1.9	-11.2	11.5	-96.9	0.3	6.8	3.5	0.9
Western_Canadian Select_Crude Monitor	72.9	7.5	-2.2	-12.0	28.0	-108.7	0.0	9.1	4.5	0.9
Western_Canadian Blend_Crude Monitor	71.5	12.0	-2.1	-12.3	26.6	-109.6	-0.2	8.8	4.4	1.0
Wabasca_Heavy_Crude Monitor	69.0	5.5	-1.8	-11.3	25.0	-99.6	-0.1	8.3	4.1	0.9
Syncrude_Synthetic_Crude Monitor	41.5	-11.4	-0.9	-18.1	0.3	-14.8	0.0	2.0	1.2	0.3
Suncor_Synthetic H_Crude Monitor	177.4	-120.0	-1.1	-42.4	1.3	-28.0	0.0	7.8	4.3	0.8
Suncor_Synthetic A_Crude Monitor	50.9	5.9	-1.9	-36.9	0.2	-21.8	0.0	2.1	1.3	0.2
Smiley-Coleville_Crude_Monitor	71.0	6.2	-2.2	-11.5	27.4	-105.2	0.0	9.0	4.4	0.9
Seal_Heavy_Crude Monitor	71.6	13.0	-2.4	-9.8	30.8	-117.9	0.0	9.4	4.6	0.8
Midale_Crude_Monitor	40.7	5.5	-1.5	-9.5	12.3	-54.8	-0.1	4.5	2.4	0.6
Lloyd_Kerrobert_Crude Monitor	76.3	-2.6	-2.2	-11.2	27.0	-101.8	-0.1	9.2	4.5	0.9

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Lloyd_Blend_Crude Monitor	71.3	7.5	-2.0	-10.2	28.9	-110.0	0.0	9.2	4.5	0.9
Husky_Synthetic Blend_Crude Monitor	67.7	21.5	-3.0	-45.4	0.4	-45.9	0.0	2.7	1.7	0.4
High_Sour Edmonton_Crude Monitor	31.3	10.0	-1.2	-9.1	7.8	-44.2	0.0	3.3	1.8	0.5
Cold_Lake_Crude Monitor	67.4	5.9	-1.7	-10.9	28.8	-103.0	-0.1	8.5	4.3	0.9
Bow_River North_Crude Monitor	66.1	2.1	-2.0	-12.7	22.3	-88.0	-0.2	7.7	3.8	0.9
Albian_Residual Blend_Crude Monitor	62.7	12.0	-2.4	-12.0	25.0	-98.0	-0.1	8.1	3.9	0.7
Albian_Heavy Synthetic_Crude Monitor	85.9	-28.1	-2.2	-12.4	23.6	-80.8	0.7	8.2	4.2	0.9
Wyoming_Sweet_COA	46.6	25.1	-2.3	-15.8	7.6	-67.9	0.0	3.8	2.2	0.9
Venezuela_Leona_COA	66.0	29.7	-2.1	-8.4	22.6	-122.6	0.2	9.2	4.6	0.8
Siberian_Light_COA	45.3	22.8	-2.0	-15.1	7.7	-65.6	0.0	3.8	2.2	0.8
Olmecca_COA	29.9	14.6	-1.1	-10.3	3.3	-40.0	0.0	2.0	1.2	0.5
Iranian_Heavy_COA	42.6	21.1	-1.5	-9.4	13.4	-74.8	0.2	5.1	2.7	0.6
Iran_Ardeshir_COA	53.3	23.1	-2.4	-10.1	18.0	-92.7	0.1	6.5	3.5	0.8
Fateh_COA	41.2	17.5	-1.0	-11.9	10.8	-63.7	0.0	4.2	2.3	0.7
East_Texas Sweet_COA	48.5	25.5	-2.4	-17.5	6.2	-66.4	0.0	3.3	2.0	0.9
Dukhan_Qatar_COA	26.9	13.5	-1.1	-7.9	4.3	-39.9	0.0	2.4	1.4	0.4
Cusiana_COA	25.9	11.7	-0.9	-13.8	2.3	-28.2	0.0	1.6	1.0	0.4
Basrah_Medium_COA	40.0	15.4	-1.5	-8.8	15.2	-68.4	0.0	4.9	2.6	0.6
Tengiz_Chevron	22.5	11.1	-1.2	-8.9	1.5	-27.7	0.0	1.5	0.9	0.3
Sumatran_Light (Minas)_Chevron	183.7	30.9	-7.3	-50.0	18.4	-195.8	4.5	8.0	5.4	2.2
Qin_Huang Dao_Chevron	133.3	11.3	-2.4	-22.3	30.9	-179.9	4.4	15.8	7.6	1.5
Nigeria_Pennington_Chevron	61.5	22.7	-2.5	-24.3	4.6	-69.0	0.0	3.8	2.3	1.0
Nigeria_Escravos_Chevron	113.6	49.7	-2.7	-41.0	7.5	-143.2	0.2	9.2	5.0	1.8
Nigeria_Agbami_Chevron	70.3	28.2	-4.4	-31.1	4.1	-72.8	0.0	2.9	2.0	1.0
Nanhai_Light_Chevron	163.8	-5.5	-7.9	-46.7	9.3	-123.6	1.7	4.3	3.3	1.4
Kuwait_Ratawi_Chevron	98.9	42.4	-3.9	-8.4	47.7	-202.1	2.5	14.6	7.4	1.0
Kuwait_Eocene_Chevron	136.6	48.4	-2.8	-10.5	54.9	-260.5	3.4	19.8	9.2	1.4
Indonesia_Duri_Chevron	171.1	68.9	-3.3	-9.2	48.5	-327.8	11.6	26.6	12.1	1.4
Forties_Chevron_	43.0	22.7	-2.7	-10.4	5.8	-65.3	0.2	3.9	2.2	0.6
Ekofisk_Chevron_	94.4	50.6	-3.2	-28.3	11.4	-140.1	1.1	8.0	4.5	1.7

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Cossack_Chevron	108.1	1.7	-4.4	-29.7	5.5	-86.2	0.2	2.1	1.8	1.0
China_Bozhong_Chevron	124.2	17.4	-2.5	-22.1	33.0	-179.3	4.9	15.4	7.5	1.5
Canada_Hibernia_Chevron	70.1	31.7	-3.0	-10.0	12.4	-115.7	1.0	8.3	4.2	0.9
Brent_Chevron	48.0	25.8	-1.9	-18.0	6.5	-67.1	0.0	3.7	2.2	0.9
Brazil_Frade_Chevron	135.1	34.0	-4.0	-11.5	31.0	-218.3	5.0	18.8	8.6	1.2
Bonny_Light_Chevron	40.7	12.9	-0.3	-19.3	3.0	-41.7	0.0	2.6	1.5	0.6
Azeri_Light_Chevron	77.2	35.1	-4.0	-32.4	6.2	-89.7	0.0	4.0	2.6	1.2
Angola_Kuito_Chevron	115.7	37.3	-4.3	-10.8	32.0	-200.5	5.1	16.4	8.0	1.0
UAE_Murban_BP	20.4	9.3	-0.7	-9.5	5.1	-27.8	0.0	1.7	1.0	0.4
UAE_DAS Blend_BP	21.7	8.2	-0.7	-9.4	2.6	-25.3	0.0	1.6	0.9	0.3
Thunderhorse_BP_	36.5	10.1	-1.1	-10.4	8.9	-50.6	0.0	4.0	2.1	0.5
Norway_North Sea Skarv_BP	48.1	23.3	-2.0	-22.5	4.1	-56.5	0.0	2.9	1.7	0.8
Mars_USA-Gulf of Mexico_BP	50.3	12.8	-1.4	-6.3	16.6	-82.5	0.0	6.5	3.3	0.6
Iraq_Basra_BP	47.1	11.6	-1.0	-9.8	16.1	-73.3	-0.1	5.7	3.0	0.6
Indonesia_Tangguh_BP	4.1	2.1	-0.2	-2.2	0.1	-4.3	0.0	0.2	0.2	0.1
Forties_Blend_BP	24.1	7.3	-0.6	-7.8	3.8	-30.7	0.0	2.3	1.2	0.3
Ekofisk_BP	46.3	23.7	-2.0	-17.3	5.6	-62.6	0.0	3.5	2.0	0.8
Brent_BP	43.7	19.8	-1.5	-16.5	5.7	-57.2	0.0	3.3	1.9	0.8
Brazil_Polvo_BP	84.7	-4.4	-2.8	-10.8	26.2	-111.0	1.5	10.6	5.1	0.8
Brazil_Lula_BG Group	55.3	19.5	-1.3	-26.4	3.9	-56.3	0.0	2.8	1.7	0.9

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