Research Report – UCD-ITS-RR-13-40

Modeling the Environmental Impacts of Cellulosic Biofuel Production in Life Cycle and Spatial Frameworks

December 2013

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Modeling the Environmental Impacts of Cellulosic Biofuel Production in Life Cycle and Spatial Frameworks

by

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DISSERTATION

Submitted in partial satisfaction of the requirements for the degree of

DOCTOR OF PHILOSOPHY

In

Transportation Technology and Policy

in the

OFFICE OF GRADUATE STUDIES

of the

UNIVERSITY OF CALIFORNIA, DAVIS

APPROVED

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2013

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September 2013
Transportation Technology and Policy

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Abstract

Biofuels may be able to reduce greenhouse gas (GHG) emissions from the transportation sector, expand domestic energy production and spur rural economic development. Lignocellulosic biofuels are of particular interest because they can use waste or residual biomass as feedstock, or feedstock grown on marginal cropland. Research on lignocellulosic biofuel production pathways has revealed risks of environmental impacts, such as land transformation, loss of soil carbon and air pollutant emission.

This dissertation examines areas of uncertainty regarding the environmental impacts of biofuel production systems through four research studies, three which focus on the environmental impacts of biofuels within a life-cycle analysis framework, and the fourth which uses large-scale spatially explicit technoeconomic modeling to evaluate interactions between biofuel production systems and air-quality policy. These will help inform decisions on how best to minimize environmental impacts, particularly a biofuels' GHG balance, as large-scale biofuel production expands.

Results show that life-cycle environmental impacts of biofuels are often dominated by the feedstock production phase. Soil organic carbon changes are among the most important and most uncertain of all processes from biofuel production. In corn stover production systems, sustained removal of biomass from a field reduces the amount of carbon sequestered in soil, which can dominate other GHG emissions. This decrease can exceed one tonne of CO_2 equivalent per hectare of corn from which stover is removed. Fertilizer production and conversion facility energy demands are also major sources of environmental impact. Cellulosic biofuels have the potential to reduce GHG emission, when displacing conventional fuels, but substantial uncertainty remains within the production system.

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Acknowledgements:

This work was supported by the Department of Energy under Award Number DE-EE0002881, a USDA Coordinated Agricultural Project Grant, and a University of California Transportation Center Dissertation Fellowship. Portions of this work describe production processes developed by EdeniQ Inc. and Ceres, Inc.; no endorsement of this or any other commercial interest is intended.

In addition to the Dissertation Committee the author would like to thank Nathan Parker, Dan Sperling, Joan Ogden, Adjith Kaduwela, Stephen Kaffka, Rob Williams, Gabriel Lade, Boon-Ling Yeo, Lindsay Price, Quinn Hart and Peter Tittman for their insights and assistance with various elements of this work over the last five years.

Finally, and most importantly, a deep and heartfelt thanks to my wife, Melissa Murphy, for her patience and understanding over the long journey which turned this research into reality.

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Nomenclature

dLUC – Direct Land Use Change

GBSM – Geospatial Bioenergy Systems Model

GHG – Greenhouse Gas

GIFT – Geospatial Intermodal Freight Transport (model)

GWP – Global Warming Potential

iLUC – Indirect Land Use Change

IPCC – Intergovernmental Panel on Climate Change

K - Potassium

LCA – Life Cycle Analysis

LCI – Life Cycle Inventory

LDV- Light-Duty Vehicle

LUC –Land Use Change

Mg—Megagrams. Equivalent to a tonne or metric ton.

N – Nitrogen

NAA – EPA Non-Attainment Areas

NO_x – Nitrogen Oxides

P – Phosphorous

RFS2 – U.S. Revised Renewable Fuel Standard

SOC – Soil Organic Carbon

SOx- Sulfur Oxides

Ton—A short or imperial ton (2000 lb).

Chapter 1: Introduction

Biofuels hold promise for reducing greenhouse gas (GHG) emissions from the transportation sector. Substituting biofuels for petroleum-based fuels may also reduce the external costs of petroleum dependence, reduce criteria air pollutant emissions and promote rural economic development (Delucchi & McCubbin, 2010; U.S. EPA, 2010). As understanding of global climate change improves, it becomes more apparent that policy measures to address GHG emissions are necessary in the near term (Philibert, 2004) to avert some of the worst climate-related impacts. Biofuels are likely to be a significant element of many nations' plans to address climate change and though they are not without risk, biofuels have demonstrated the potential to be deployed at large scale. Despite potential benefits, biofuels have, in some circumstances, been found to increase GHG emissions relative to petroleum fuels and can also adversely affect ecosystem health, food markets and water quality (Fargione, Hill, Tilman, Polasky, & Hawthorne, 2008; Farrell, Sperling, & et. al., 2007; Reijnders & Huijbregts, 2008; Searchinger et al., 2008).

For future biofuel developments to avoid similarly unfavorable outcomes and achieve a climate change benefit, analysts must improve their ability to prospectively model biofuel and bioenergy systems and support timely and informed policy decisions. This dissertation is driven by a desire to help understand and accurately identify what makes a biofuel system environmentally beneficial. Careful examination of biofuel production systems and the development of a useful analytical toolkit can improve policy making, though few definitive conclusions can be drawn until these systems are more mature and better-understood.

Researchers have already evaluated the starch or sugar-based (first generation) biofuels available for widespread production in the U.S. and concluded that they offer a limited benefit towards GHG mitigation and energy security, and pose a substantial risk to food markets and water quality. This dissertation will focus on environmental characteristics of some of the cellulosic (second generation) biofuels. Second generation biofuels are thought to have superior environmental and energy-balance characteristics than first generation fuels (Delucchi, 2010; Hsu et al., 2010; von Blottnitz & Curran, 2007). They are expected to enter fuel markets in substantial quantity over the next several decades (Advanced Ethanol Council, 2013). This dissertation will help evaluate what impact their introduction may have on climate change emissions and other environmental indicators.

1.1 Sustainability of Biofuel Systems

Biofuels have historically been viewed as a more sustainable alternative to petroleum transportation fuels (Sperling & Gordon, 2009). Early policy failures, such as the European biodiesel mandate, which inadvertently promoted the conversion of tropical land to energy crop use, in this case palm oil, led to increases in emission of GHGs from land use change (LUC) and other environmental harms (Bonin & Lal, 2012; Cherubini & Strømman, 2011; Reijnders & Huijbregts, 2008). This example demonstrates the importance of improved understanding of biofuels' impacts prior to commercial scale production to craft better policy.

Life cycle analysis (LCA) evaluates the environmental flows and consequent impact of a product or service over each life cycle stage, beginning with primary resource extraction and terminating at its end-of-life. LCA has demonstrated that for petroleum fuels pre-combustion impacts typically represent less than 25% of total impacts (Hill et al., 2009; M. Wang, Lee, & Molburg, 2004). Biofuels, on the other hand, tend to have a majority of their environmental impacts concentrated in upstream phases of production, especially cultivation and harvest of feedstock, and inputs for the conversion facility. LCA is therefore a critical tool for understanding the actual environmental impacts of biofuel production. LCA also allows evaluation of tradeoffs between different categories of environmental impact, such as GHG emissions and water pollution or between production phases. For example, a particular variety of biomass feedstock crop may require more fertilizer than other varieties, but have a chemical composition that improves conversion efficiency. The increased fertilizer demand carries with it environmental harms, but improved yields reduce the impact of the conversion facility. LCA is the preferred tool for weighing the impacts of changes to productions systems like this.

The primary environmental concern discussed in this paper is global climate change, due to its scope and potential for severe impacts (IPCC, 2007). Biofuels change the CO_2 footprint of transportation and energy consumption during combustion, by substituting for fossil fuels, as well as during production, by altering carbon cycling through agricultural systems. In addition to CO_2, biofuel production emits other GHGs which have higher global warming potentials (GWPs) than CO_2, namely CH_4 and N_2O. Both are emitted during fertilizer production and N_2O emissions occur on fertilized fields (Goorahoo, S, Ashkan, Mahal, & Salas, 2012; Odlare et al., 2012). Methane is also emitted during the decomposition of organic matter, including agricultural residues as they are incorporated into soil, though these emissions tend to be much smaller than field N_2O emissions.

Biofuels also can affect the formation of secondary organic aerosols through emission of volatile reactive organic species from field emissions, agricultural equipment activity and fuel evaporation (Eller et al., 2011), as well as primary aerosols through suspended dust or smokestack emissions at conversion facilities. Recent research has demonstrated the strong warming potentials of some particulates, notably black carbon (Bond et al., 2013), while also finding that other particulates can have cooling effects or contribute to net climate variability (Booth, Dunstone, Halloran, Andrews, & Bellouin, 2012; Ramanathan & Feng, 2009; Shindell et al., 2009). Particulate GHG effects are not included in this dissertation because of this uncertainty in their effect.

GHG emissions are also affected by changes to pools of carbon in soil, which can be caused by increased feedstock production (Anderson-Teixeira, Davis, Masters, & Delucia, 2009; Huggins, Allmaras, Clapp, Lamb, & Randall, 2007; Reijnders & Huijbregts, 2008). These changes in soil carbon are often precipitated by land use change (LUC), such as conversion from natural grassland to managed agriculture, which can disturb pools of soil organic carbon (SOC), stimulating microbial activity which releases carbon as CO_2 and CH_4. Most soil also contains some inorganic carbon, though most studies of carbon in agricultural soils find the inorganic component to be an order of magnitude smaller than the organic component. Chapter 4 discusses soil carbon in greater detail and examines the effect on SOC of removing stover for cellulosic ethanol production using a meta-analysis (J. Johnson, Acosta-Martinez, Cambardella, & Barbour, 2013).

Some biofuels may reduce tailpipe emissions in light-duty engines, due to their lower concentrations of particulate-forming components, such as sulfur, and their inhibitory effect on in-cylinder combustion temperatures, which reduces NO_x formation (Canakci, Ozsezen, Alptekin, & Eyidogan, 2013; Hsu et al., 2010). The consensus in literature is that biofuels are likely to be an improvement over their petroleum equivalents as far as air pollutants from combustion are concerned. The consensus in literature regarding upstream impacts is not quite as settled, but generally agrees that the net impact of biofuel production causes, or at least risks, increased criteria pollutant emissions. A critical question is: Are the benefits from biofuels' cleaner combustion greater than the upstream harms from their production? Understanding the upstream harms is difficult due to the spatially distributed nature of biofuel production; feedstock may come from many different fields spread over a substantial area and possibly located in different airsheds (Hill et al., 2009; Tittmann, Parker, Hart, & Jenkins, 2010). Some authors have begun to examine air pollutant emissions from biofuels in a spatially explicit fashion (which is discussed in more detail in Chapter 2) but the field is still emerging.

Additional complexity is added by market-mediated effects, known as indirect land use change (iLUC), in which the change in agricultural or harvest practices in one area creates demand for a given product, which may be met by conversion of land in a distant area. Agricultural residues and grassy energy crops are thought to minimize potential iLUC because they do not consume portions of the plant, or utilize land, that is currently used for productive purposes (though the use of stover to maintain soil condition is arguably a productive purpose). This dissertation cannot hope to conclusively answer the question of iLUC and discusses the subject only briefly.

Biofuels also have raised significant concerns for water quality and availability. One common characteristic of marginal land is lack of water; energy crops on these lands might require irrigation for some part of their growing cycle, which places them in competition with food, feed and fiber crops for scarce irrigation water, even if they are not competing with food crops for land (Delucchi, 2010; Mishra & Yeh, 2011; Yeh et al., 2011). This phenomenon may stimulate iLUC changes through a completely new pathway, as agricultural production shifts in response to water availability patterns in response to biofuel production. Beyond the question of water availability, there is substantial concern about biofuels' effect on water quality. Cultivation of feedstocks, even when feedstocks are derived from residues of other crops, requires fertilizer, some of which typically runs off into surface waters. Corn stover, which is a potential biofuel feedstock in the U.S., is particularly affected by this problem due to the high nitrogen (N) requirements of corn cultivation and wide use of tile drainage systems in the Corn Belt. Over 30% of all N applied to high-intensity corn fields may run off into surface water (Powers, 2005); since the Mississippi river watershed is a major corn-growing region, this significantly contributes to the Gulf of Mexico's Hypoxic Zone (Costello, Griffin, Landis, & Matthews, 2009; Syswerda, Basso, Hamilton, Tausig, & Robertson, 2012).

1.2 Environmental Impacts of Biofuel Production

Biofuels could reduce net GHG emissions from transportation by displacing fossil carbon with biogenic carbon. Producing the biomass for biofuels, however, emits GHGs and other pollutants through fertilizer production, SOC loss, LUC, equipment activity and transportation. Even if biofuels yield net reductions in GHGs through displacement of fossil fuels, other air and water quality impacts mean that large scale adoption of biofuels may trade an energy and GHG problem for an environmental quality one.

Several main research questions guided the research contained in this dissertation.

- Are cellulosic, or second generation, biofuels likely to offer GHG reductions compared to the petroleum fuels and/or first generation biofuels they seek to displace on a life-cycle basis?
- What phases of the biofuel life cycle contribute the greatest amount of GHG emissions?
- What phases of the biofuel life cycle most contribute to other categories of environmental impacts?
- How do different impact categories (e.g. air pollutants, GHGs, water quality) trade off against each other in the biofuel production system?
- How should biofuel production systems be developed to minimize environmental harm?

The broader goal of this dissertation is to contribute to policymakers' understanding of some of the tradeoffs associated with biofuel production, so that policies more accurately anticipate their real impacts. There is simply too much uncertainty in the system for conclusive answers to be produced here, but this dissertation will reduce the uncertainty in several areas, notably the effect of different allocation methods on LCA of biofuels, the relative effect of different production parameters on the net GHG footprint, the expected changes in SOC from corn stover harvest and interactions between existing air quality policy and biofuel system development.

1.3 Structure of this Dissertation

This dissertation consists of four chapters, each of which represents a paper that examines the life-cycle impacts of biofuel production systems. As research progressed during early phases of the project, the relative importance of certain impact categories or phases of production became apparent, as did the uncertainty in particular processes or stages. These findings guided the selection of chapter topics

The first paper, Chapter 3, entitled "Life Cycle Inventory Development for Corn and Stover Production Systems under Different Allocation Methods" evaluates the effect of allocation methods on the life cycle inventory (LCI) of corn grain and stover. This paper contributes detailed life cycle inventories (LCIs) of corn grain and stover, and provides insight on allocation for residual feedstocks. One goal of this paper is to improve understanding of the uncertainty within LCAs of biofuel production systems, by describing the range of outcomes possible from decisions on allocation methods and simplifying the process of translating LCIs made under one set of allocation assumptions into a different set.

The second paper, Chapter 4, entitled "Aggregated Analysis of Soil Organic Carbon Changes Resulting from Corn Stover Harvest" reviews literature and data on soil carbon changes from stover collection. As the LCA model documented in Chapter 5 was being developed, it became apparent that soil carbon changes are extremely uncertain, and important, for determining the life-cycle GHG footprint of the biofuels studied in this dissertation, in particular, corn stover. Accordingly, this paper is a meta-analysis of existing literature that seeks to quantify some of the key relationships between SOC change and agronomic factors, clay content in soil, stover removal rate, fertilization, tillage practices, etc. The results of this research help determine whether stover-based biofuels have the potential to reduce GHGs when used as transportation fuel.

The third paper, Chapter 5, entitled “Life Cycle Inventory Development for Biochemical Cellulosic Ethanol Production Under Several Scenarios”, describes the development of an LCA of biochemical cellulosic ethanol production system. In particular, it analyzes a novel low-input system under development by EdeniQ, Inc. This paper is framed as the development of a LCI of cellulosic ethanol, since the untransformed inventory of environmental flows, rather than the impact of those flows are reported. This paper contextualizes the importance of allocation methodology, discussed in Chapter 2, and soil carbon changes, discussed in Chapter 3, into the full cellulosic ethanol biofuel life cycle.

The final paper, Chapter 6, entitled “Effects of Air Pollution Control Costs on National Biofuel Industry Development,” combines spatially explicit modeling of biofuel industry development based on technoeconomic modeling, with spatial data on air quality to examine the interaction of the U.S. Clean Air Act and biofuel industry development costs. Energy policy is typically modeled on large, often nation-wide scales; whereas the health effects of pollutant emissions are largely dependent on conditions in the location where they are emitted. At present, few models attempt to explore the interactions between these two domains and so, overlook parameters which could affect biofuel production, such as air quality regulations. In the U.S., the Clean Air Act functionally limits the locations where air pollutant emission sources can locate; facilities can technically locate in polluted areas, but often cannot economically do so due to emission limits and cost of abatement. This policy has been described as an obstacle to large-scale biofuel development in the U.S. (Youngs, 2011), since the cost of obtaining permits for novel technology can be substantial. No independent research has tested whether air pollution regulations are, in fact, obstacles to biofuel industry development. Chapter 6 hopes to inform this discussion by adding consideration of air pollutants to a spatial predictive model of biofuel conversion facility locations, using the cost of air pollution control devices and nitrogen oxides (NO_x) offsets as its mechanism. This paper demonstrates a method by which some environmental considerations can be added to existing technoeconomic models and also helps answer questions about the effects of U.S. air quality policy on the ability of a biofuel industry to meet RFS targets.

Chapter 2: Background

2.1 Feedstock

Ethanol production worldwide has been dominated by pathways that use starch or sugar as feedstock. This allows easy fermentation using well-known processes, but causes competition between food and fuel for limited supplies of agricultural products (Carriquiry et al., 2009; Hattori & Morita, 2010). In some places, such as Latin America, this has disrupted agricultural markets, leading to price rises and malnutrition (Food and Agriculture Organization, 2012; Wise, 2012). Converting land to agricultural uses typically causes significant emissions of carbon dioxide (CO_2) from disturbed soils, as well as the loss of any biomass carbon from the land prior to conversion, which contributes to climate change. These LUC effects can be of sufficient magnitude to outweigh the theoretical benefits of biofuels (Searchinger et al., 2008).

While corn continues to supply the overwhelming majority of U.S. ethanol production (Office of Transportation and Air Quality, 2011), there has been an effort by both researchers and policymakers to find alternative biomass feedstocks and shift to second-generation conversion pathways. The dominant biofuel policy in the U.S., the Revised Renewable Fuel Standard (RFS2), defines a set of characteristics which classify a biofuel as "renewable," including using non-fossil organic matter as feedstock, minimizing potential competition against food crops and direct LUC and life-cycle GHG targets (Office of Transportation and Air Quality, 2010; U.S. EPA, 2010; U.S. House of Representatives, 2007). RFS2 also caps the amount of corn ethanol that can qualify as a renewable fuel and creates life-cycle performance targets for second generation biofuels. While the biofuel industry has not yet been able to meet the second-generation biofuel targets laid out in RFS2, this policy defines the landscape in the U.S. biofuel sector. RFS2 requirements, along with economic and technical characteristic s of the conversion processes dictate that preferred feedstocks for sustainable biofuel production share three primary characteristics (Alvira, Tomás-Pejó, Ballesteros, & Negro, 2010; Gallagher et al., 2011; Hill et al., 2009; Parish et al., 2013; U.S. EPA, 2010):

- They must be able to be produced in large quantities at low cost.
- They must be compatible with likely cellulosic ethanol production technologies
- Their production should minimize environmental harms.

Since few systems have yet been developed to supply biomass on the scale required for commercial biofuel production, such as that mandated by the RFS2, current research of these production systems is largely based on modeling (e.g. Hess *et al.* 2009; Ebadian *et al.* 2012). Several possible feedstocks have been identified which may meet the criteria required for biofuel production, however substantial uncertainty remains. Predicted costs to supply biomass are often higher than that which is believed to be economically viable for large scale production (National Research Council, 2011). Several promising feedstocks, such as palm kernel oil, turned out to have higher environmental impacts than anticipated (Cherubini & Strømman, 2011).

2.1.1 Agricultural Residues

Most agricultural activity produces a substantial amount of residue: non-saleable fractions of seasonal or annual crops, pruning or removal of perennial ones, hulls, spoilage, etc. Residues typically have little economic value and are considered a byproduct or waste. For seasonal grassy crops, such as corn, rice or wheat, straw residue is typically left on the field and plowed under or burned in place. When removed from the field, this material has historically been disposed of in the same manner as other organic waste, often by open pile burning or landfilling. A small amount of it is used as feedstock for controlled combustion with energy recovery, such as electricity or heat generation. Alternatively, some residues have been used for animal feed, animal bedding, compost or mulch; however, this is generally a small fraction of total agricultural residue in the U.S.

This lack of competitive uses gives agricultural residues potentially favorable economic characteristics since biofuel producers would not have to compete against other users for much of this material. Because residues are routinely produced during food crop cultivation, they would not compete against food crops for land (Cherubini & Strømman, 2011). There is evidence, however, that large-scale residue removal, particularly in the case of straws from cereal crops, might lead to reduced soil quality, including soil carbon losses (Lal, 2006; Lemke, VandenBygaart, Campbell, Lafond, & Grant, 2010). The low value of residues also means that residues can be subject to supply uncertainty due to changing market conditions or producer behavior for the primary crop.

Corn stover is the above-ground biomass of the corn plant, excluding grain. Corn stover deserves special attention as a biofuel feedstock for several reasons. The U.S. produces a large amount of corn stover, estimated at almost 200 Million Mg per year, though not all of this resource can be sustainably or economically collected (Graham, Nelson, Sheehan, Perlack, & Wright, 2007). At present, almost all corn stover is left on the field and eventually reincorporated to the soil, around 2% is harvested as silage, a moist, fermented animal feed (U.S. EPA, 2013a) and another small amount is grazed by cattle or used for other purposes. The lack of demand for corn stover implies lower costs as a biofuel feedstock, compared to a material which is in demand for multiple uses, and also minimizes the potential iLUC impacts, since stover used for biofuels would not need to be replaced by alternative types of biomass. Corn producers are interested in using stover for feedstock since it increases the per-acre revenue of their crop, though the expected price of stover is likely to be a small fraction of the price received for grain grown on the same acreage (see Chapter 3 for a longer discussion of this topic).

At present most corn stover is left on the field, to return nutrients to the soil and improve tilth. In routinely tilled fields, it is typically shredded and plowed under. Under reduced tillage, some part of it is left on top of the soil as mulch. At present, about 25% of U.S. corn acreage operates under no-till practices; this is often done to reduce erosion and maintain water retention capacity. Only 15% of current corn acreage is irrigated, most is grown in the "corn belt" where average precipitation is sufficient for high yields, though recent droughts have raised concerns about future water supplies (U.S. Department of Agriculture, 2009).

Corn stover harvest typically requires one or more additional passes across the corn acreage by agricultural machinery, one to mow the stover and arrange it in windrows, then, after a suitable drying time, another pass to gather it into bales (Shinners, Bennett, & Hoffman, 2012). More equipment activity is often required to collect the bales from the field and transport them to near-field storage locations, where they await pickup. In addition to substantial operating costs, additional agricultural equipment activity can compact soil and impair future water infiltration. Weather conditions may also interfere with stover harvest. A transition to single-pass harvesting, in which grain and stover are collected simultaneously, will likely improve the economics and reduce energy intensity of large-scale stover collection (Shinners et al., 2012).

Empirical studies of corn production with stover harvest generally find reductions in SOC, compared to corn production without stover harvest (Anderson-Teixeira et al., 2009; Guzman, 2013; Hooker, Morris, Peters, & Cardon, 2005; D. L. Karlen, Birell, & Hess, 2011; D. L. L. Karlen et al., 1994). Soil microbial activity and erosion reduce levels of soil carbon, while plant growth tends to increase them through root expansion and fallen litter (leaves, branches, etc.). Over long periods of time, these pools tend to come into equilibrium in which the flows into soil carbon equal the flows out (Anderson-Teixeira et al., 2013; Gollany et al., 2010; Sarkhot, Grunwald, Ge, & Morgan, 2012). Changes to soil, from changes in agricultural practices for example, tend to upset the equilibrium and result in changes in SOC. When stover or other biomass is routinely removed from agricultural soils where it was previously left in place, there is a reduction in the carbon flows into SOC pools, usually without a corresponding reduction in flows out of the same pools. The flow rate of carbon out of SOC pools depends on several factors, including SOC levels; soils with high levels of SOC tend to lose SOC more quickly (Anderson-Teixeira et al., 2013). This implies that sustained biomass removal is likely to lead to reductions in SOC until a new equilibrium is reached, a conclusion that is generally, but not universally seen in reviews of empirical studies (Anderson-Teixeira et al., 2009; Lemke et al., 2010). Furthermore, modeling studies often predict less soil carbon loss than empirical ones (Meki et al., 2011; W. Smith & Grant, 2012).

Fertilization also contributes to the environmental impacts of corn stover production. There are a wide range of fertilization regimes, depending on local soil, climate and economic conditions; producers are generally advised to test their soil's baseline nutrient levels and tailor fertilizer applications to match plant needs (Sawyer & Mallarino, 2007; Wortmann & Klein, 2008). The impacts of fertilizer use on fields include both on-field, upstream and downstream components. On-field impacts primarily focus on volatilization of N_2O and NO_x. There is substantial uncertainty regarding the magnitude of these impacts, though several estimates are available in literature (Brentrup, Küsters, Lammel, & Kuhlmann, 2000; Dufossé, Gabrielle, Drouet, & Bessou, 2013; Hoben, Gehl, Millar, Grace, & Robertson, 2011; IPCC, 2007; Linquist, Groenigen, Adviento-Borbe, Pittelkow, & Kessel, 2012; Powers, 2005).

Upstream impacts are largely focused on the production of petrochemical fertilizers, which requires substantial energy; this energy is typically provided from fossil fuels. Non-petrochemical fertilizer, such as manure or compost is available, but requires more energy-intensive transport and application methods than concentrated liquid petrochemicals. Most common fertilizer compounds have available LCIs in commercial databases, such as GaBi (PE International & LBP, 2008) or Ecoinvent (Ecoinvent Centre, 2011), though these data are often outdated and may not reflect production practices in a given study area. For example, Ecoinvent has a fairly complete database of agricultural chemicals, but the constituent LCIs are almost entirely based off a European study from 1986. There will almost certainly be differences between the production and distribution patterns in that study and current production systems in the U.S. due to technological advancement and changes in supply chains (Ingram et al., n.d.; Lieberman, 1984). Still, this dataset represents one of the only comprehensive compilations of such data available to researchers.

Downstream effects are primarily eutrophication and eco-toxicity of fertilizer compounds which volatilize or leach to surface and ground water. These effects are often mediated by secondary reactions in the air or water and can be complicated to model (Delucchi, 2010; Hill et al., 2009; C. Murphy, 2008; Powers, 2005; Schnoor et al., 2008; Tsao et al., 2012; Wagstrom & Hill, 2012). This dissertation will generally not address exposure and ecological or health impacts, though many of the LCIs generated as a result of the work described herein are directly relevant for future studies on the subject of downstream impacts.

The other critical factor affecting corn stover's environmental impacts is post-harvest processing. At present, corn stover is generally baled and stored in outdoor stacks, sometimes with a tarp or plastic wrapping (Shinners & Binversie, 2007; Sokhansanj, Turhollow, & Perlack, 2008). This has relatively low costs and uses readily available technology, but subjects stover to degradation from exposure to weather and often requires transport at below-optimal bulk densities (Hess et al., 2009a). Several methods of addressing the issues of storage stability and efficient transport have been proposed, including pelletization, torrefaction or conversion to pyrolysis oil. The energy requirements for most of these processes are substantial and uncertain (Kaliyan & Morey, 2010; Mani, Tabil, & Sokhansanj, 2006; Mani, 2005; Morey, 2012). The Idaho National Laboratory developed a model for commodity-scale uniform feedstock processing, which uses technologies that are likely to be energy-efficient in the near term while also allowing the benefit of feedstock tradability across production systems (Hess et al., 2009a; Searcy & Hess, 2010). This Uniform feedstock model is the basis for biomass processing in this dissertation.

While corn stover has been a main focus of biofuel researchers in the U.S., many other agricultural residues have been evaluated as well. Other cereal crops, such as wheat or sorghum, have been evaluated as biofuel feedstocks since they, like stover, are produced in large volumes but are generally not in great demand at present. A particularly notable study of wheat straw was conducted by Ebadian, *et al.* (2012), in which feedstock production was modeled under uncertainty from multiple sources, including weather, yield, markets and equipment failure. This sort of modeling addresses many of the critical areas of uncertainty that affect every agricultural system. The papers presented in this dissertation do not utilize stochastic uncertainty to the same degree as Ebadian *et al.*'s work but do address uncertainty through scenario analysis. Most cereal straws are subject to many of the same considerations that affect corn stover, including the need for fertilization, harvest and post-processing and potential SOC loss.

Orchard waste is also thought to be a promising feedstock for biofuel and bioenergy systems; however, the physical and chemical characteristics of wood are generally considered to be better matched for thermochemical conversion than biochemical (Dutta et al., 2011; French, Hrdlicka, & Baldwin, 2010; Phillips, Aden, Jechura, Dayton, & Eggeman, 2007; Shah et al., 2012). This dissertation only examines- biochemical conversion pathways, and thus does not study wood feedstocks.

2.1.2 Purpose-Grown Energy Crops

In addition to agricultural residue, purpose-grown crops have been studied as possible feedstocks for biofuel production. In order to avoid iLUC concerns, many proposed biofuel production systems grow energy crops on degraded or marginal land which is not suitable for food production (Gopalakrishnan et al., 2009; Hattori & Morita, 2010). Three main classes of crops have been identified:

oilseeds, grasses and purpose-grown trees. Only grasses are discussed in this dissertation in depth, though the modeling in Chapter 6 includes some non-grassy crops.

Several warm-season native grasses have been proposed as possible biomass feedstocks, including switchgrass (*panicum virgatum,* far right in Figure 2-1*)*, elephant grass (*miscanthus giganteus,* commonly known as miscanthus) and big bluestem (*andropogon gerardii* sixth from right in Figure 2-1). While agricultural practices have historically been optimized for monoculture, recent evidence indicates that mixtures of these grasses may produce better yields and reduced fertilizer demands, possibly due to the presence of nitrogen-fixing rhizomicrobes in some species (Jasinskas, Zaltauskas, & Kryzeviciene, 2008; Tilman, Hill, & Lehman, 2006). These grasses share many common characteristics, but like all crops, produce optimal yields when specific species or cultivars are selected to match local conditions. Chapter 5 will discuss the characteristics of switchgrass as a biomass feedstock; many of the conclusions are applicable to other warm-season grasses as well, however specific research is required to confirm this.

Warm-season grasses can grow without fertilization, but this may not produce sufficient yields for economical biofuel production. In most soils, N is the limiting factor for high yields and switchgrass typically displays a positive response to increasing N applications (Jung & Lal, 2011). This response is not always linear and depends on a variety of other climate and soil factors; further research is required to consistently determine the optimal level of fertilization. Switchgrass can be harvested with existing forage harvest equipment and, like corn, typically requires multiple passes and a period of field-drying to produce stable bales (Brechbill & Tyner, 2008). This can subject yields to uncertainty based on weather, in addition to the inherent yield uncertainty of agriculture. Warm-season grasses are typically grown in 8-15 year rotations, with a year or two of establishment during which little or no biomass is harvested, then several years of maturity with harvests once or twice per year which harvest the above-ground biomass down to approximately 30cm stubble height.

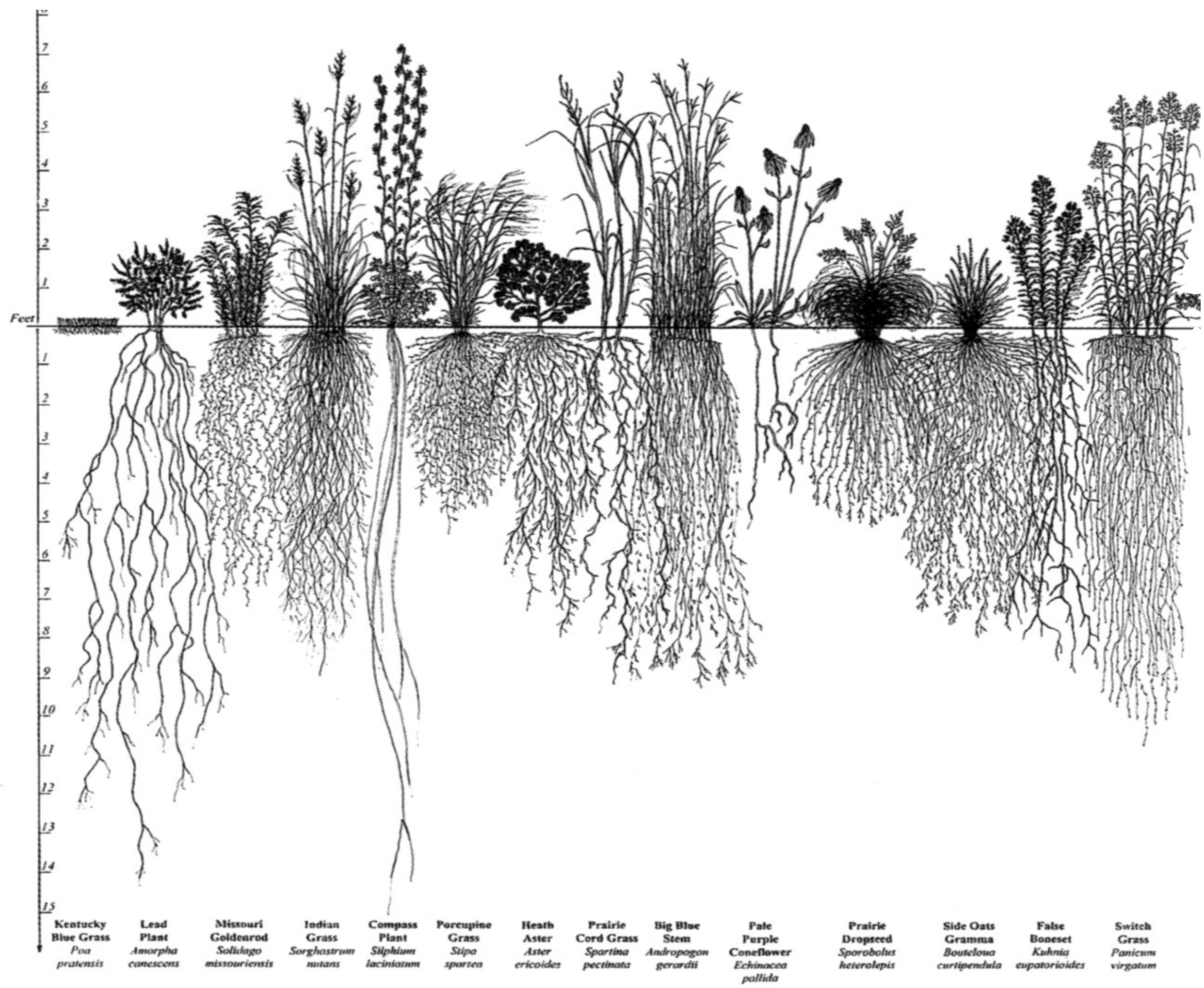


Figure 2-1 - Grasses are often considered for bioenergy crops. Deep root systems help minimize the need for irrigation and sequester carbon in soil. Source: Heidi Natura, Living Habitats, used with permission.

Warm-season grasses have another highly desirable characteristic as a biofuel feedstock: the ability to sequester substantial amounts of carbon in soil as root mass. Figure 2-1 shows the typical vertical profile of these plants; most develop root systems stretching more than 2 meters (6 feet) below ground at full maturity. The carbon which forms the structure of these roots is removed from the air and transported by the plant into the ground. Deep roots may durably sequester carbon even as above-ground biomass is harvested, though these effects depend strongly on local conditions (Liebig, Johnson, Hanson, & Frank, 2005; Monti, Barbanti, Zatta, & Zegada-Lizarazu, 2012). Some authors, notably Tilman, *et al.* (2006) conclude that the root carbon sequestration of grassy energy crops is sufficient to allow the production of carbon-negative biofuels. Tillman's conclusion is speculative and depends on high yields, substantial root carbon sequestration and very efficient conversion technology. Under more reasonable conditions, warm-season grasses may allow for durable carbon sequestration for many years, until a new carbon equilibrium is reached (Cherubini & Strømman, 2011). This effect can substantially decrease the life cycle carbon footprint of resulting biofuels.

2.2 Conversion Technologies

Ethanol is the dominant biofuel at present and is positioned to be the primary biofuel for light-duty vehicle (LDV) applications over the near term. Other liquid biofuels, such as butanol, dimethylether (DME), dimethylfuran (DMF) or "drop-in" hydrocarbons are under consideration by researchers, but the technologies and supply chains needed to produce these fuels at commercial scale is still immature. As ethanol is more widely adopted, researchers are also discovering some previously-unconsidered ancillary benefits, such as its high octane number which allows for engines to improve efficiency through higher compression ratios (Anderson et al., 2012). For the purposes of this dissertation, ethanol will be considered the end-point fuel. This is not an endorsement of ethanol as compared to other alternatives, but rather a reflection of the likely course of renewable fuel policy over the next 10 years. Additionally, the processes to produce other fuels are functionally similar to those for ethanol, so many of the key characteristics of ethanol production systems described in this dissertation would apply elsewhere.

There are two broad families of lignocellulosic biofuel conversion technology: thermochemical and biochemical. Thermochemical pathways use heat to partially decompose elements of biomass into liquid or gaseous intermediate products, which are then either combusted for direct energy recovery or converted into fuels or chemical precursors. Biochemical technologies use various methods of hydrolysis, including steam, strong acids or bases and rapid pressure shifts, to produce simple sugars that can be fermented by microbes. Ethanol is the most common end product from biochemical production pathways, largely because ethanol fermentation is well understood, having been used in the production of alcoholic beverages for most of human history.

Thermochemical pathways typically heat biomass in the absence of oxygen, which facilitates the degradation of some volatile carbohydrates and emits a liquid or gaseous hydrocarbon intermediate. The remnant after the emission of volatile components is a charcoal-like solid remnant called biochar. Thermochemical processes require substantial amounts of energy, which is usually obtained by combusting some of the produced gases or biochar. Gasification pathways have theoretical yields that are often predicted to be higher than biochemical ones (Dutta et al., 2011; Phillips et al., 2007), but the technology for synthesizing fuels from syngas has been difficult to scale to commercial size in biomass-fueled facilities.

Biochemical conversion involves breaking carbohydrate polymers, primarily cellulose and hemicellulose, into monomeric and dimeric sugars, which can be consumed by fermentation microbes which produce ethanol or another useable product. Commonly, biochemical conversion processes use strong acids or bases combined with high pressure and temperature to begin the conversion process by disrupting the cellular structure of plant material and partially hydrolyzing some carbohydrates (Andy Aden, 2008; Viikari, Vehmaanperä, & Koivula, 2012). Enzymatic hydrolysis, typically using externally applied cellulase enzymes results in the hydrolysis of most of the remaining cellulose and hemicelluloses. The resulting sugar solution is then fermented, commonly by strains of *zymomonas mobilis,* an ethanogenic yeast, to convert free sugars into ethanol. During this process, several byproducts of hydrolysis and fermentation can inhibit desired activity; managing conditions within reaction vessels to minimize the concentration of these inhibitors is key to achieving high yields (Ishola, Jahandideh, Haidarian, Brandberg, & Taherzadeh, 2013; Sánchez & Cardona, 2008). Most biochemical cellulosic conversion processes are thought to yield between 70 and 80 gallons of ethanol per dry ton (290 to 330 liters per tonne) of feedstock, though substantial uncertainty remains. Some systems claim much higher efficiencies; for example the process designed by ZeaChem, which uses acetogenic microbes for fermentation followed by high temperature catalytic conversion to fuels, claims to yield as much as 135 gallons per dry ton (560 liters per tonne) (ZeaChem, 2012).

Given the lack of empirical data from operational biochemical cellulosic ethanol plants, modeling of future biofuel scenarios should focus on comparatively well-understood technological pathways and make conservative assumptions, otherwise substantial uncertainty regarding technological parameters is added to the normal uncertainty of prospective models (Kazi, Fortman, Anex, & Kothandaraman, 2010). Accordingly, the baseline biochemical production model used in these studies is the one described in NREL's *Process Design and Economics for Biochemical Conversion of Lignocellulosic Biomass to Ethanol - Dilute-Acid Pretreatment and Enzymatic Hydrolysis of Corn Stover* (Humbird et al., 2011). This design has several advantages over other designs described in the literature. First, it is comprehensively and transparently described in publicly available literature. Second, it reflects the evolution of previous models developed at NREL (A Aden et al., 2002; Andy Aden & Foust, 2009; Wooley et al., 1999) and the projections of novel technologies. Third, it shares many commonalities with other likely commercial biochemical cellulosic ethanol pathways, including on-site manufacturing of enzymes, hydrolysis pre-treatment with separate fermentation and on-site power generation using process byproducts (lignin cake and biogas from wastewater treatment). The paper presented in Chapter 5 uses elements of a proprietary low-input conversion process, but even in this case, a substantial amount of the model was based on the NREL design due to the new technology still being in an early phase of development.

2.3 Previous Evaluations of Biofuels' Environmental Impact

As large scale production of ethanol from corn increased, along with concern regarding climate change, life cycle GHG emission (or carbon footprint) and energy balance became the primary focus of research (Farrell et al., 2006; von Blottnitz & Curran, 2007; M. Wang, Wu, & Huo, 2007). These papers generally concluded that corn-grain based ethanol had the potential to reduce GHG emissions from transportation (though most did not include LUC effects), but that cellulosic fuels were more promising. From the late 2000s to the present, the consensus in most published literature was that corn-grain based ethanol was an environmentally inferior option than cellulosic fuels, or sugar cane ethanol from areas where sugar cane grew efficiently, such as Brazil (Andress, Nguyen, & Das, 2011; CARB, 2012; Farrell, Sperling, et al., 2007; Hsu et al., 2010; Shapouri, Duffield, & Wang, 2002).

From the mid-2000s to the present, publications that considered the environmental impacts of cellulosic biofuels have typically focused on life-cycle energy balance and GHG emissions. Comparatively fewer papers have directly evaluated environmental impacts and indicators other than GHGs or energy, and particularly non-air pollution impacts. Powers (2005) produced a very detailed study of water-quality impacts from fertilizer runoff from corn production in Eastern Iowa, by creating a model of the processes involved and calibrating against water quality measurement data. Costello, *et al.* (Costello et al., 2009) also evaluate fertilizer run-off to surface water and conclude that switching from corn to cellulosic ethanol will reduce the eutrophication of the Mississippi river and Northern Gulf of Mexico, but do not model the likely growth of future biofuel production, which would likely see cellulosic ethanol supplementing, rather than replacing, existing corn grain production.

Several papers attempt to quantify the water usage of biofuel production (Andy Aden, 2007; Delucchi, 2010; Mishra & Yeh, 2011), though this impact is often examined in the context of production costs or capacity, rather than environmental harm.

Hill (2009) attempts to estimate the health costs of air quality degradation from biofuel production by using response-surface modeling based on a proposed spatial distribution of biofuel production activity. This study concluded that aggregate costs, from health and climate impacts, are significantly lower for cellulosic biofuels, but that the spatial distribution of air pollution would significantly change as a result, since cellulosic feedstocks (and presumably, the conversion facilities) are often located in areas with little pollution-causing industry at present.

While the literature on human and environmental health impacts of biofuels is somewhat sparse, there is a much deeper body for energy and GHG impacts. Accurate estimation of environmental impacts is complicated by substantial uncertainty in the technological and biological systems being studied, as well as a wide range of modeling and measurement assumptions that vary between studies (Guinee et al., 2002; Huijbregts et al., 2001; Mullins, Griffin, & Matthews, 2011; Venkatesh, Jaramillo, Griffin, & Matthews, 2011; Wardenaar et al., 2012; Zamagni, Guinée, Heijungs, Masoni, & Raggi, 2012). Extracting policy guidance from these uncertainties can be made somewhat easier by comparing prospective production pathways or scenarios against better-understood baselines. LCA is a very common methodological choice for this comparison. Table 2-1 shows a selection of studies with strong emphases on LCA and a comparison between a prospective pathway and a baseline fuel. In the course of the research for the papers described in this dissertation, many other studies of cellulosic biofuels were evaluated but omitted from this table due to lack of clear indicators, methodological assumptions or lack of a comparison against a baseline fuel (e.g. Fu *et al.* 2003; Kim & Dale 2005b; Sassner *et al.* 2008; Foust *et al.* 2009; Delucchi 2010).

Study	Feedstock	Indicators	Baseline?	Results	Notes
Pimentel & Patzek (2005)	SG, WR	Energy	Corn Ethanol	+	
Spatari, *et al.* (2005)	CS, SG	GHG, Air	Gasoline	+	
Malça & Freire (2006)	OR	Energy	None	+	Concludes that wheat straw ethanol has positive energy balance
Wu, *et al.* (2006)	SG, OR, WR	GHG, Energy	Gasoline	+	
Aden (Andy Aden, 2007)	CS	Water	Corn Ethanol	|	
Granda, *et al.* (2007)	FW	Energy, GHG, Air	Gasoline, Corn Ethanol	+	
Kalogo, *et al.* (Kalogo, Habibi, MacLean, & Joshi, 2007)	MSW	Energy, GHG, Air	Gasoline, Corn Ethanol	|	Found MSW ethanol superior to gasoline but inferior to landfill with LFG recovery.
Pimentel & Patzek (2008)	SG, WR	Energy	Corn Ethanol	-	
Aden & Heath (2009)	CS, SG, WR	GHG, Air, Water	Corn Ethanol	+	Comparison is primarily for feedstock production
Luo, *et al.* (2009)	CS	Many	Gasoline	+	
Hsu, *et al.* (2010)	CS, SG, OR	GHG, Energy	Gasoline, Corn Ethanol	+	Includes uncertainty through Monte Carlo Simulation
Kusiima & Powers (2010)	CS, SG, WR	GHG, Air, Water, Erosion, Toxicity	Corn Ethanol	+	Includes uncertainty through Monte Carlo Simulation
Hoefnagels , *et al.* (2010)	SG, FW	GHG, Energy	Gasoline, Diesel, Corn Ethanol	+	
Irribaren, *et al.* (2012)	FW	GHG, Energy, Air, Water, Land-Use	None	|	
Kendall & Yuan (2013)	CS, SG	GHG	Sugarcane Ethanol	-	Compared recent studies with varying modeling assumptions
Maleche, *et al.* (2013)	CS, WR, OR	GHG, Energy	Gasoline, Diesel	+	

Table 2-1 - Comparison of Studies that Evaluate Cellulosic Biofuels' Energy or GHG Balance and Compare Against a Baseline Fuel. Feedstocks Abbreviations: CS = Corn Stover, SG = Switchgrass, OR= Other Agricultural Residue, FW = Farmed Wood, WR = Wood Residue, MSW = Municipal Solid Waste. Results: + : Indicates cellulosic biofuel superior to baseline, -: Indicates cellulosic biofuel inferior to baseline, | : Indicates unclear or indeterminate comparison.

In addition to the papers discussed above, there are several published review articles on the subject, which confirm the general conclusion and do a great deal to provide both depth and context to the field. Many reviews find a general consensus that cellulosic biofuels have the potential to reduce life-cycle GHG emissions substantially, when compared to petroleum-based fuels, though the magnitude of this effect is still quite uncertain (Borrion, McManus, & Hammond, 2012; von Blottnitz & Curran, 2007). Similarly, review papers have demonstrated that most studies of cellulosic ethanol predict a net positive energy balance (Hammerschlag, 2006).

Many reviews find reduced environmental impacts, according to most indicators, for cellulosic biofuels compared to gasoline, though several studies have reported significantly higher acidification and eutrophication potentials, due largely to the effect of fertilizers when applied to agricultural fields (Kim, Dale, & Jenkins, 2009; Powers, 2005).

Taken as a whole, the body of literature on cellulosic biofuels tells a fairly consistent story. There are a wide range of technological pathways and feedstocks that show promise for the production of cellulosic biofuels. Many of these pathways have the potential to produce fuel with a net positive energy balance and fewer GHG emissions than a comparable amount of gasoline. Distinguishing between these pathways and feedstocks is difficult, in large part because only one commercial-scale conversion facility has been built, and it closed as soon as its external funding source ran out (Chapman, 2012; Range Fuels Inc., 2007). Without empirical data, all LCAs must use models to predict future environmental impact, which adds uncertainty.

Current models predict that cellulosic biofuels have the potential to substantially reduce GHG emissions compared to petroleum-based fuels, though the magnitude of this reduction is uncertain. Many models foresee feasible reductions in life-cycle GHG intensity on the order of 50%, with similar reductions in fossil energy consumption. Cellulosic biofuels are likely to be superior on most other environmental indicators, except those strongly affected by the use of fertilizers during biomass cultivation, such as eutrophication potential and acidification potential. In order to achieve favorable GHG balances, it is imperative that the facilities power themselves by utilizing process byproducts; importing fossil energy or grid electricity quickly overwhelms the benefit of any resulting fuels. The impacts of feedstock production are the other common area of major GHG emission. Conversely, transportation and facility construction are generally found to be minor factors in determining life cycle GHG impact.

2.4 Policy Landscape

In the U.S. and Europe, biofuels have never been sufficiently cost-competitive to enter the market without substantial impetus from policy; this trend is almost certain to continue for the foreseeable future (Tao & Aden, 2009). In the U.S., the dominant biofuel policy is the RFS2, which mandates certain amounts of biofuels enter the market according to a schedule. This is coupled with a set of subsidies for fuel producers along with loan programs to ease the burden of capital costs (National Research Council, 2011; Office of Transportation and Air Quality, 2011). Revisions to the renewable fuel standard have capped the quantity of corn ethanol that can qualify for the favorable "renewable fuel" designation and shifted emphasis to advanced or cellulosic biofuels. No commercial-scale manufacturing capacity has yet emerged to produce a sufficient volume of advanced or cellulosic fuels to meet these targets (Bracmort, 2012), a state that is likely to continue for the next several years at least; this has caused the U.S. EPA to substantially reduce the biofuel targets in every year they have ostensibly been binding. RFS2 volumetric targets are often the default value used in large-scale modeling studies (Parker, Hart, et al., 2010), despite the growing realization that they are unlikely to be met for several years, at least.

California has taken the lead in GHG policies by implementing a Low-Carbon Fuel Standard (LCFS). This policy evaluates fuels sold in the state based on their life-cycle GHG impacts and proscribes a reduction in the sales weighted average GHG intensity over time. By targeting the carbon intensity of a sales weighted average, rather than implementing a volumetric target, net GHG reduction targets can be met in the most cost efficient manner and also will reward innovative producers for bringing very low-carbon fuels to market (Farrell, Sperling, et al., 2007). California's LCFS policy has been credited with modestly reducing GHG emissions over the time it has been in place, though there is still concern about trans-boundary effects such as "fuel shuffling," in which identical fuels are traded between markets to obtain the benefit of low carbon values in California (Yeh, Witcover, & Kessler, 2013). Similar policies are starting to be adopted in other regions and there is movement towards standardization across regions. LCFS policies serve as an incentive for advanced, highly efficient biofuel makers, since very low-GHG fuels enjoy an economic benefit when they are brought to market.

While biofuel policy is a relatively recent development, air quality policies have been well developed for decades now. In the U.S., the Clean Air Act is the dominant regulation to protect air quality. While it does not directly affect biofuel production, it has a significant indirect impact, by limiting the potential locations and technologies available to a conversion facility (Sheehan et al., 2003). Regulatory authority for air-quality decisions derives from the Federal Clean Air Act, but most air-quality policy decisions are actually made at the local level, through the air pollutant emission permitting process. Specific requirements for permits vary by region, since each air district is allowed some discretion in setting its own policies. Ethanol conversion facilities generally emit pollutants from their power generation systems, which combust process byproducts. Combustion of solid, wet, heterogeneous biomass, such as that which would occur at biofuel conversion facilities, can be relatively dirty, but several types of emissions control technologies are available to reduce these (U.S. EPA, 2002, 2003, 2007). The study of air pollutant emissions from cellulosic ethanol production is still relatively new. Table 2-1 gives an overview of some of the papers which consider air pollutants, though they are the primary focus of only a select few. Jones (2010) predicts the pollutant emissions of several proposed cellulosic ethanol facilities and Hill, *et al.* (2009) quantify the health costs of these emissions. The literature tends to indicate that air pollutant emissions from cellulosic ethanol production, across the full scope and life cycle of the biofuel system, are unlikely to be worse than those of gasoline and potentially superior. The greatest risk of harm comes from increased fertilizer production and use from biomass production activity.

Chapter 3: Life Cycle Inventory Development for Corn and Stover Production Systems Under Different Allocation Methods

3.1 Introduction

Biofuels may offer an opportunity to reduce fossil fuel consumption and greenhouse gas (GHG) emissions from the transportation sector. To compare the performance of biofuels against conventional fossil fuels, their environmental impacts must be evaluated from a life cycle perspective. Production of biomass for biofuel feedstock can contribute a significant fraction of total environmental and energy impacts from the biofuel life cycle. Using agricultural residues as biofuel feedstock may avoid many of the unintended consequences of purpose-grown energy crops (Johansson & Azar, 2007), as discussed in Chapter 2.

This study defines agricultural residues as the non-saleable parts of a plant left over after harvest; animal waste or byproducts can also be considered a residue but they are not considered in this study. For corn, the above-ground biomass, other than grain (cob, husk, stem and leaves) are residue, commonly known as corn stover. Corn stover is a promising source of biomass for biofuel or bioproduct processes, since it is grown in large quantities during corn production and does not directly compete against food crops for land; there may be indirect competition as stover harvest affects the over-all economic conditions for growers, but the trade-off is mediated through agricultural markets. This will be discussed later in this chapter. The U.S. produces well over 300 million tonnes of corn per year (U.S. Grains Council, 2013), and stover is produced at approximately a 1:1 ratio to corn on a dry-mass basis.

Cereal crop residues, such as corn stover, are either unused at present, or used in very low-value applications such as animal bedding or plowed under to maintain soil condition. This is important since if there was a competing use for stover, diverting for use as a biofuel feedstock could lead to unintended consequence, such as spurring demand for a purpose grown crop. At present, most cereal straw, including over 95% of corn stover is plowed back into the soil. This yields no direct revenue for the former, but may increase or maintain soil fertility, which can improve future yields. Incorporating corn stover into soil can also help maintain soil organic carbon (SOC) levels, which affects net carbon balance in the atmosphere and thereby, climate change. With little economic or nutritional value being generated by these residues, using some fraction of them for biofuel production would not require replacement by another crop and therefore, would not contribute to iLUC.

In the current corn production system, stover is rarely harvested, but when harvested, it becomes a co-product of the corn production system. In life cycle assessments (LCAs) of cultivation systems that produce multiple products, or co-products, by rotating crops or processing multiple parts of a plant for different uses, the whole system's impacts are typically allocated among all co-products (van Zeijts, Leneman, & Wegener Sleeswijk, 1999). This need for allocation is not limited to cropping systems or agricultural products; in LCAs of any system that generates multiple products or services, some method for attributing environmental impacts to each co-product is required. Harvesting stover causes environmental impacts from additional fertilization, equipment activity and changes to soil biogeochemistry. These impacts must be assigned to stover, which necessitates some sort of attribution.

In this study, the term *allocation* is used to describe all processes and methods that might be used to divide or otherwise attribute environmental impacts to a single co-product. This usage is broader than its official use in LCA (such as its definition in the ISO 14040 standards) because, strictly speaking, allocation refers to division of the total environmental impacts between products in proportion to some value (economic, energetic, etc.). However, allocation has, in much of current LCA literature, come to mean any method of attributing impacts between co-products; this study will adopt this usage even though it may not be correct in the strictest possible sense. Defining allocation in this more expansive form includes other common methods for treating co-products in LCA, such as subdivision and system expansion, which are actually approaches that avoid allocation.

Not surprisingly, allocation methodology can significantly affect the life cycle environmental impacts attributed to stover-derived products (Hsu et al., 2010). This chapter describes three different approaches, economic allocation, energy allocation and system expansion, to allocating impacts from the corn and stover production system to stover alone, and produces life-cycle inventories (LCIs) for the production of corn stover. The results of applying the three approaches are compared to evaluate their effect on the performance of corn stover as a biomass resource. This comparison helps characterize the variability introduced by the selection of a particular method for co-product treatment in LCA. In addition, this study creates LCIs for corn grain and stover production under different allocation approaches, which are available in the online supplemental material for the article.

3.2 Literature Review

Biofuel and bioenergy systems are extremely complex; accurate assessment of environmental impacts is recognized as a challenge by a wide range of researchers (Luo et al., 2009). Several authors in the body of existing LCA literature have begun to address this issue in conceptual terms (Guinee et al., 2002; Wardenaar et al., 2012; Weidema, 2008). The International Standards Organization (ISO) promulgated the most widely acknowledged guidelines for LCA, the ISO 14040 and 14044 standards, which dictate a preference for avoiding allocation by subdivision or system expansion when assessing systems that produce co-products (ISO, 2006a, 2006b). If allocation is required, because subdivision and system expansion are not possible, then value-based allocation of environmental flows using a physical basis such as energy content or mass is preferred. As a last resort, economic allocation may be used. Rather than using system expansion or subdivision, some LCA researchers have indicated alternative hierarchies to ISO for selecting methods for handling co-products, including designating system expansion as an allocation process, rather than as a process for avoiding allocation, and preferring economic allocation over other allocation approaches (Ekvall & Finnveden, 2001).

Ekvall and Finnveden discuss several allocation methodologies and conclude that the method should reflect a real-world causal relationship underpinning the system under study (Ekvall & Finnveden, 2001). Linking to a causal relationship helps improve a LCA's ability to answer relevant policy questions; the same values which shape the actual design of a system also shape the analysis of the system. If a system is designed to produce profit, then environmental impacts are assigned proportionately to economic value. In biofuel systems, energy could be preferred as a physical basis for allocation because energy production is the system's primary product. However, since corn and stover may be used for different energy purposes - corn grain for nutritional calories and stover for thermal energy - a direct comparison based on energy may not be reasonable. In market economies, economic value may be even more important in shaping the formation of systems. However, because prices for any given product change, economic allocation can lead to temporal variability in the outcome of a study even when the production system remains unchanged. Despite the limitations of these two value-based allocation approaches, both are examined in this chapter. Mass-based allocation for the corn production system is not considered. The economic and energy value for corn and stover is not strongly tied to their relative mass; a cultivated hectare typically produces an equal or greater mass of stover than corn, yet the energy content and economic value of the grain is typically much higher (Table 3).

One of the techniques to address allocation issues, system expansion, brings all of the co-products of a system within the system boundaries of the LCA. This method may be preferred when there is an alternative case against which to compare the modeled system. For example, in near-term stover production, assigning stover the impacts of additional or changed activities that take place only when stover is harvested , but not those in which stover is left on the field is one way to divide the activities between those done for corn grain and those done for stover. In this case there is a clear counterfactual based on a well-described *status quo*. However, as farmers acclimate to a system in which stover is routinely harvested and used for biofuel production, their practices will likely change to reflect the new economic and agronomic reality. At present, farmers make decisions regarding the specific cultivar of plant, fertilization, irrigation and harvest scheduling based on a wide range of factors designed to maximize returns while minimizing risk; this functions as a multi-attribute decision-making problem (MADM) (Romero & Rehman, 1987). For example, farmers must balance the desire to meet short term financial obligations, achieve long term financial goals, sustain the biogeochemical system upon which their success depends and minimize risk from both market and natural forces. In addition, they have personal goals and desires, which may not be effectively captured by analyses that solely evaluate economic costs. These various goals and attributes must be balanced against each other in a risk-weighted fashion. MADM problems create uncertainty in the assignment of responsibility to individual factors, since many factors are at play and often in complex, non-transparent ways. Assignment of responsibility for environmental impacts within a LCA framework is therefore complicated because the causal relationships, upon which allocation assumptions should be based, are difficult to define.

LCAs that evaluate multi-function systems must make certain assumptions regarding allocation. These assumptions may strongly affect the results of these studies. These practitioner decisions can lead to differences among studies and can lead to confusion during interpretation. To address this, the modeling in this chapter attempts to transparently report the allocation assumptions and methods, and describe their effect on the LCI for stover.

Previous research on corn stover for use as a bioenergy resource has largely adopted approaches that reflect a consequential LCA perspective (Guinee et al., 2002; Spatari et al., 2005). In other words, the researchers assume a business-as-usual production system where stover is left unharvested, and then assign only the additional processes required by stover harvest, such as stover collection activities and extra nutrient requirements. This consequential approach essentially describes a subdivision method. Though recent scholarly literature seems to view consideration of market-mediated effects as a necessary element of consequential LCA (Earles & Halog, 2011), the approach of only considering the additional processes required for generating a new co-product from an existing system clearly takes a consequential approach. This study does not consider market mediated effects; however, the subdivision case described here models changes to an existing system, the basic concept underlying consequential LCA.

Analyses in the transportation fuel sector have typically focused on allocation of impacts between the multiple products of a petroleum refinery (M. Wang et al., 2004) or corn ethanol (K. Edwards & Anex, 2009; Kendall & Chang, 2009). The body of literature on the subject of allocation within grain and straw or stover production systems is comparatively smaller. With few exceptions (e.g. (Cherubini, Strømman, & Ulgiati, 2011; Spatari et al., 2005)), existing LCAs of corn stover ethanol select one allocation approach, and do not compare different approaches. Of these studies, the majority have considered stover production from existing corn fields and have used nutrient replacement methods to attribute environmental impacts to stover (Spatari et al., 2005).

While most studies simply assume the nitrogen (N), phosphorus (P), and potassium (K) nutrients removed in stover must be replaced, Van Zeijts, *et al.*, expand on this simple nutrient replacement approach, and assign nutrient burden based on nutrient uptake by successive generations of plants on a field instead of the amount of fertilizer placed on a given crop (van Zeijts et al., 1999). This method requires data about soil conditions and microbial activity. When the necessary data are available, this approach may be preferable, but it is impractical when production systems are aggregated over large areas, due to differences in cultivation practices, climate, biogeography and soil type. Because this study attempts to develop LCIs based on national average conditions, the nutrient uptake approach is not considered.

Current LCA literature on biofuels often simplifies the feedstock production phase or uses values from literature. Comparatively fewer comprehensive LCI's exist for feedstock on its own. Among them Adler, *et al.* (2007) and Kim and Dale (2009) stand out. Both studies use DAYCENT (Del Grosso et al., 2000), a soil model, to predict SOC changes and emissions of N_2O. Adler, *et al.*'s study goes into detail regarding step-by-step GHG emissions from the processes associated with corn and stover production, but assumes significantly less fertilization and fuel consumption by equipment than what is typically used on corn in the U.S. (Economic Research Service, 2012; Perlack, Ranney, & Wright, 1992). Adler, *et al.*'s study does not focus on corn stover, but rather the total energy product from a given area; disaggregating the results to derive a figure for stover alone is difficult. Kim and Dale's study also uses DAYCENT modeling, for eight counties in the U.S. and reports relatively similar values to Adler and those presented later in this chapter. In contrast to Adler, *et al.*, and most other studies in this field, life-cycle GHG emissions on a per-mass basis are provided for both corn grain and stover. Both studies agree that the largest source of GHG emissions from the corn system is N_2O emitted from soils and that corn stover systems can result in net SOC increase, even with sustained stover removal of up to 50%, which is in contrast to many other studies in the field.

The most directly comparable study to the one presented here is that of Luo *et al.*, which examines the effects of different allocation methods on life cycle environmental impacts of corn stover production (Luo et al., 2009). They examine economic and energy-based allocation as well as a system-expansion approach that is similar to the subdivision approach used in this paper. Luo *et al.* assess the full fuel cycle (i.e. field-to-wheels) and use pre-existing database values for many of the system inputs. The study described in this paper focuses specifically on the feedstock production phase and uses a more detailed model of corn and stover production.

3.3 Methodology

3.3.1 Scope and System Definition

The system boundary for this study is limited to the agricultural system for producing corn and stover, in essence on-farm activity and the production of fuels and fertilizer. The functional unit of analysis is one hectare of corn and stover production. This study assesses the production of stover from U.S. corn cultivation by modeling an average field based on national statistics. All of the activity described in this section is considered the baseline value for corn cultivation in the U.S. and is assumed to yield the U.S. national average of 147.2 bushels/acre (9.24 tonnes/hectare) of corn and 3.95 dry tonnes of stover/hectare, at sustainable stover collection rates (Hess, Kenney, Ovard, Searcy, & Wright, 2009b; National Agricultural Statistics Service, 2012). Collection of stover, which is uncommon at present, requires the following additional inputs and activities: addition of N, P and K fertilizers in sufficient quantity to replace the N, P and K removed in stover biomass, and additional farm equipment activity required for cutting, baling and moving baled stover to field-side for temporary storage.

3.3.2 Life Cycle Inventory Development

Life-cycle impacts of corn production systems are typically dominated by the fertilizers and herbicides required to produce corn at high yields (Kim et al., 2009; Luo et al., 2009). Corn requires high inputs of N and while some of this demand can be met by rotation with nitrogen fixing crops, 97% of U.S. corn acreage receives synthetic nitrogen fertilizer. In addition, approximately 80% and 60% of corn fields receive phosphate and potassium fertilizers, respectively (Economic Research Service 2012, Tables 9, 11, 13). Fertilizer application rates used in this study are based on national averages as reported by the USDA Economic Research Service (2012). Since these rates are based on current practice, in which stover is seldom collected, the subdivision scenario adds additional fertilizer to replace the removed nutrients based on the chemical composition of stover, as reported in Wortmann & Klein (2008).

The specific fertilizer compounds used to deliver particular nutrients vary depending on local supplies, cost, and soil conditions. This study uses the most common forms of N, P and K fertilizer as reported by the USDA Economic Research Service (Table 3-1) (Economic Research Service, 2012). Ammonium Phosphate Nitrate was applied in sufficient quantity to meet P demand, which also satisfied part of N demand; the balance for N was met with liquid ammonia. K demand was satisfied with Muriate of Potash (potassium chloride). Limestone was applied at the rate specified in West and McBride (2005).

	Fertilizer	Percent of Corn Fields Treated [19]	Average Application Rate (kg /ha*yr) [19]	Amount Required to Replace Stover Nutrients (kg/ha*yr)
Nitrogen (as N)	Ammonium Phosphate Nitrate, Liquid Ammonia	97%	156.9	31.6
Phosphorous (as P_2O_5)	Ammonium Phosphate Nitrate	78%	67.3	7.9
Potassium (as K_2O)	Muriate of Potash (Potassium Chloride)	61%	88.5	57.3

Table 3-1 - Average Use of Fertilizer in the U.S. Addition of N fertilizer is almost ubiquitous, while the majority of fields also receive P and K.

Most LCA studies of corn production use the Intergovernmental Panel on Climate Change (IPCC) methods for estimating N_2O emissions, which assumes that 1.25% of N fertilizer volatilizes as N_2O (Kendall, Chang, & Sharpe, 2009). A small number of LCAs of corn production have used detailed modeling of biogeochemical systems in determining life-cycle environmental impacts from corn production, including N_2O (Kim & Dale, 2005a, 2003). Using a different approach, Powers calculated N_2O volatilization based on the fraction of fertilizer that undergoes denitrification, as opposed to total fertilizer mass as in IPCC methods (Powers, 2005). This approach has high data and analytical requirements; Powers' model was calibrated against many years of water quality monitoring data from the East Iowa watershed. The majority of LCA studies neither calibrate their leaching and volatility factors using such detailed empirical data, nor use biogeochemical modeling to estimate N_2O field emissions.

Multiple studies have confirmed that N_2O flux increases with additional fertilizer N, though the precise relationship is likely non-linear and not completely understood (Hoben et al., 2011). Despite the limitations and uncertainty in the IPCC methods, some still argue that it may be the best choice where no more detailed analytical data exist (Brentrup et al., 2000). In an analysis of multiple studies of gaseous emissions from cereal crops, Lindquist and colleagues found N_2O volatilization to be, on average, 1.06% of applied N; which will be the value used in this study (Linquist et al., 2012).

Pesticide and herbicide application rates are based on national averages reported by the USDA National Agriculture Statistics Service (2011). The diversity of local corn growing conditions leads to many pesticide and herbicide combinations. This study included any formulations that were applied to >50% of U.S. corn acreage at their average application rate. These include: atrazine at 1.16 kg active ingredient/hectare and glyphosate at 1.19 kg active ingredient/hectare. Uncertainty introduced by this assumption is likely to be limited, since this analysis finds pesticide production and application accounts for only about 2-3% of net energy consumption or GHG emissions from corn production. Energy demands of agricultural equipment for corn cultivation were estimated based on data from GREET (M. Q. Wang, 2008). LCIs for other model inputs are taken from the Ecoinvent or GaBi Professional databases (Ecoinvent Centre, 2011; PE International & LBP, 2008).

Changes in soil carbon may exert a significant effect on the GHG emissions of stover production; however, there is significant uncertainty regarding the magnitude of these effects. Sequestration of carbon in cultivated soil is heavily dependent on local climatic and biogeochemical conditions, as well as the specific cultivar grown, the amount of biomass harvested, and fertilization practices. Recent research indicates that soil carbon changes from biomass cultivation may extend deeper than 30 cm, the typical cut-off depth for soil carbon analyses in literature (Follett, Vogel, Varvel, Mitchell, & Kimble, 2012). Basic principles of soil carbon dynamics imply that removal of stover is likely to reduce soil carbon sequestration as compared to cultivation practices that leave all stover on the field, even where the absolute effect of the corn and stover system may still increase soil carbon. A review of existing literature finds a diversity of conclusions spanning a range from net soil carbon gains (Clay et al., 2012) and losses (Anderson-Teixeira et al., 2009) for soil subject to stover collection and removal.

Clearly, more research is required to quantify the relative change in soil carbon, and significant geographic, agronomic and climate uncertainty may persist even if more conclusive results are obtained. Because of this uncertainty, soil carbon changes are not included in the LCI of stover reported in this paper – but they should not be ignored in LCAs which model systems that utilize stover.

3.3.3 Allocation Methodology

At present, the majority of stover is left on the field to decompose and maintain soil condition, though some is collected for use as cattle fodder (W. Edwards, 2011). Current research indicates that as much as 68% of stover can be sustainably harvested for biofuel production under no-till production practices (Hess et al., 2009a; Powers, 2005), though less than 40% is sustainable under typical current practices. Following the methodology described as current state-of-practice by the Idaho National Laboratory Advanced Uniform Feedstock Model, a stover yield of 3.95 dry tonnes/hectare (1.6 dry tons/acre) is assumed (Hess et al., 2009a). Although, repeated removal of large fractions of stover may degrade soil quality, this represents 38% of total stover available, which meets current sustainability criteria and is a reasonable estimate of the economically available stover which can be collected with current equipment (Graham et al., 2007). Grain yields were assumed to be the 2011 national average, 9.23 tonnes/hectare (147 bushels/acre)(National Agricultural Statistics Service, 2012). It is assumed that no additional soil conditioning treatments are required as a result of the removed or retained stover.

Three allocation scenarios are presented: the first based on energy content, the second based on economic value, and the third on subdivision. The first two methods require modeling the corn and stover production system as a whole, then allocating impacts to each product. The subdivision method models stover and grain production separately; when summed together, the impacts of the two subsystems equal those of whole corn production system.

3.3.3.1 Energy-Based Allocation

Energy allocation uses the lower heating value of the stover (16.5 MJ/kg) compared to corn (413.6 MJ/bushel, 16.3 MJ/kg) to allocate environmental flows (Forest Products Laboratory, 2004; Morey, Tiffany, & Hatfield, 2005). This results in allocation of 70% of total impacts from corn cultivation to corn grain and 30% to stover. For comparison, Luo *et al.*, found a allocation of 62.5% and 37.5% for corn and stover when they used what they called a “mass/energy” based allocation method (Luo et al., 2009).

3.3.3.2 Economic Allocation

The price of corn was taken from the average market price of corn in 2011, $196.36/tonne ($6.06/bushel) (Economic Research Service, 2011). Since the corn price typically reflects delivered product, the price was adjusted downward to reflect the cost of transportation from the field to the delivery site. This assumes transport in a heavy-duty diesel combination truck pulling a 12.2 meter (40 foot) grain trailer with 26.3 tonnes (1035 bushels) per truck-trip, with empty back-haul paid at 50% of the loaded rate. The distance traveled was assumed to be the average distance for grain transport by truck in the U.S. according to the Commodity Flow Survey, 331.5 km (206 miles) (Bureau of Transportation Statistics, 2009). Per-mile costs were based off national average operational costs of truck transport from the American Transport Research Institute, $0.93/km ($1.49/mile) (ATRI, 2011). This yields a corn price to the grower of $182.09/tonne ($5.40/bushel). While corn price fluctuates on a daily basis, the difference between corn price and stover prices is so great that even relatively large fluctuations (+/- $1.00 per bushel) result in only minor changes to allocation (less than 2% of total burden). The stover price is based on the mean, field-side willing-to-accept price of corn stover, $92/dry ton ($101.41/dry tonne), as described by the National Research Council (2011). This resulted in allocation of 85% of total impacts to grain and 15% to stover. All prices were calculated in 2011 dollars, as this was the last year consistent data was available for all necessary prices.

3.3.3.3 Subdivision

Many studies have only assigned stover the processes that occur as a result of adding stover harvesting and transport to a corn production system; they essentially divide the stover-specific activities from the corn production system and quantify them independently; in other words, subdivision (Wardenaar et al., 2012). In the case of corn stover, this reflects likely real-world production practices, since in the near-term stover collection would occur separately from grain harvest.

The stover production processes include (1) additional equipment operation for harvesting, baling, and transport of stover to a field-side location; and (2) replacement of nutrients removed from the field in stover, with the assumption that 100% of the N, P and K removed in stover must be replaced. Stover is comprised of 0.8% N, 0.2 % P (as P_2O_5) and 1.45% K (as K_2O) (Wortmann & Klein, 2008). Stover harvesting activity uses values from Idaho National Laboratories' Uniform Feedstock Model; yield was taken as 3.95 dry tonnes/acre (Hess et al., 2009a). Table 3-2 shows a comparison of the different allocation methods.

	Economic Allocation	Energy Allocation	Subdivision
Allocation to Grain	85%	70%	Baseline corn cultivation
Allocation to Stover	15%	30%	N, P, K in stover + extra harvest activity

Table 3-2 - Allocation methods. Energy allocation attributes almost twice as much impact to stover as economic.

3.3.4 Impact Assessment

Since two motivations for expanding biofuel use are GHG reduction and energy security, this study evaluates the life cycle 100-year global warming potentials from the IPCC (GWP_{100}) and fossil fuel use. In addition, acidification potential (AP) and eutrophication potential (EP) are presented as indicators for pollution to the air and water, respectively (Guinee et al., 2002). A comprehensive emissions inventory is available in the supplementary material. Impacts of feedstock production, relative to the total fuel cycle for cellulosic ethanol are discussed in Chapter 4.

3.4 Results and Discussion

One hectare of corn and stover production requires approximately 23 GJ of fossil energy inputs and results in the emission of approximately 2.5 tonnes of carbon dioxide equivalent (CO_2e) (Table 3-3). Fertilizer production effects generally dominate total GHG and fossil energy impacts. GHG emissions from fossil energy production and combustion represent about 19% of total emissions from stover, in the subdivision case and about 17% for grain.

For most indicators, subdivision produces impacts approximately equal to those of economic allocation. Both economic allocation and subdivision assign significantly less impact to stover than energy allocation. For most impact categories, the ratio of stover impacts to total system impacts was within the range of 0.12-0.17, very similar to economic allocation (Table 3-4). GHG emissions from stover were 13.5% of the total under subdivision, as compared to 14.5% under economic allocation (100 year IPCC equivalents).

	Total per Hectare	Grain Econ	Grain Energy	Grain Alone	Stover Econ	Stover Energy	Stover Subdivision
Air Pollutants							
CO (kg)	13.0	11.13	9.09	11.80	1.90	3.94	1.23
NO_x (kg)	15.7	13.43	10.97	13.71	2.29	4.75	1.84
SO_x (kg)	2.50	2.14	1.75	2.22	0.36	0.76	0.28
$PM_{2.5}$ (kg)	0.97	0.83	0.67	0.85	0.14	0.29	0.11
PM_{10} (kg)	1.21	1.03	0.84	1.06	0.18	0.36	0.15
Pb (air, kg)	0.00	0.0003	0.0003	0.0003	0.0001	0.0001	0.0001
Ozone (kg)	0.00	0.0008	0.0007	0.0009	0.0001	0.0003	0.0001
NMVOC (kg)	4.87	4.16	3.39	4.05	0.71	1.47	0.81
GHGs							
CO_2 (kg)	1,449	1,238	1,011	1,276	211	438	172
CH_4 (kg)	4.22	3.60	2.94	3.49	0.61	1.28	0.72
N_2O (kg)	3.16	2.70	2.21	2.63	0.46	0.96	0.53
SF_6 (kg)	0.00	0.00001	0.00001	0.00001	0.00000	0.00000	0.00000
GWP100 (kg CO_{2e})	2,496	2,133	1,741	2,148	364	755	348
GWP20 (kg CO_{2e})	2,666	2,278	1,860	2,288	388	806	378
Indicators							
AP (kg SO_{2e})	13.68	11.68	9.54	11.96	1.99	4.14	1.59
EP (kg PO_{4e})	28.73	24.55	20.05	24.14	4.19	8.69	4.59
Fossil Energy (MJ)	22,653	19,353	15,803	19,339	3,300	6,850	3,283

Table 3-3 - Results of allocation between grain and stover for three allocation scenarios. The Grain Alone scenario represents current Business-as-Usual (BAU) practices.

N_2O emissions comprised about two fifths of total GHG impact under most scenarios and were almost entirely due to volatilization of fertilizer. Some models predict that the removal of stover may actually decrease N_2O emissions from corn fields by reducing N inputs from stover decomposition (Kim et al., 2009), though other analyses conclude that removing stover will increase N_2O emissions by exacerbating soil temperature cycling (Németh, 2012). This uncertainty highlights the need for additional research into the subject of nitrogen volatilization from agricultural activity.

	Subdivision Method		System Total
	Value	**% Total**	
GWP 100 – Corn (Mg CO_2e)	**2.15**	**86%**	**2.50**
GWP 100 – Stover (Mg CO_2e)	**0.35**	**14%**	
AP – Corn (kg SO_2e)	**12.0**	**88%**	**13.6**
AP – Stover (kg SO_2e)	**1.59**	**12%**	
EP – Corn (kg $PO_4^{3-}e$)	**24.1**	**84%**	**28.7**
EP – Stover (kg $PO_4^{3-}e$)	**4.59**	**16%**	
Fossil Energy – Corn (GJ)	**19.4**	**86%**	**22.7**
Fossil Energy – Stover (GJ)	**3.28**	**14%**	

Table 3-4 - Comparison of grain and stover production impacts by subdivision method and total system impacts. Both methods yield very similar net values.

Soil carbon effects are highly uncertain and likely depend strongly on local conditions. Existing literature reports soil organic carbon losses that range from -3 to 2 Mg C/hectare* year (Anderson-Teixeira et al., 2009; Follett et al., 2012). At either end of this range, soil carbon changes dominate all other GHG effects by more than an order of magnitude. Even at a comparatively moderate sequestration value for fields where small amounts of stover are removed, 368 kg C/hectare* year (Clay et al., 2012), the SOC changes equate to approximately 1.4 tonnes of CO_2e per hectare per year of sequestration; far greater than the combined impacts of all other elements in the stover production process. SOC changes, if they are at the extreme ends of published ranges, far outweigh all other elements in the stover LCI. This has several critical implications: First, potential SOC changes should be foremost on the mind of policy makers when deciding policies which may affect the spatial distribution of corn production for biofuels. Second, in soils where a SOC increase could be reasonably be expected, such as marginal soils with low natural SOC, there may be opportunity for carbon sequestration through SOC increase that could yield a favorable life-cycle GHG input even if the corn farming requires substantial agrochemical input. Finally, tillage practices have a critical effect on net SOC changes; no-till production has repeatedly been demonstrated to have a positive effect on SOC, when compared to conventional tillage (Humberto Blanco-Canqui, Stone, & Stahlman, 2010; Clapp, Allmaras, & Layese, 2000; Reicosky & Evans, 2002). While the effects of tillage vary with local conditions, as a rule, SOC loses can be minimized by sourcing corn stover from fields under no-till management.

The results of the analysis presented in this study generally agree with previous literature in the field, but direct comparison against studies is difficult because most studies examine the full fuel cycle as opposed to crop production alone. However, Luo *et al.*, also found economic allocation to result in significantly less impact from stover production than energy-based allocation, though the magnitude of difference was greater in their study (Luo et al., 2009). Luo *et al.* also found higher impacts to stover under their system expansion case, which is likely attributable to differences in LCI methodology. The results of this study generally agree with those of Kim and Dale (2005b), who report higher per-hectare GWP emissions and fossil energy consumption, but evaluate all activity on a plot of land over multiple years; the difference is essentially one of system boundaries.

While ethanol production is not modeled in this study, at typical conversion efficiencies (330 L/dry tonne for stover and 366 L/dry tonne for corn (Sánchez & Cardona, 2008)) implies an effective feedstock burden under subdivision of 270 g CO_2e/L from feedstock for stover-based ethanol and 635 g CO_2e/L for corn. For comparison, total lifecycle emissions of gasoline and corn ethanol are 3100 g CO_2e/L and 3200 g CO_2e/L, respectively, based on the California Air Resources Board's Low Carbon Fuel Standard methodology (California Air Resources Board, 2011). This reinforces the generally-accepted conclusion that stover-based cellulosic ethanol may have significant GHG advantages over corn ethanol, if the energy and GHG intensity of conversion are sufficiently low.

The analysis conducted in this paper concludes that the environmental impacts of the combined corn and stover system are very similar to the sum of the corn-only system and the effects of stover as estimated by the subdivision method (see Table 5, summed values are < 1% different). This is largely due to the way current stover collection practices are modeled. At present, corn is assumed to be collected by a combine harvester, after which the stover is cut and windrowed by a forage harvester, this is known as a two pass system. Single-pass harvesting, in which one machine both harvests grain and creates windrows of cut stover, may be common in the long-term, but as yet, very few single pass harvesters are in operation and two-pass systems are likely to dominate over the near term. As such, combined grain and stover operations are likely to have very similar impacts to the grain-only plus subdivision scenarios for analyses based on current technology.

This analysis assumes that enough stover is left on the field to prevent erosion and soil degradation. This may not hold true in all situations and stover removal may have significant effects on soil condition and soil carbon (Graham et al., 2007; Powers, 2005; W W Wilhelm, Johnson, Karlen, & Lightle, 2007). Further research is required to determine whether large-scale stover removal can be accomplished without harmful soil condition impacts.

Ultimately, life cycle analysts, researchers, and policymakers must select a co-product treatment method that is most appropriate for the analysis of stover-based biofuel or bioproduct systems. There may be no objectively “right” answer to these questions, however several guiding principles may be drawn from this study along with existing LCA literature (Table 3-5).

	Economic Allocation	Energy Allocation	Subdivision Method
Advantages	• Reflects motivation of producers • Cost data generally available	• May reflect the motivation of energy policies • Does not fluctuate with markets	• May require lower data burden than allocation • Direct link between activity and consequences
Disadvantages	• Requires modeling of complete system • May not accurately reflect non-monetizable factors	• Requires modeling of complete system • May require modeling of conversion system	• May not reflect stakeholder values or decision criteria • May not be appropriate in retrospective LCAs* • May not accurately reflect activity that improves both systems

*Only as subdivision is applied here; where stover collection is evaluated as an addition to corn-only production.

Table 3-5 - Comparing characteristics of the allocation methods evaluated in this study.

In the case of corn stover, economic allocation and the subdivision method yield similar results, while energy-based allocation assigns significantly more impact to stover. The analysis conducted in this study cannot determine whether the similarities between economic allocation and subdivision are coincidental, or whether they reflect an underlying conceptual linkage. One would expect that over the long term, economic allocation and a properly subdivided production system will converge to similar values, as production practices become more efficient and markets settle around prices that reflect actual costs of production (Hopehayn, 1992). By this interpretation, subdivision represents the marginal costs of stover collection, while economic allocation represents the average cost. Over the long run, the difference between subdivision and economic allocation should be minimal, if rational, undistorted and efficient markets are assumed.

At a purely conceptual level, if or when, mature corn and stover production systems and markets exist, economic allocation may best align allocation methods with the motivation behind real-world decision making (Ekvall & Finnveden, 2001), since economic value drives most decisions regarding production systems. In the near-term, subdivision may be preferable, since it is strongly tied to actual field activity and the data requirements may be better understood and less volatile than for economic allocation. Nevertheless, the subdivision method has several potential flaws, especially here where it is applied as a consequential analysis. Some systems may be impractical to prospectively model without a full consequential approach that includes market-mediated effects. For example, growers may value the flexibility of having multiple markets (biofuels, animal fodder and food) for their crop and as a result, might view the benefits of stover collection as greater than the direct economic value of the stover itself. In addition, if growers add stover collection to an existing corn system, they may decide to invest in process upgrades that improve yield in both systems, such as more intensive soil management or different formulations of fertilizer. Since consequential methods would only allocate the impacts that directly arise from collection of stover, this would create a mismatch between growers' motivations and the analytical approach

Energy-based allocation faces a particular challenge because the forms of energy in the two products are not substitutable. The final products from each feedstock may provide different energy services; in the case of corn grain, nutritional energy and for stover, transportation energy as ethanol. Estimating net energy value of corn versus stover thus requires knowledge about the intended use and, where required, the conversion efficiency. Where final products are dissimilar or conversion efficiencies are uncertain, energy-based allocation will struggle to accurately reflect true energy value of corn and stover. Energy-based modeling is unlikely to be preferable to the other methods unless it is clear that maximizing energy production was a dominant factor guiding the development of biofuel supply systems.

This study does not consider the effect of crop rotation on fertilizer impact attribution. In the U.S., corn is often grown in rotation with nitrogen-fixing crops such as soybean, or cover crops which are incorporated into the soil. In the case of crop rotation, some of the fertilizer applied to corn, particularly

P and K compounds, will likely remain resident in the soil to be utilized by subsequent crops (van Zeijts et al., 1999). This presents an additional allocation problem should be considered in future research.

3.5 Implications

The study discussed in the preceding sections helps characterize three different methods of assigning impacts to stover in corn production systems, system expansion, energy-based allocation or economic value allocation. This characterization offers some guidance for policymakers who have to set policy regarding biofuel production, but it does not answer the critical question of which method should be used? Further research on this subject may not be able to provide a categorical answer to this question, because of the difficulty in matching modeling methodology to real-world decision making (Huijbregts et al., 2001), as discussed earlier.

The question is then, what method should be used when no categorically "correct" answer exists, as is the case. It is quite possible to assign impacts to co-product streams with high accuracy, as this paper demonstrates; such accuracy may be impossible when selecting *which* allocation method to prefer. This ultimately rests upon how one conceives of the causal relationships which shaped the system under study and there may be no categorically correct answer here; it may be impossible to say whether producers are behaving purely in response to long-term economics, which would imply economic allocation, or viewing stover as a marginal change to existing practices, which would imply system expansion. Some level of arbitrariness in allocation may be unavoidable, but recent research, including the study described in this chapter, imply that system expansion is likely preferable in the short term, because of its clear physical connection to the activities associated with stover harvest and a reasonable match with producer decision-making. Economic allocation is likely to be preferable as stover harvesting becomes a routine part of the corn production system. Over the long term, econometric modeling of empirical data can improve models of average producer behavior and tighten the link between stover pricing and producer behavior (Gillingham, Newell, & Palmer, 2009; Lee &

Chambers, 1986; Lin, Dean, & Moore, 1974). These methods may not completely achieve the goal of accurately matching models to decision-making rationale, but they can be sufficient to inform discussion on the subject and make a decision that at least partially achieves policy goals; in the words of Charles Lindblom, “muddling through,” (Lindblom, 1959).

In addition to the study of allocation methods, this paper has two other immediately practical implications. First, the LCI produced here will contribute to the main LCI paper discussed in Chapter 5, as well as contribute to the work of other researchers. The second immediate implication arises from the general agreement on GHG impacts between this paper and others in recent literature. While some differences are to be expected, arising from measurement or modeling assumptions as well as differing data sources, the values produced here are similar to those in other studies in this field notably Luo, *et al.* (2009), and Kim and Dale (2009). While this study does not consider the critically important element of SOC change (which will be addressed in the next chapter) the agreement on the other elements of stover production implies an emerging consensus on the subject, which is important for policy making.

Chapter 4: Analysis of Soil Organic Carbon Changes from Corn Stover Harvest

4.1 Introduction

Biofuels are thought to be a promising technology for reducing greenhouse gas (GHG) emissions from the transportation sector. The U.S. Revised Renewable Fuel Standard (RFS2) calls for a substantial increase in biofuel utilization over the next 10 years. At least 16 billion gallons (61 billion liters) of biofuels made from lignocellulosic feedstocks ("cellulosic biofuels") are specifically mandated by RFS2 (Renewable Fuels Association, 2010). Cellulosic biofuels have the potential to meet RFS2 GHG reduction goals (Bracmort, 2012; Farrell et al., 2006; C. Murphy & Kendall, n.d.; Tao & Aden, 2009; Viikari et al., 2012), but substantial uncertainty remains, particularly surrounding soil organic carbon (SOC) changes from producing and harvesting lignocellulosic feedstocks (Anderson-Teixeira et al., 2009; Lemke et al., 2010; P. Smith, 2007). In fertile soils, organic matter from root growth and above-ground litter is incorporated into the soil over time. Some of this carbon remains in the soil for long periods of time (Humberto Blanco-Canqui & Lal, 2009; J. M.-F. Johnson, Barbour, & Weyers, 2007). When undisturbed, carbon content in soils often reaches equilibrium, where the amount of soil carbon being added approximately equals that being lost (Buyanovsky & Wagner, 1997).

Disturbing these pools of SOC through changes in land coverage or agronomic management, such as removing large amounts of biomass for biofuel production, can alter soil carbon balances. This is of particular interest to biofuel analysts and policy makers, since the magnitude of these changes can be quite significant (Fargione et al., 2008). Cultivating feedstock crops for cellulosic biofuels typically requires a substantial change in management since, at present, virtually no cellulosic biofuel capacity is operating in the U.S. (Advanced Ethanol Council, 2013). Even where specific agronomic practices for biofuel crops are similar to food ones, biomass harvest removes much more biomass from the field than food harvest.

Corn stover, the above-ground, non-grain part of the corn plant, is thought to be a promising feedstock for biofuel production because substantial acreage of corn is already cultivated in the U.S. and stover is typically left on the field as residue (Graham et al., 2007). If harvesting stover causes a loss of soil organic carbon, through oxidation or reduction and volatilization to CO_2 or CH_4, then the life-cycle GHG impact of stover-based biofuels would increase. SOC changes are affected by local soil and climatic conditions as well as the type of organic matter in the soil, some forms, such as lignin, are typically much more recalcitrant than others. Understanding the SOC change is, therefore, an important element in accurate life-cycle assessment of biofuels.

This paper focuses on the following question: Does removing some part of the corn stover from corn fields reduce SOC? If so, under what conditions and by how much is it reduced? To answer this, we collect data from 21 studies of corn stover removal and SOC changes. 17 of these studies were from peer-reviewed publications, two were unpublished data from authors which had published in this field before (and which are intended for publication in the future), one was a M.S. thesis and one a PhD Dissertation.

4.2 Methodology

4.2.1 Data Collection

A literature search was conducted of studies quantifying changes in SOC from the harvest of corn stover. Google Scholar and ISI Web of Science were searched using the keywords “soil carbon” and “corn stover”. This returned several hundred results, so a set of criteria was established to limit the inclusion to papers which would most directly reflect the effects of corn stover removal on SOC. These criteria were:

- Inclusion of at least two levels of stover removal, including zero.
- Corn must be grown continuously or must represent at least 50% of any crop rotation.
- Sampling depth must be at least 5 cm.

- Agronomic parameters including soil classification, tillage and nitrogen (N) fertilization must be reported or obtainable through other sources.
- Must be unique data; literature reviews and meta-analyses were used to identify potential studies, though all data in the dataset was copied from the original publication.

Only studies reporting empirical data were selected for this analysis; a comparison between measured and modeled studies is planned for future work. The 5cm sampling depth was picked to minimize the transient effects of surface litter. The crop rotation condition was set to allow corn-soy rotations, which are common. When a paper met these criteria, the relevant data were extracted to a MS-Excel data file (Microsoft, 2006). Additional papers were discovered by examining the works citing and cited by papers which were included in the study, as well as several literature reviews on the subject (Anderson-Teixeira et al., 2009; Humberto Blanco-Canqui, Lal, Post, Izaurralde, & Owens, 2006; Powlson, Glendining, Coleman, & Whitmore, 2011; W W Wilhelm, Johnson, Hatfield, Voorhees, & Linden, 2004; Zanatta, Bayer, Dieckow, Vieira, & Mielniczuk, 2007). When many sampling depths were reported in the same study and field, no more than two were included in this study, to avoid overrepresentation of any single study.

21 suitable studies were identified, which included data from 22 experimental fields (Appendix 8.2). These studies identified several factors thought to impact SOC changes from stover removal: soil clay content, biomass removal rate, initial SOC content, crop rotation practice, N fertilization, tillage practice, sampling depth, soil bulk density and duration of the study. Values for these parameters were extracted from the papers in the study. Where data were not reported, study authors were contacted to attempt to fill in gaps. If this failed, values were estimated from other sources, such as companion studies or earlier or later work from the same research plots. Soil conditions, such as bulk density and clay content were estimated by referencing the soil series and study location in the USDA Web Soil Survey (Soil Survey Staff, 2013).

Residue removal rates were given in the constituent papers, however not all were given as the fraction of above-ground biomass; some were based on surface area measurements or on the percent of mechanically-harvested stover, which excludes a stubble under the cutting height of a harvester. These were converted to mass fractions based on the 1:1 relationship between cut height and stover mass reported in Wilhelm, et al. (2010) and the average "Low-Cut" height for mechanical silage harvesters reported by Wu and Roth (Z. Wu & Roth, n.d.). Where corn height was unavailable, it was assumed to be equal to that of the average in the nearest test field reported in Wilhelm, et al. (Wally W. Wilhelm et al., 2010).

SOC is typically reported in one of two forms, as a mass fraction (g SOC/kg soil, or % SOC) or as a mass-per-area (typically Mg SOC/ha). The mass fraction form was used as the functional unit for our analysis, which reduces covariance between SOC levels and sampling depth. Where mass fractions were not available, the following relationship was used to convert between the two:

$$SOC_m \left(\frac{Mg}{ha}\right) = 10{,}000\frac{m^2}{ha} \times SD\ (m) \times BD\left(\frac{Mg}{m^3}\right) \times SOC_f\left(\frac{kg_{SOC}}{kg_{soil}}\right) \qquad (1)$$

where SOC_m is SOC mass per area, SD is sampling depth, BD is soil bulk density and SOC_f is SOC mass fraction.

Tillage practices were grouped into three classes: (1) conventional tillage (CT - which includes continuous tillage using moldboard plow); (2) reduced tillage (RT - which includes conservation tillage; chisel plow; strip tillage; mulch tillage; ridge tillage); and (3) No tillage (NT). Conventional tillage has been widely reported as contributing to SOC loss; several studies find that tillage has a greater affect on SOC than residue removal (Clapp et al., 2000; Dick et al., 1998; Reicosky & Evans, 2002). This effect varies with soil depth, since tillage induces mixing of soils and rapidly moves stover carbon downwards, as well as reducing particle size (Anderson-Teixeira et al., 2009; Dolan, Clapp, Allmaras, Baker, & Molina, 2006). We control for the different tillage classes using indicator variables for which tillage method was used on a field.

Nitrogen fertilization may have an effect on SOC concentrations; this is examined in this study. The effect of nitrogen fertilizer on soil microbial activity and carbon dynamics will depend strongly on biogeochemical conditions, including the amount of available nitrogen in the soil prior to fertilization. Previous literature has been mixed and uncertain regarding the effect of nitrogen on SOC levels (Dolan et al., 2006). There is relatively little variation in nitrogen treatment rates, so it is uncertain whether treating this as a continuous parameter will identify any meaningful effects. Accordingly, two specifications are presented, one with nitrogen treated as a binary qualitative variable and one as a numeric rate (Specifications 4 and 5, respectively).

Soil classes are grouped into 7 categories, corresponding with USDA soil textural classes (Soil Conservation Service, 1987); not every class was observed in this dataset. Indicators for each class and type are included in regressions with appropriate exclusions to avoid perfect multicollinearity.

4.2.2 Analytical Methods and Identification

A reduced form regression approach was used to study the effect of various factors on SOC content in soil. The approach allows for flexible control of a number of factors which may affect SOC. In addition, cluster robust standard errors, clustered at the study level, were used to construct confidence intervals which account for idiosyncratic differences across studies as well as correlation in observations over time within studies (Cameron & Trivedi, 2005). In order to produce results that are relevant for prospective modeling of SOC changes, two types of SOC change are considered. In some cases, the important characteristic is the net gain or loss of SOC after a period of corn stover recovery. This "Within-Field" (WF) change is estimated using a differences-in-differences regression, where the dependent variable is the initial SOC and the initial SOC is controlled for as an explanatory variable.

Sometimes the critical characteristic for models is the difference between SOC in a field in which stover is collected and a hypothetical *status quo*. In the case of corn stover, the *status quo* is assumed to be corn production with stover left on the field, as it is in over 95% of all U.S. corn fields(U.S. EPA, 2013a). This "Between-Field" (BF) change is analyzed using a differences estimation. The basic regression used takes the form

$$y_{it} = h(\boldsymbol{x}'_{it}\beta) + \epsilon_{it} \qquad (2)$$

where y_{it} is the final SOC percentage for field i in time t and $\boldsymbol{x}_{it}$ are explanatory variables including percent biomass removal, initial percent SOC, nitrogen treatment, tillage practice, clay content, sampling depth, and study duration. β is the coefficient estimated by regression, ϵ is the error term and *h* is the functional form of the parameter, which can be non-linear, such as quadratic or logarithmic. The purpose of the regression is to identify the causal relationship between $\boldsymbol{x}_{it}$ and final SOC. This requires a number of assumptions.

The data collected represent averages across a number of replications such that

$$\overline{y_{\iota t}} = \frac{1}{n_j}\sum_{j=1}^{n_j} y_{ijt} \qquad (3)$$

where j is the number of replications on field i. In order to be able to identify the relationship of interest, the estimates must have linear parameters. To see this, note that the average change in y_i from a change in variable x_i is given by

$$\Delta\, \overline{y_\iota} = \frac{1}{n_j}\sum_{j=1}^{n_j} \Delta y_{ij} = \frac{1}{n_j}\sum_{j=1}^{n_j} h(\Delta x'_{ij}\beta) \qquad (4)$$

So long as $h(\cdot)$ is linear in the parameters, then

$$\Delta \bar{y}_j = \beta \frac{1}{n_j} \sum_{j=1}^{n_j} h(\Delta x_{ij}) \qquad (5)$$

Note that $h(x_{ij})$ can be a non-linear in the variables x_{ij}, so the assumption is not unduly restrictive.

A second key assumption to identify the causal relationship is that the conditional expectation of the errors is zero. The assumption would be violated if important explanatory variables are omitted, which correlate with an explanatory variable x_{ij} and affect final SOC percent, known as omitted variable bias. The condition may also be violated if the functional form is mis-specified. The robustness of the estimated effects to the inclusion of a number of control variables and specifications is checked to test the sensitivity of our results to potential omitted variable bias.

A last concern relates to the nature of the dependent variable. The SOC content in fields, as a percentage of mass, is constrained to be within the interval (0,1). Linear regressions do not restrict predictions to be between (0,1) and could lead to biased results (Kieschnick & McCullough, 2003). A popular approach to dealing with this is to use a logistic transformation of the dependent variable given by

$$\ln\left(\frac{y_{jt}}{1 - y_{jt}}\right) = h(\boldsymbol{x}'_{it}\beta) + e_{jt} \qquad (6)$$

If the errors follow an additive logistic normal distribution, then e_{it} will follow a normal distribution and standard Gaussian statistical inference applies. All proceeding results were run under both a linear model and a logistic model. In general, the logistic model had limited if any advantage over the linear model, and the linear model allowed for more precise estimates because of its assumption of linear marginal effects.

4.3 Results

Variable	Mean	Std. Dev	Min	Max	N
Final Soil Organic Content (kg/kg)	0.0202	0.0064	0.0072	0.0473	251
Initial Soil Organic Content (kg/kg)	0.0233	0.0082	0.0091	0.0544	185
Biomass Removed (fraction of total)	0.4735	0.4187	-0.1800	1	251
Tilling Practice (Categorical Variable)	1.7540	0.6850	1	3	212
Clay Content (kg/kg)	0.2156	0.1002	0.0580	0.4370	251
Sampling Depth (cm)	23.4821	13.4621	5	60	251
Study Duration (years)	10.075	9.99	2	34	251

Table 4-1 - Summary Statistics for Corn Stover Removal Dataset. 81% of plots in the study were treated with nitrogen fertilizer.

Table 4-1 presents the summary statistics of the key variables of interest. As can be seen, final SOC is slightly lower than our initial observed SOC; however, directly comparing differences in means can be misleading for a number of reasons. First, we do not observe initial SOC for 47 of our observations. Second, as can be seen from the summary statistics, there is substantial heterogeneity across studies such as the type of tilling practice, the soil class, sampling depth, soil density and the duration of study.

Direct evaluation of WF and BF changes may lead to incorrect inference if there are other factors which led to changes in SOC in addition to biomass removal. Using a regression approach, we measure WF and BF changes flexibly, controlling for a number of factors which may also determine final SOC percentage. Included in our analysis are nitrogen application rates, duration of the study, clay content, sampling depth, and tillage practices. The effect of different parameters and combinations of parameters are checked in several forms, or "specifications" of the linear regression model.

Study and field effects are also considered, since agronomic practices, as well as local soil and climate conditions would be strongly correlated with the study they are reported in. If different studies are associated with different methodologies which are not captured in the dependent variables of interest, our results may be biased. These are controlled for in the same way as the qualitative variables above. Namely, for some specifications we include indicators for each study, with appropriate exclusion restrictions. In these regressions, identification is based on within-study variation as including indicator variables for each study effectively demeans all variables by their respective within-study or within-field means. By checking for study effects, the effect of variation within a study or field is lost, so this approach can identify whether there are systematic differences between studies, but cannot simultaneously identify the effects of other parameters.

Specification	[1]	[2]	[3]	[4]	[5]
Biomass Removed (%)	-0.00113***	-0.00150***	-0.00146***	-0.00126***	-0.00129***
	(0.000382)	(0.000290)	(0.000295)	(0.000374)	(0.000379)
Nitrogen Treatment Indicator				-0.000123	
				(0.000756)	
Nitrogen Rate (‘00 kg/ha/year)					0.000726
					(0.000534)
Log Duration (log years)				0.000242	0.000168
				(0.000668)	(0.000634)
Clay Content (%)				0.00348	0.00578
				(0.0102)	(0.0110)
Sampling Depth (cm)				-0.0000763	-0.0000861
				(0.000238)	(0.000229)
Sampling Depth Squared (cm^2)				-0.00000115	-0.000000900
				(0.00000396)	(0.00000380)
Till 1 (CT)				0.0231***	0.0216***
				(0.00387)	(0.00450)
Till 2 (NT)				0.0247***	0.0230***
				(0.00317)	(0.00365)
Till 3 (RT)				0.0250***	0.0237***
				(0.00386)	(0.00412)
Constant	0.0208***	0.0176***	0.0176***	(Omitted)	(Omitted)
	(0.00176)	(0.000139)	(0.000142)		
N	251	251	251	211	207
R Squared	0.006	0.588	0.590	0.958	0.959
AIC	-1824.2	-2047.3	-2042.8	-1651.2	-1623.8
Study Effects?	N	Y	N	N	N
Field Effects?	N	N	Y	N	N

Table 4-2 Difference Estimators (BF SOC changes) for Linear Regression of SOC concentration (%) as dependent variable. Asterisks indicate significance, *: p<0.1, **: p<0.05, ***: p<0.01. Standard errors are in parenthesis.

The first three specifications for each model, [1-3] and [6-8], check for the presence of bias introduced by study-specific or field-specific effects. Table 4-2 shows the result for the linear difference estimator (BF SOC changes). Specification [1] presents the basic BF effect with no control variables. If the experiments were properly randomized, the estimated effect should be unbiased. Results including study fixed effects are shown in specification [2]. Control for the effects of the experimental field, rather than the study in which results were reported, was done using the same methods and shown in specification [3]. Similar analyses are done for WF SOC change in specifications 6-8. The relatively similar coefficients generated for each of these specifications, combined with clear statistical significance for all, indicates that there are no significant biases introduced by study or field effects.

All of the linear models with more complete sets of parameters, specifications [4], [5], [9] and [10], indicate a very consistent effect of SOC removal; every 1% of additional residue removal leads to a 0.0013% reduction in SOC, with all other factors being held equal. All SOC change values are significant to $p<0.01$. While this SOC reduction appears small, when one considers that the average corn field in this study had 57 Mg/ha at the start of residue removal treatments, this implies a loss of around 50 kg C per hectare for every percent of residue removal. The duration term has a negative sign under both linear (not shown) and logarithmic forms, which indicates that continuing treatment also tends to reduce SOC.

All specifications show a significant negative effect at the 1 percent level of residue removal on SOC. Importantly, this effect does not vary substantially between specifications. The stability in the point estimate indicates that biomass removal treatment was well randomized and was not correlated with other important determinants of final SOC. Few other parameters reach statistical significance in the

Specification	[6]	[7]	[8]	[9]	[10]
Biomass Removed (percent)	-0.00112**	-0.00140***	-0.00135***	-0.00130***	-0.00134***
	(0.000387)	(0.000342)	(0.000344)	(0.000358)	(0.000360)
Initial SOC (%)	0.619***	0.625***	0.639***	0.496***	0.494***
	(0.0948)	(0.0717)	(0.0772)	(0.0734)	(0.0736)
Nitrogen Treatment Indicator				-0.000431	
				(0.000796)	
Nitrogen Rate (‘00 kg/ha/year)					0.000324**
					(0.000135)
Log Duration (log years)				-0.000303	-0.000264
				(0.000612)	(0.000616)
Clay Content (%)				0.000411	0.000582
				(0.00707)	(0.00738)
Sampling Depth (cm)				-0.000372	-0.000354
				(0.000272)	(0.000273)
Sampling Depth Squared (cm^2)				0.00000507	0.00000480
				(0.00000440)	(0.00000440)
Till 1 (CT)				0.0170***	0.0159***
				(0.00273)	(0.00274)
Till 2 (NT)				0.0165***	0.0155***
				(0.00238)	(0.00245)
Till 3 (RT)				0.0159***	0.0148***
				(0.00379)	(0.00357)
Constant	0.00731***	0.00903***	0.00518**	(Omitted)	(Omitted)
	(0.00224)	(0.00180)	(0.00211)		
N	185	185	185	165	165
R Squared	0.686	0.829	0.808	0.981	0.981
AIC	-1565.8	-1680.2	-1654.9	-1413.3	-1414.1
Study Effects?	N	Y	N	N	N
Field Effects?	N	N	Y	N	N

Table 4-3 - Difference-in-Difference Estimators (WF SOC changes) for Linear Regression of SOC concentration (%) as dependent variable. Asterisks indicate significance, *: p<0.1, **: p<0.05, ***: p<0.01. Standard errors are in parenthesis.

specifications, however, which generally supports the common impression in literature on the subject: that SOC in corn production systems is variable and uncertain. The signs of most parameters agree with other studies. Sampling depth and study duration are negative, which is to be expected, since both treatment duration and the mass of soil sampled would be expected to correlate with the magnitude of effects noticed; repeated corn cultivation is generally associated with declining SOC (D. L. L. Karlen et al., 1994; W. Smith & Grant, 2012). Clay content has a positive sign, indicating that increasing clay content generally reduces SOC loss, as reported by multiple studies (e.g., 29).

Table 3 shows the difference-in-difference estimator, which controls for initial levels of SOC and describes WF changes If removal treatments were not randomly assigned and there were important differences between treated and untreated fields which affect final SOC levels, the differences regression may lead to biased point estimates. The difference-in-differences estimator is robust for these concerns. Like the difference estimator discussed above, the effect of biomass removal is significant and negative, and does not substantially vary when alternative control variables are included. Unsurprisingly, the parameter with the greatest effect on final SOC concentration is initial SOC concentration. Parameters are generally of similar magnitude, sign and significance as in the BF analysis discussed above, suggesting the studies properly randomized treatment.

For most of the complete specifications (numbers [4], [5], [9], [10]), the results indicate each additional percent of biomass removal results in SOC decreasing an average of 0.0013% with a standard error of approximately 0.0004%, which yields a 95% confidence interval of approximately 0.0005 to 0.002% decrease. We tested for the presence of nonlinear effects using both the logistic model as well as quadratic terms in the linear model; however, the nonlinearities across biomass removal rates were not found to be statistically significant. The result is likely driven by lack of heterogeneity in removal rates across studies. Most studies reported removal rates only for no or near complete removal of biomass, and few had intermediate removal levels. As a result, the estimates are best thought of as an average effect of biomass removal.

Very few parameters besides biomass removal, initial SOC and the model coefficient (which is omitted in favor of tillage practice dummy variables in several specifications) achieve statistical significance, however those parameters are significant to $p<0.01$ certainty. Nitrogen treatment rate is significant on the WF model, but not on the BF model. Several of the non-significant parameters have been identified by other studies, or theoretical understanding of SOC dynamics, as affecting SOC changes. It is uncertain whether the results here are merely artifacts of this experimental design or call into question previous results.

4.4 Discussion

The results demonstrated above show a loss of 0.0005% to 0.002% in SOC per year for every 1% of residue removed. Using equation (1) and assuming a removal rate of 30%, which has been proposed by several sources in literature as a sustainable rate of stover removal (e.g. 41, 42), over a sampling depth of 30 cm and soil density equal to 1.31 (the average found from this dataset), this equates to a loss of 197-786 kg SOC/ha*year, which if emitted entirely as CO_2 yields 0.72 to 2.9 Mg CO_2/ha*year. In the context of life cycle analysis, this CO_2 emission is highly significant. Assuming an approximately 4 dry tonne/ha yield of stover and 292 liter/tonne conversion efficiency, this adds approximately 30 grams of CO_2e per megajoule (MJ) of delivered fuel. The RFS2 requires fuels that achieve the “cellulosic” designation achieve 50% reductions in life cycle GHG intensity compared to the petroleum fuels they displace. This implies targets of around 50 grams CO_2e/MJ for cellulosic biofuels, depending on the fuel being evaluated and the life cycle analysis methodology. The results of this study indicate that for stover based fuels, SOC change alone accounts for most of the allowable GHG emissions.

One area where substantial uncertainty remains is temporal effects. The treatment duration term was highly uncertain (the estimate was much smaller than the standard error) for both linear and logarithmic transformations of duration (Table 4-2 and Table 4-3, specifications 4, 5, 9, 10. Linear parameters were estimated, but not shown). Under commonly accepted models of soil dynamics, SOC concentrations in a field under a positive or negative SOC flux, such as residue removal, will come to an equilibrium over time (Anderson-Teixeira et al., 2013; Buyanovsky & Wagner, 1997). The lack of significance in this parameter may be a result of incorrect model specification, omission of other factors which affect SOC (such as total biomass production on the field), of a misunderstanding regarding the nature of SOC equilibria

SOC changes from stover harvest is a critical issue for determining the life-cycle GHG footprint of biofuels and bioproducts in the U.S. The U.S. grew over 34 million ha (84 million acres) of corn in 2011; which produces over a hundred million tonnes of residue as well. This residue could potentially be used for a wide range of bioprocesses and since it is currently left on the field on over 95% of farms. If SOC decreases from moderate levels of stover harvest are as high as earlier studies predict (Anderson-Teixeira et al., 2009), any bioprocess using corn stover is likely to be a significant net emitter of GHGs.

The results from the regressions above clearly show a significant and robust negative correlation between residue removal and SOC concentration. This matches the expected behavior of systems according to current understanding of SOC dynamics (Anderson-Teixeira et al., 2013; Humberto Blanco-Canqui, Lal, Post, Izaurralde, et al., 2006; Hooker et al., 2005), which strongly implies that the statistical correlation, in fact, reflects a causal relationship. By aggregating the results of many studies, the analysis presented above was able to overcome some of the statistical uncertainty described by previous authors in the field.

Few other parameters achieve statistical significance, which confirms the common conclusion in literature that SOC dynamics are highly uncertain. For WF changes, initial SOC was significantly correlated with final SOC, which is to be expected, since SOC changes are incremental increases or decreases upon previously existing SOC pools. The WF analysis also showed a significant relationship between nitrogen fertilization rate and SOC change. Previous research has been divided on the subject of the relationship between N fertilization and SOC (Dolan et al., 2006; Pikul, Johnson, Schumacher, Vigil, & Riedell, 2008).

One finding of this analysis contradicts well-established opinion in this field. For both WF and BF changes, SOC did not significantly differ between different tillage practices (CT, RT and NT were within a range less than any of their standard errors). Multiple previous studies have concluded that tillage, particularly conventional tillage (CT in this study), are strongly associated with reductions in SOC (e.g. 27, 38, 39). Further analysis is required to determine whether this is an artifact of the regression parameters used in this study, or whether tillage effects are more uncertain than previous literature indicated.

It is possible that the current model does not effectively capture differences in biomass production between fields. Of the parameters considered, only nitrogen fertilization is strongly associated with more biomass being produced. Changes in SOC levels are determined by the balance between inputs to soil, largely from plant matter, and flows out, from erosion and microbial metabolism. Rapid plant growth can increase SOC in two ways, by facilitating rapid root growth and creating a larger pool of above ground biomass, some of which may be incorporated into the soil. If the model, as currently formulated, is insensitive to the total biomass production of corn plants, then the categorical variables for tillage may be absorbing some unintended effects. Additionally, in areas with very high biomass production, tillage is sometimes required to minimize the insulating effects of surface residue, which can slow soil warming in spring and retard germination (Nielsen, 2010). This may imply an interaction between biomass production effects and tillage which is not captured in the current model.

Understanding SOC changes within the framework of life cycle analysis is complicated because accurate estimation of these changes is typically based on a consequential assessment framework. That is to say, the characteristic of interest is what changes a proposed production system would cause on the world. So, for a stover based production system the absolute magnitude of emissions from SOC change must be evaluated in a context which also considers any emissions from SOC change that would occur had the stover not been removed. This is usually done by a comparison between systems in which stover is harvested and the *status quo* in which it is generally not harvested. The analysis presented in this paper can help future analysts by presenting models for WF and BF changes. In general, the BF case better matches the needs of consequential LCA. BF comparison evaluates the difference between fields in which stover is removed and those in which it is retained on the soil. The WF comparison, on the other hand, may be less vulnerable to uncertainty stemming from soil conditions or measurement practices. BF comparisons in this study implicitly assume that all fields in a study have approximately equal SOC concentrations at the start of the study, which is not always the case, as is demonstrated by some of the studies in this review (Clapp et al., 2000; Wilts, Reicosky, Allmaras, & Clapp, 2004). Since initial SOC levels clearly affect SOC dynamics under residue removal, this means that BF comparisons suffer from at least one source of uncertainty that WF would likely avoid.

There are several areas of uncertainty which may affect the conclusions of this analysis. Climate conditions and the cultivars grown substantially affect total biomass production, which is the maximum amount of biomass that could be returned to the soil. Not all studies quantify total biomass returned, future work will attempt to evaluate whether mass of carbon entering the soil is more strongly correlated with maintaining SOC levels than residue removal rates.

While many studies have reviewed the impact of crop residue removal on SOC (Anderson-Teixeira et al., 2009; Humberto Blanco-Canqui, Lal, Post, Izaurralde, et al., 2006; Powlson et al., 2011; W W Wilhelm et al., 2004; Zanatta et al., 2007) most have not looked at agricultural management strategies that can help offset SOC lost due to crop residue removal. Blanco-Canqui (2013) recently reviewed the potential of several agricultural practices to counteract the SOC lost due to residue removal. No-till cover crops or applying C-rich substances such as manure, compost or the solid byproduct of cellulosic ethanol production (e.g. lignin cake or biochar) can all have beneficial impacts on SOC levels in soils from which lignocellulosic biomass is harvested.

The substantial uncertainty surrounding the SOC effects of sustained stover collection clearly demonstrate the need for further research in this area. LCA of biofuel production shows the critical importance of providing relatively low-GHG feedstocks for biofuel production systems. Likely near-term technology can achieve the goals of climate change mitigation policies, like RFS2, but they do not clear the GHG target thresholds for advanced biofuels by much; if feedstock production results in SOC loss at the higher end of its uncertainty range, there is virtually no chance for biofuels to achieve their GHG reduction targets and, in fact, at the high ranges of SOC loss, biofuels may be worse than the petroleum fuels they hope to replace.

Further study is needed to answer these critical questions. Most pressingly, there needs to be more empirical studies of SOC change under a variety of management conditions. Already, there is a multi-center research effort, coordinated by the USDA under the Sungrant program to directly address this research need (D. L. Karlen, Varvel, et al., 2011; Stott, Jin, & Ducey, n.d.). Additionally, better guidance regarding the most relevant methods for quantifying SOC change and measurement standards would help facilitate meaningful comparisons between studies.

Chapter 5: LCA of Cellulosic Ethanol under Multiple Scenarios

5.1 Study Context

Cellulosic biofuels have been a subject of interest to researchers for over several decades (Delucchi, 2010; Fu et al., 2003; Hsu et al., 2010; Pimentel & Patzek, 2008; Spatari et al., 2005; M. Wu et al., 2006). They may have the potential to displace a meaningful fraction of petroleum-based transportation fuels and reduce transport-related GHG emissions, but this conclusion is not yet fully settled (Bonin & Lal, 2012; Campbell, Lobell, & Field, 2009; Searchinger et al., 2008). Significant uncertainty remains about the life-cycle GHG impacts from cellulosic biofuels. Lab and pilot scale studies of several second-generation biofuel technologies indicate that many of the proposed conversion pathways have the potential to produce low-carbon fuels, but some second generation fuels have higher life-cycle GHG impacts than the petroleum fuels they seek to displace (Kendall & Yuan, 2013). Awareness of the importance of feedstock production on biofuels' life-cycle GHG footprint is increasing, as studies have revealed feedstock production practices can create a massive "carbon debt" that offsets years of potential benefits from biofuel use (Fargione et al., 2008)

Over a dozen commercial scale cellulosic ethanol facilities are currently planned or under construction, though at present only a handful of pilot plants have been completed in the U.S. (Advanced Ethanol Council, 2013). The environmental impacts of each pathway is a subject of importance to policymakers. Agreement on a common set of modeling assumptions, system boundaries, co-product allocation practices and environmental accounting standards would help facilitate comparisons between pathways (Bonin & Lal, 2012; Wardenaar et al., 2012).

Life cycle analysis (LCA) can serve a critical role in the development of advanced biofuels, by determining the carbon intensity of a fuel and by linking particular environmental impacts to a particular process, which could then be targeted for improvement. LCAs also highlight areas of uncertainty within the production cycle. For biofuel production, direct and indirect land-use change (LUC) and associated soil carbon fluxes, nitrous oxide (N_2O) emissions from soils, bio-refinery conversion efficiencies and the material inputs to bio-refineries have all been identified as areas of significant uncertainty (Anderson-Teixeira et al., 2009; Humberto Blanco-Canqui & Lal, 2007; Cherubini & Strømman, 2010; Hoben et al., 2011; Hoskinson, Karlen, Birrell, Radtke, & Wilhelm, 2007; Kendall & Chang, 2009; Khanna, Crago, & Black, 2011; Sanchez et al., 2012; Sheehan et al., 2003).

This study adds to existing literature in three main ways. First, most published LCAs of cellulosic ethanol production pathways omit substantial detail regarding the full production cycle; most focused their attention on one element such as feedstock production (e.g. Spatari *et al.* 2005; Kim *et al.* 2009) or conversion processes (e.g. Fu *et al.* 2003; Iribarren *et al.* 2012; Borrion *et al.* 2012). To fill the gaps in analysis, the Argonne National Laboratory's GREET model is commonly used for part or all of the biofuel production chain (Burnham, Wang, & Wu, 2006). GREET maximizes its flexibility to compare a wide variety of fuel production pathways and consider national-level energy policy. Independent analyses are needed to confirm or challenge those of GREET. The LCI presented in this chapter is meant to provide additional depth and also serve as a comparison for GREET or other large-scale models. The comprehensive nature of this model also better allows examination of how subunits of the conversion process affect the field-to-blending terminal performance of the biochemical cellulosic ethanol production system over its whole life cycle.

The second major advance is the evaluation of a process design philosophy for the production of cellulosic ethanol. Most producers and much of the current literature on lignocellulosic ethanol production seeks to increase the yield of fuel for every unit of feedstock added to the process (Ishola et al., 2013; Lau & Dale, 2009; Unruh, Pabst, & Schaub, 2010; ZeaChem, 2012). EdeniQ's proposed design seeks to minimize the chemical inputs to the process, instead. Rather than achieving a positive cost and carbon balance by increasing output, this design concept seeks to reduce inputs (Lane & Derr, 2011).

This offers an interesting opportunity to compare more standard (if such a term can be used to describe and industry that does not yet exist) approaches against this low-input one. This can allow “hot-spots” of environmental impact to be identified and helps inform the discussion regarding which, if any, designs offer superior environmental performance.

Finally, this study produces one of the most comprehensive LCIs available in published literature. Over 1,100 mass and energy flows are tracked for each scenario and are made available in the supplementary material associated with this paper (Appendix B). This allows future researchers to evaluate the impacts of biofuel production across several scenarios without having to develop their own LCIs.

This study seeks to extend the research community’s understanding of the interaction between various phases of production and the decisions made during the design of the biofuel production system. As discussed in Chapter 3, this often requires presenting the results in a disaggregated fashion (even if only in supplementary material) so that the effect of modeling assumptions are more transparent. For example, when study scopes are “well-to-wheel” or “field to wheel”, the combustion of a fuel in a vehicle is included. Different vehicles can have vastly different fuel economies and pollutant emission profiles. Thus, comparing fuels on a well-to-wheels basis embeds assumptions about vehicle performance in the results, complicating interpretation of the study results and comparison with other studies. A well-to-pump, or well-to-distribution terminal model removes any assumptions about fuel combustion characteristics from the analysis. California’s Low-Carbon Fuel Standard (LCFS) is a good model for how to accomplish this; the LCFS evaluates fuels on a well-to-pump basis for this reason, using emissions per MJ of fuel as its functional unit of analysis (CARB, 2012; Farrell, Sperling, et al., 2007; Farrell, Berkeley, et al., 2007).

Many LCAs of biofuels narrowly focus on GHG emissions, yet other pollutants are certainly a concern. This study includes a comprehensive evaluation of environmental flows to air, water and soil, and provides access to the full LCI, rather than simply a subset of pollutants or summary impacts. It also breaks the production process into separate phases, to facilitate comparison across different parts of the production process and evaluate tradeoffs that come along with process design decisions.The LCIs presented in the following paper are meant to be a resource for researchers to develop the advanced tools necessary to evaluate as-yet-undeveloped biofuel production systems.

Materials and Methods

5.2.1 Goal and Scope Definition

This model evaluates the environmental flows consumed and generated during the production of biochemical cellulosic ethanol on a field-to-blending-terminal basis, using a mixture of process-based and consequential LCA approaches. The system boundaries (Figure 5-1) include the agronomic processes and for feedstock production (equipment use, agrochemical production and application, and biogeochemical field emissions), transport of feedstock to the conversion facility , the conversion process, and transport of anyhydrous ethanol to the blending terminal where ethanol is mixed into retail motor vehicle fuels. This system boundary (field-to-blending terminal) allows for fuels to be compared on an energy-equivalent basis, independent of any effects from vehicle fuel economy.

Other system boundary considerations in this model include simplified modeling of the ethanol production facility’s construction, which assesses major construction materials only (concrete, steel, and aggregate) and does not consider facility decommissioning. Previous studies have shown that the construction and demolition of buildings has negligible life cycle impacts compared to materials production and building operation (Scheuer, Keoleian, & Reppe, 2003). Production of mobile equipment, including farm equipment, is also excluded on similar grounds.

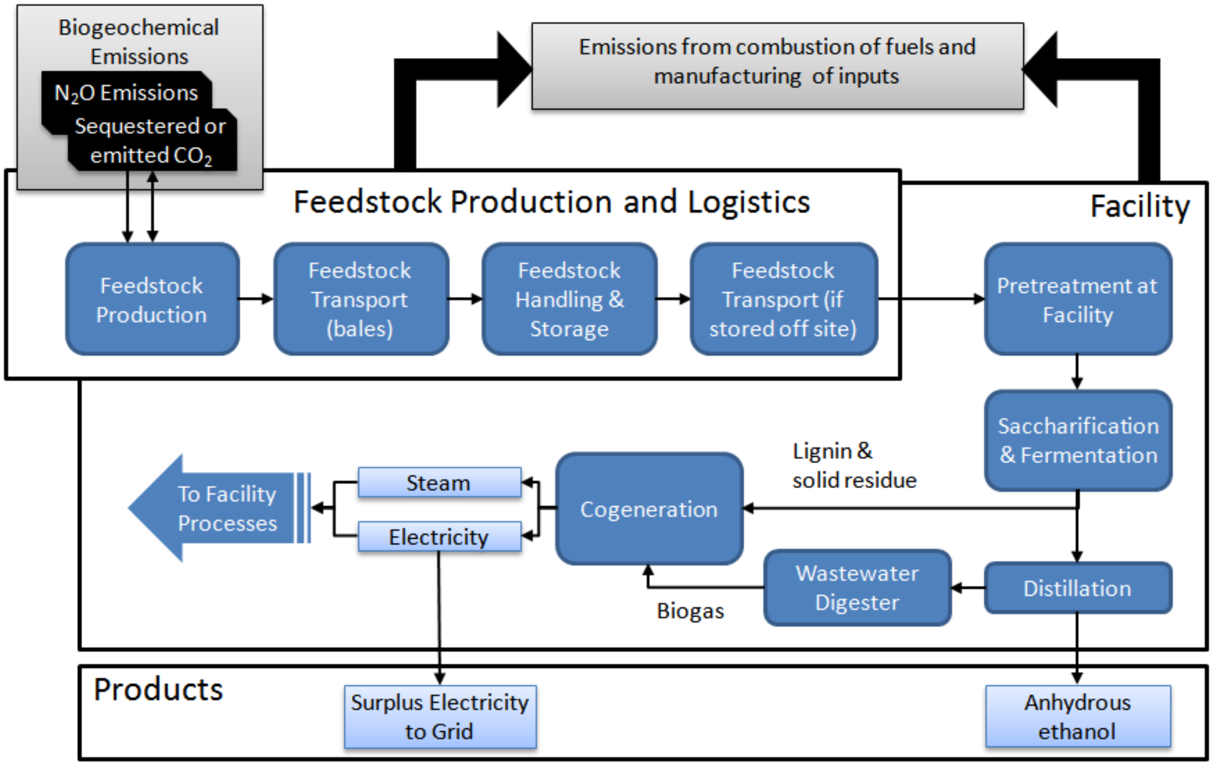


Figure 5-1 LCA system boundaries include both feedstock production and conversion into fuels.

Waste treatment at the conversion facility is likely to have minimal impact. Most of the solid waste from the conversion process is combusted to generate energy, and liquid waste is treated in an on-site wastewater treatment plant to enable water recycling. Because of water recycling, water losses are primarily through evaporation, rather than discharge. Residual ash from biomass combustion and other un-recycled materials are produced in small quantities and assumed to be disposed in a landfill where they are largely inert. In addition, ash from combustion may have value as a soil additive (Risse & Gaskin, 2010), however its value for this use is uncertain and thus excluded from this analysis (Pandey & Singh, 2010). Any other waste products are assigned neither environmental burdens, for disposal, nor credits as coproducts.

5.2.2 Life Cycle Inventory

The various life cycle inventories reported by this model are developed in Microsoft Excel, with VBA scripting used to automate some processes (Microsoft, 2006). LCI data for material and energy inputs are primarily derived from LCI databases such as Ecoinvent and GaBi Professional (Ecoinvent Centre, 2011; PE International & LBP, 2008). A detailed table describing the LCIs used in the model is provided in the supplementary information (Appendix 1). Some materials or processes use LCIs provided by manufacturers or taken from other sources in current literature.

Accurate and complete LCI datasets are critical for comprehensive and timely LCAs. Inventory datasets may not be geographically or temporally appropriate, however, which presents a challenge to researchers. The shortcomings in LCI data are well-documented and widely discussed in literature, (e.g. Huijbregts *et al.* 2001; Björklund 2002). Recent comprehensive LCIs of chemical inputs to the biofuel system, including pesticides, fertilizers, antibiotics and propagation nutrients are notably scarce. Wherever possible, recent U.S. data were used to maintain consistent geographic and temporal context, though in some cases, European data or data more than ten years old were the only available option. Uncertainty is introduced into these, and other LCA results, due to the paucity of LCIs, however, in general the flows which are most uncertain represent relatively small components of the overall process.

5.2.3 Feedstock Production

Two feedstocks are modeled in this LCA: corn stover and switchgrass.

Corn stover is the above-ground biomass left after corn harvest and has traditionally been considered a waste or residual. It is typically left on the field to reduce erosion, and is reincorporated into the soil to return nutrients and maintain soil health. When harvested for another use, stover becomes a co-product of corn production and presents several allocation challenges.

In the base case of this LCA stover is treated using a consequential approach, where only changes to *business-as-usual* (BAU) practices are allocated to stover. Alternative attribution methods are discussed in depth in (C. Murphy & Kendall, 2013). BAU is assumed to be repeated no-till corn cultivation with grain harvested and stover left on the field. When stover is removed from the field, embodied nutrients [nitrogen (N), phosphorous (P), and potassium (K)], along with carbon, are removed as well. This requires the replacement of nutrients removed in stover by additional synthetic and mineral fertilizers. The mass of N, P and K replaced is calculated using stover composition values from Wortmann & Klein (2008). Agricultural equipment activity, for collecting, baling and stacking baled stover is also attributed to the resulting biomass, since it would not have occurred in the BAU case.

Switchgrass production, in contrast to corn, has not been done for commercial purposes, so comparatively fewer data exist on cultivation and harvest practices. The switchgrass cultivation data used in this study were provided by Ceres Inc., a company that has extensively researched grassy crop cultivation (Ceres Inc., 2013). The data rely on the University of Nebraska crop budgets for agricultural equipment work rates and energy consumption (Klein & Wilson, 2013), as well as their own research into fertilization parameters. Fuel consumption values provided by Ceres approximately agree with values elsewhere in literature, including the Idaho National Laboratories' Advanced Uniform feedstock model (Hess et al., 2009a). Switchgrass differs from corn in that there may be predictable and significant differences in activity on a year-to-year basis due to its growing cycle. After a two year establishment phase, in which harvests are limited and agronomic practices are tailored to maximize the growth of young plants, there is a 6-10 year period of maturity, with full harvests each year. After this maturity period, the plot must be re-seeded to maintain high yields. These variable emission and materials use rates are averaged across the lifespan of the plot. Average yield for each post-establishment year was set at 7.8 dry tonnes per hectare, which corroborates values in literature (Hess et al., 2009a; Jung & Lal, 2011). When the limited yields from the establishment phase are considered, average annual yields over the 8 year growing cycle are 6.34 dry tonnes per hectare.

Both corn and switchgrass require fertilizer to achieve high yields. Total N, P and K application is determined by soil conditions and plant characteristics, but the choice of which formulation to apply may be determined largely by local supply, past experience and economic conditions (Nutrient Stewardship, 2011). The compounds used for corn fertilization were based on those most commonly used on corn in the U.S.A. according to USDA National Agricultural Statistics Service data (Economic Research Service, 2012). Ammonium phosphate nitrate was applied in sufficient quantities to meet P requirements. N requirements beyond what was provided by ammonium phosphate nitrate were met by liquid ammonia and K requirements were met by potassium chloride. For switchgrass, diammonium phosphate (DAP) was applied in sufficient quantities to meet P requirements. Excess N demand was met with liquid ammonia and K demand was met with potassium chloride. Total applications of N, P and K were 32, 8 and 57 kg/ha*year (28, 7 and 52 lb/acre*year) respectively, which approximately agree with the values published in Sindelar, *et al.* (2013)

Emissions from fields through volatilization or runoff of fertilizer are an important consideration. High-intensity corn production requires nitrogen (N) fertilization, even when in rotation with a nitrogen-fixing plant such as soy. Nitrogen fertilization can result in volatilization of N as N_2, NH_4, N_2O or nitrogen oxides (NO_x). Only NO_x and N_2O are tracked, because N_2 is inert and NH_4 is quickly removed from the atmosphere (Seinfeld & Pandis, 2006). Since most U.S. corn production uses tile drainage, nutrient leaching into groundwater was not considered in this model, but run-off to surface water was estimated as 31.6% of applied N (Powers, 2005). Phosphorous loss to surface water, at 4.66% of applied P, also came from the Powers study. Powers concluded that potassium loss to water was minimal due to soil microbial activity and the relatively low solubility of potassium salts under conditions found in the soil.

N_2O volatilization was estimated as 1.06% of applied N (Linquist et al., 2012) and NO_x volatilization rate of 238 mg/m^2 (Akiyama, Tsuruta, & Watanabe, 2000). All impacts from lime application to soils are allocated to grain production and so are not considered for stover-based biofuel.

Field equipment activity generally follows the feedstock harvest and processing system described by the *Pioneer Scenario* from the Idaho National Laboratories (INL) Uniform feedstock model (Hess et al., 2009a). This calls for a two-pass harvesting system in which corn grain is removed by a standard grain combine, after which a flail shredder cuts down the remaining stover and arranges it in windrows. After a drying period of about three days, a fraction of the biomass, typically 25-40%, is baled and stored at field-side. The shredding, windrowing, baling and stacking of bales are modeled and attributed to the resulting stover. Switchgrass is harvested and baled similarly, with cutting, windrowing and baling steps.

Equipment operations result in emissions of criteria pollutants and GHGs from fuel combustion. Criteria pollutant emissions other than SO_2 are calculated using the US EPA Tier III non-road emission factors based on the power output of the engine (*EPA Tier III Non-Road Diesel Engine Standards*, n.d.). Emissions of sulfur (as SO_2) and CO_2 are calculated by determining the mass of fuel consumed and typical carbon and sulfur content of diesel fuel. The life-cycle environmental impacts of diesel production, prior to combustion, are based on the GaBi PE database (PE International & LBP, 2008).

5.2.3.1 Soil Carbon Changes

Removing large amounts of biomass from a field can directly impact soil characteristics, including carbon and nitrogen content. These are highly dependent on local biogeochemical conditions and a significant amount of uncertainty exists regarding their magnitude (Lal, 2006; Spatari & MacLean, 2010). Soil carbon effects are subdivided into two categories, direct and indirect. The base case of this model assumes no significant long-term changes in soil organic carbon (SOC) as a result of feedstock collection. These assumptions are evaluated in low and high SOC change scenarios based on the models presented in a meta-analysis by Anderson-Teixeira, *et al.* (Anderson-Teixeira et al., 2009) as well as DAYCENT modeling reported by Kim & Dale (2009).

In addition to direct changes to soil conditions, biomass production activity can cause indirect changes to land use and cover, through market or policy mechanisms. For example, when corn acreage which was previously used to supply human consumption is used for biofuel, the un-met demand will be satisfied with corn or substitute grains grown elsewhere. Smith (2007), conceptualizes this indirect land-use change (iLUC) as direct land-use change that is temporally or spatially shifted from its cause. This conception of iLUC highlights the importance of having specific data about both the crop that is directly affected by a proposed biofuel system and the land affected indirectly. Similarly, changes in the value of crops can cause producers to intensify their existing growing parameters, such as by adding fertilizer or changing cultivars. Since neither corn stover nor switchgrass have been collected on large scale at present, no such data exist regarding these indirect changes. iLUC and cultivation intensity changes from stover and grassy crop utilization may be relatively small, since stover is currently a residue and grassy crops can be grown on marginal agricultural land, but it is too early in the development of large-scale biofuel production capacity to reach a firm conclusion on this subject. The results presented in this chapter omit iLUC and intensification effects due to this uncertainty and the presence of policies in the U.S. designed to minimize iLUC emissions (Schnepf & Yaccobucci, 2013).

5.2.3.2 Feedstock Pretreatment

Pretreatment operations include all processes from the point where bales of stover are stacked in road-side storage to where they enter the conversion process, excluding transportation. These are modeled based on pretreatment processes described in the INL Advanced Uniform Feedstock *Pioneer Scenario* (Hess et al., 2009a). The required energy consumption for feedstock handling and grinding is estimated using mass-based energy consumption factors for each step in the pretreatment process. The model assumes that most stationary equipment (e.g. grinders and feed systems) is powered by grid electricity. Diesel combustion emissions for mobile equipment, such as forklifts and bale handlers, are estimated using the same methodology as used for agricultural equipment and, similarly, assume EPA Offroad Tier III compliant engines (*EPA Tier III Non-Road Diesel Engine Standards*, n.d.).

5.2.3.3 Conversion Process

In this model the term "conversion process" refers to all of the material conversion activities which occur at the bio-refinery. This model reflects current understanding of cellulosic process design, which is a rapidly developing field and has not yet been successfully commercialized; accordingly the modeling parameters used here may not be applicable to other cellulosic ethanol processes.

A primary obstacle to using cellulosic feedstocks for liquid fuel production is the recalcitrance of cellulose to break down into its constituent sugars, which can then be fermented into ethanol. Most processes require significant additions of acids, or enzymes such as cellulase, to liberate sugars from cellulosic materials (e.g. Humbird *et al.* 2011). The model described in this paper reflects a production process under development and currently in pilot-scale deployment by a commercial partner, which provided process design and information to the research team. This process differs from others by utilizing a genetically engineered fermentation microorganism that produces cellulase enzymes which would otherwise have to be externally added. The process emphasizes minimizing chemical inputs, rather than maximizing yield. Accordingly, The base case scenario presented in this paper assumes that no external chemical inputs are required, other than those necessary for microorganism propagation; the effect of external chemical or enzyme inputs are estimated in one of the additional scenarios reported here, based on data from Maclean and Spatari (2009). No other chemical inputs are modeled for the conversion process. An insignificant amount of acid and caustic is required for the clean-in-place system, which is recycled through multiple uses, so its exclusion is not expected to affect the outcome of the LCA.

The conversion facility is sized to produce 40 million gallons (151 million liters) of anhydrous ethanol per year at a conversion efficiency of 70 gallons per dry ton (292 liters per dry tonne) of biomass (corn stover or switchgrass). Production of steam and electricity dominates environmental flows associated with the conversion facility. Most cellulosic ethanol process designs assume that energy needs are met by combusting process byproducts, in this case, lignin cake, spent cell mass and unconsumed carbohydrates from the conversion process, as well as biogas from a wastewater treatment digester. The methane potential of the anaerobic digester was estimated based on (Tian, Mohan, Ingram, & Pullammanappallil, 2013).

The combustion of byproducts occurs in a fluidized bed boiler, driving an extraction turbine. Overall thermal efficiency of electricity production is assumed to be 22.9% (Grass & Jenkins, 1994). Under these conditions, the facility would be able to produce sufficient electricity for internal needs and have a surplus of approximately 17 MW. Due to the developmental nature of this technology and the lack of similar commercial-scale plants, the base case scenario conservatively assumes that the plant meets its own energy needs but does not export electricity, so no value is assigned to the surplus electricity. Additional scenarios show the effects of using surplus electricity to displace grid generation, or importing grid electricity to make up for a shortfall. Since electricity production or consumption would be approximately continuous, electricity consumption and displacement were assigned impacts that reflect U.S. grid average electricity.

Several nutrients and growth promoters are required for microorganism propagation and are included using LCIs from the GaBi Professional or Ecoinvent databases (Ecoinvent Centre, 2011; PE International & LBP, 2008). Air pollutant emissions from the boiler are assumed to be controlled with a multiclone and baghouse (for particulate matter) and by good combustion practices and exhaust gas recirculation for reducing NO_x emissions. Emissions from the boiler are modeled after a similar biomass boiler from another proposed cellulosic ethanol facility (AMEC Earth & Environmental, 2009). VOC emissions from hydrolysis and fermentation tanks are controlled with a wet scrubber and leakage of VOCs from the process or during transfer between vessels is assumed to be negligible.

5.2.3.4 Facility Construction

A simplified treatment of facility construction impacts is included in this LCI. The two largest elements of environmental impact from construction are the production of concrete and steel, which represent the greatest mass of material within the proposed bio-refinery. The life cycle inventories for these materials were obtained from the Portland Cement Association and the World Steel Association, respectively (Marceau, Nisbet, & VanGeem, 2007; World Steel Association, 2011). Facility lifespan was, upon recommendation from industry partners, conservatively assumed to be 20 years and no building decommissioning was considered. Impacts were distributed over the facility lifetime by simple straight-line amortization.

This analysis indicated that these two construction materials accounted for less than 0.5% of total GHG impact of each unit of resultant fuel, in the base case.

5.2.3.5 Transportation

Transport emissions and energy consumption are estimated based on standard assumptions for freight logistics (e.g. Winebrake *et al.* 2008). Previous work at UC Davis in the area of geospatial modeling of biofuel systems has indicated that average transport distances for feedstocks between field and processing facility can exceed 50 miles (Parker, Hart, et al., 2010). The *Pioneer scenario* envisions processing and storage facilities located relatively near to fields in order to minimize the distance across which bale transport, which is less efficient than bulk transport, must be utilized. This study assumes an average bale transport distance of 25 miles and an average bulk transport distance of 75 miles.

Feedstock transport was modeled as described in the uniform feedstock model (26 bales per 53 foot trailer, or 21.8 metric tons of minimally compressed bulk feedstock). Agricultural transport trucks are typically older than the fleet average, since they travel shorter distances and haul lower value goods. Feedstock transport trucks are assumed to have California 2002 model year compliant engines with 120,000 engine hours per truck. Using representative values for fuel economy and assuming empty back haul at 1.4 times the fuel economy of loaded trucks (Frey, Rouphail, & Zhai, 2008), estimates of diesel consumption were generated. Emission factors for the criteria pollutants were derived from EMFAC (CARB, 2007), carbon and sulfur emissions were estimated based on the mass of fuel combusted.

Results

The baseline scenario for ethanol production makes the following key assumptions. A more detailed list of parameters used in the base case scenario is available in Appendix 2.

- Feedstock production:
    - Average annual yields of approximately 4 dry tonnes per hectare (1.8 tons per acre) for corn stover and 6.3 dry tonnes per hectare (2.8 tons per acre) for switchgrass.
    - No significant change in soil organic carbon or nitrous oxide emissions from feedstock production and harvest
- Conversion Facility:
    - A conversion process yield of 265 liters per tonne (70 gallons per dry ton) feedstock
    - No significant chemical inputs are required beyond those necessary for microbe propagation
    - The facility generates sufficient energy from combusting process byproducts to be energy-neutral; no electricity, heat or fossil fuels enters or exits the facility.

      All carbon dioxide emitted from combusting process byproducts is biogenic and assumed to not to contribute to changing atmospheric GHG levels

Under these conditions, producing one megajoule (MJ) of ethanol emits 36.6 grams of CO_2-equivalent (g CO_2e) over its life-cycle for stover-based fuel, and 38.3 g CO_2e for switchgrass based fuel using 100-year GWPs from the IPCC's *Fourth Assessment Report* (IPCC, 2007). Table 1 shows key results for both base cases. For comparison, California Reformulated Gasoline has life-cycle emissions of approximately 99 grams CO_2e per MJ when calculated according to the California Low Carbon Fuel Standard (LCFS) methodology (CARB, 2012). By the same methods and including indirect land-use change, corn ethanol has emissions typically between 80 and 100g CO_2e.

	Corn Stover(g / MJ)	Switchgrass (g / MJ)
Criteria Air Pollutants		
CO	1.81E-01	1.70E-01
NOx	4.07E-01	3.36E-01
Sox	1.42E-01	1.40E-01
$PM_{2.5}$	5.30E-02	5.16E-02
PM_{10}	5.56E-02	5.32E-02
Ozone	4.38E-06	2.32E-06
Lead (to air)	8.76E-05	8.38E-05
Non-Methane VOCs	8.93E-02	1.01E+02
Greenhouse Gases		
CO_2	2.82E+01	2.77E+01
CH_4	6.57E-02	6.95E-02
N_2O	2.27E-02	2.97E-02
SF_6	8.02E-08	2.94E-08
100 Year IPCC GWP	3.66E+01	3.83E+01
20 Year IPCC GWP	3.95E+01	4.13E+01
Indicators		
Acidification Potential[1]	4.33E-01	6.45E-01
Eutrophication Potential[2]	1.90E-01	2.49E-01
Fossil Energy Consumption[3]	4.92E-01	5.06E-01

Table 5-1 Base case results for multiple flows and indicators. 1 - Reported in units of g SO2 equivalent, (Guinee, et al. 2002). 2- Reported in units of PO4 equivalent (Guinee, et al. 2002). 3- Reported in units of MJ fossil energy per MJ delivered ethanol.

Under base case conditions, both pathways have the potential to yield life-cycle GHG reductions compared to petroleum gasoline of around 60%, though it must be stressed that this study considers national average or typical conditions; actual evaluations of biofuel GHG impacts should be made on a geographically and technologically explicit basis. Corn stover has a slight advantage in feedstock production impacts, due to lower nitrogen requirements. It is important to note that the amount of N fertilizer allocated to corn stover depends on the allocation methods used during LCI development for corn stover; different allocation methods can assign more or less of the total fertilizer impact from corn cultivation to the stover (Murphy & Kendall, In Press).

Despite the common perception that switchgrass requires less fertilizer than stover, switchgrass' N requirement for high biomass yields is are approximately the same as stover on a per-dry-ton basis (Bonin & Lal, 2012; Sanderson, Read, & Reed, 1999; Vogel, Brejda, Walters, & Buxton, 2002). In addition, switchgrass has one or two establishment years, in which there is little or no harvest, which reduces the effective yield without a commensurate drop in fertilizer demand. Finally, while switchgrass may not demonstrate a significant benefit when only on-field processes and N are modeled, switchgrass is likely to have a substantially more beneficial impact on SOC than corn stover, due to its extensive root system, which is not included in the base case scenario.

Production and preprocessing (grinding to a 10 mm (0.4 in) maximum particle size) of feedstock dominates the life cycle GHG impacts of this cellulosic ethanol production process; over 79% of base case GHG emissions are attributed to these phases. With transportation of feedstock, this number jumps to 97%. This is largely due to the conversion facility's ability to meet its own energy needs by combusting process byproducts, and reflects the design philosophy behind a low-input conversion process. Since very few chemicals are required at the conversion facility, energy is the main input to the process, which is ultimately provided by the feedstock.

The life cycle GHG and energy flows for the base case scenario generally agree with other LCAs of cellulosic biofuels; they somewhat lower than those of Wang, *et al.* (2007) and Spatari & MacLean

(2010) and higher than that of Aden & Heath (2009). The variability between estimates reported in different studies is well within the range of uncertainty anticipated given data limitations and differing modeling assumptions. Both stover and switchgrass-derived ethanol yielded similar results for non-GHG flows and indicators; the notable exception being significantly higher switchgrass VOC emissions due to the different fertilizer compounds used. Because the selected fertilizer compounds are based on test plots rather than commercial production, they might change in the future.

5.3.1 Sensitivity Analysis

Sensitivity analysis was conducted by analyzing possible alternative scenarios. Many of the processes modeled in this paper are subject to uncertainty; however, the distribution of this uncertainty is not yet well understood, limiting the usefulness of stochastic analysis. Table 1 shows the list of scenarios that were evaluated as sensitivity cases for corn stover ethanol. Table 2 shows the list of scenarios for switchgrass ethanol. These scenarios are not intended to be an exhaustive set of possibilities, but rather reflect important conditions for future cellulosic ethanol production systems. These scenarios highlight some of the important characteristics of a cellulosic ethanol production system.

The effects of stover collection on soil condition and soil chemistry are still being researched and debated (Anderson-Teixeira et al., 2013; J. Johnson et al., 2013; D. L. Karlen, Birell, et al., 2011; D. L. Karlen, Varvel, et al., 2011). Accordingly, scenarios C1 and C2 evaluate the effects of SOC depletion based on the meta-analysis of field tests reported in Anderson-Teixeira (2009); scenarios C3 and C4 evaluate N_2O and SOC parameters based on DAYCENT modeling reported in Kim & Dale (2009).

Scenario Number	Scenario Name	Changes from Base Case
C1	Corn Stover High SOC Change	Corn Stover SOC changes per Anderson-Teixeira (2009) Full-Form model, 30cm sampling depth, 25% residue removal, 10 year sample
C2	Corn Stover Low SOC Change	Corn Stover SOC changes per Anderson-Teixeira (2009) Reduced-Form model, 30cm sampling depth, 25% residue removal, 10 year sample
C3	Corn Stover w/ N_2O Reduction	Reduces N_2O emissions by .5 kg N_2O-N per hectare-year, based on average from Table 3 Kim & Dale (2009)
C4	Corn Stover w/ DAYCENT Soil Change Parameters	Applies N_2O, NO_x and SOC changes based on average of all sites reported in Table 3, Kim & Dale (2009)
C5	Corn Stover 5MW Electricity Deficit	As base case, except facility requires 5MW of additional electricity from grid, using Ecoinvent US average grid LCI
C6	Corn Stover 5MW Electricity Surplus	As base case, except facility exports 5MW of additional electricity to grid, displacing using Ecoinvent US average grid LCI generation
C7	Corn Stover 17MW Electricity Surplus	As base case, except facility exports 17MW of additional electricity to grid, displacing using Ecoinvent US average grid LCI generation
C8	Corn Stover, High Conversion Process Efficiency	As base, except facility produces 10% more ethanol per unit of feedstock (77 gallon / dry ton) input, with no other changes to system
C9	Corn Stover, Low Conversion Process Efficiency	As base, except facility produces 10% less ethanol per unit of feedstock (63 gallon / dry ton) input, with no other changes to system
C10	Corn Stover, External Enzymes Needed	As base, but requires 10 g / kg dry matter of cellulase enzymes, with LCI as reported by (Dunn, Mueller, Wang, & Han, 2012)
C11	Corn Stover, Dilute Acid Pretreatment	As base, but adds additional acid and neutralization chemicals per (Humbird et al., 2011)

Table 5-2 - List of sensitivity case scenarios for corn stover based production.

Coproduct credits are also a source of uncertainty in the life cycle of biofuels. The cellulosic biofuel described in this paper has only one important potential coproduct; electricity. Scenarios C5, C6 and C7 evaluate the impacts of the facility providing or demanding grid electricity. Finally, there is uncertainty surrounding the conversion process itself, so scenarios C8-C12 evaluate the impacts of different conversion process yields or a need for additional enzymes or chemicals. A complete LCI for each scenario, except the external enzyme ones, is provided in tables S1-S23. Since no complete LCI has yet been published for cellulase enzymes, the GHG impact of this scenario is reported in the text of this paper, but it is omitted from the supplementary material since it is identical to the base case in every respect except for 100-year GWP.

Scenario Number	Scenario Name	Changes from Base Case
S1	Switchgrass with SOC Change	SOC changes per Anderson-Teixeira (2009) Reduced-Form model, 30cm sampling depth, 10 years harvest
S2	Switchgrass 5MW Electricity Deficit	As base case, except facility requires 5MW of additional electricity from grid, using Ecoinvent US average grid LCI
S3	Switchgrass 5MW Electricity Surplus	As base case, except facility exports 5MW of additional electricity to grid, displacing using Ecoinvent US average grid LCI generation
S4	Switchgrass 17MW Electricity Surplus	As base case, except facility exports 17MW of additional electricity to grid, displacing using Ecoinvent US average grid LCI generation
S5	Switchgrass, High Conversion Process Efficiency	As base, except facility produces 10% more ethanol per unit of feedstock (77 gallon / dry ton) input, with no other changes to system
S6	Switchgrass, Low Conversion Process Efficiency	As base, except facility produces 10% less ethanol per unit of feedstock (63 gallon / dry ton) input, with no other changes to system
S7	Switchgrass, External Enzymes Needed	As base, but requires 10 g / kg dry matter of cellulase enzymes, with LCI as reported by (Dunn et al., 2012)
S8	Switchgrass, Dilute Acid Pretreatment	As base, but adds additional acid and neutralization chemicals per (Humbird et al., 2011)

Table 5-3 - List of sensitivity case scenarios for switchgrass based production

There are, at present, fewer data available about the soil effects of switchgrass cultivation, so fewer scenarios are evaluated for this feedstock. The scenarios reported for switchgrass are, otherwise, essentially the same as those for corn stover.

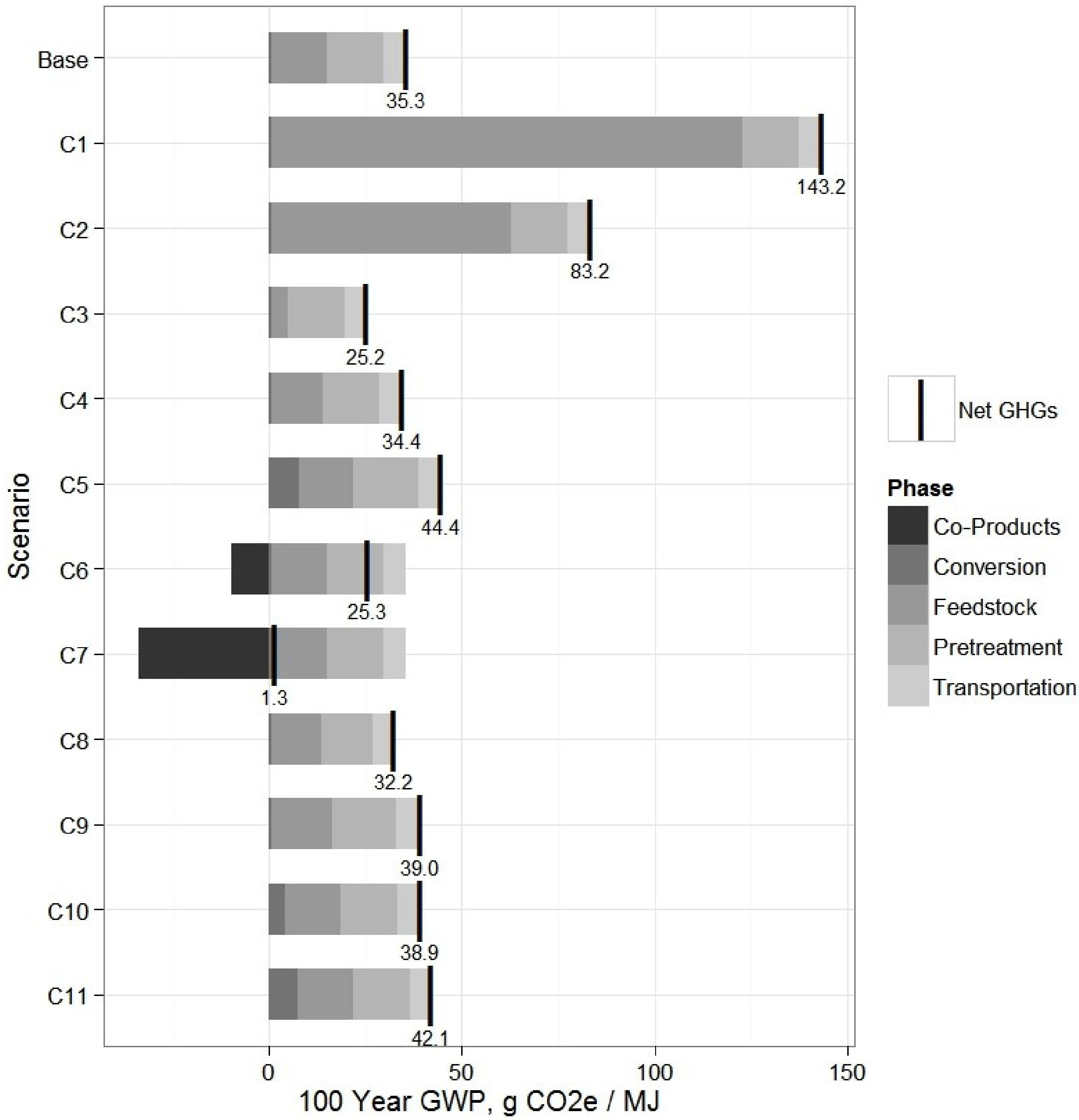


Figure 5-2 - GHG Impacts by Phase of Life Cycle for Corn Stover Scenarios. See Table 5-2 for scenario list.

Figure 5-2 shows the life cycle GHG impacts of the corn stover scenarios described in Table 5-2, with the impacts of different phases of the production life cycle highlighted by shading. Soil carbon effects are an element of substantial uncertainty and there is substantial disagreement between the effects modeled by DAYCENT, as reported by Kim & Dale (2009) and the meta-analysis of field studies reported by Anderson-Teixeira, *et al.* (Anderson-Teixeira et al., 2009). Excluding soil carbon effects, most scenarios fall in the range of 36-46 g CO_2e pr MJ of delivered fuel.

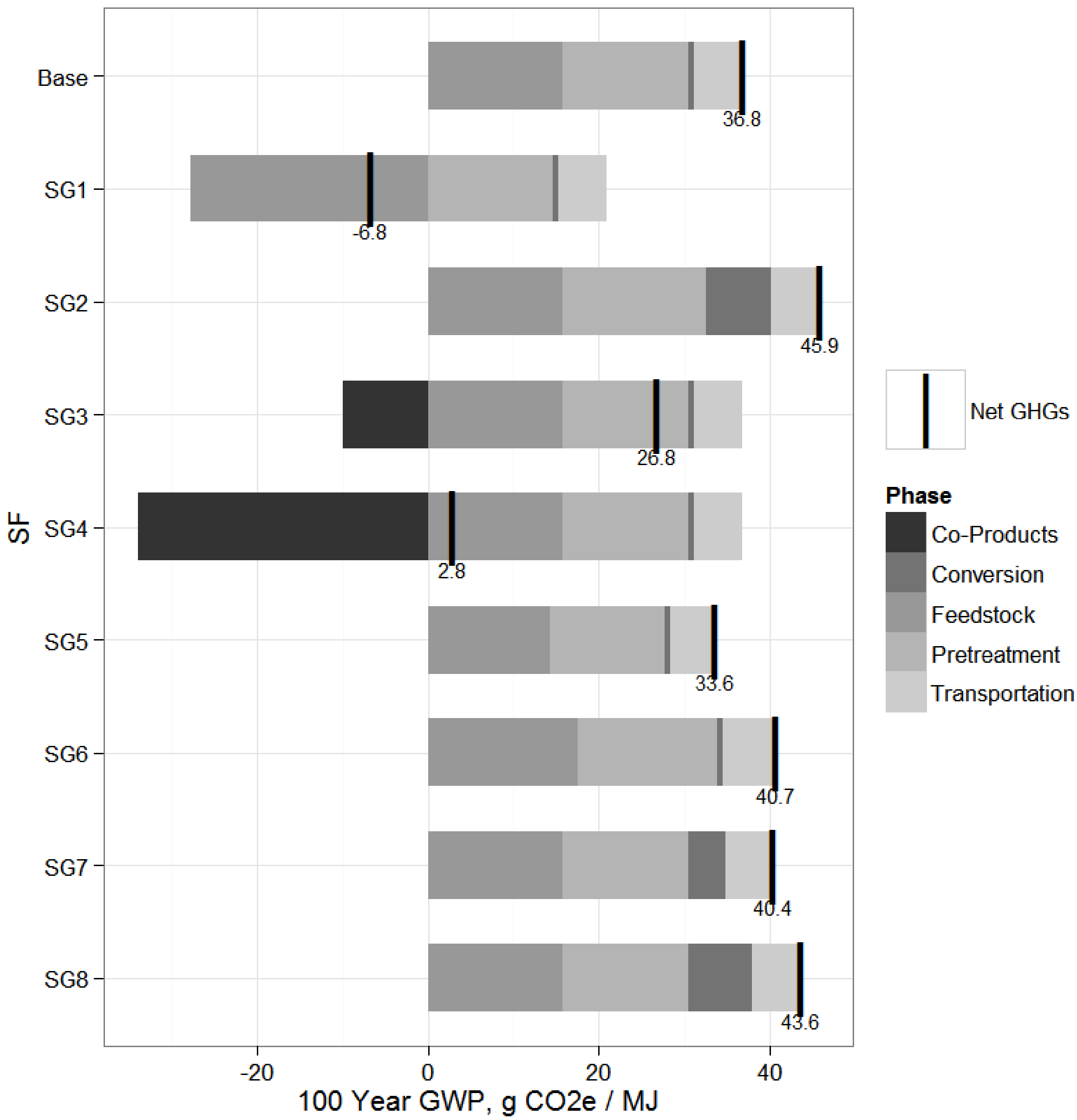


Figure 5-3 - GHG Impacts by Phase of Life Cycle for Switchgrass Scenarios. See Table 5-3 for scenario list.

Soil carbon changes have a greater effect on GHG intensity than any other parameters in this study, particularly in the case of corn stover (Figure 5-2). The base-case analysis assumed that a limited amount of stover could be removed without reducing SOC levels, as has been claimed by multiple authors in this field (Follett et al., 2012; Hess et al., 2009a). In contrast, when integrated with the LCA modeling, the soil carbon model from Anderson-Teixeira (2009) demonstrated SOC losses of a magnitude greater than all other GHG impacts in the stover ethanol production system combined, even under its more optimistic reduced-form model. The less optimistic, full form model predicted SOC losses so high as to render stover based ethanol more carbon-intensive than petroleum gasoline under any realistic production process (Figure 5-3). Unfortunately, there are a limited number of studies on the SOC effects of stover removal, so the meta-analysis results from the Anderson-Teixeira *et al.* paper may not reflect real-world SOC changes due to small-sample error.

The alternative source for modeling SOC changes, DAYCENT modeling by Kim and Dale (2009), also predicted a loss of SOC under sustained stover harvest, though the magnitude was significantly smaller than that predicted by Anderson-Teixeira and colleagues. In addition, DAYCENT accounted for reductions in N_2O emissions due to stover removal, which ultimately outweighed SOC losses on a CO_2e basis. These N_2O reductions are highly uncertain and depend largely on local conditions; Németh (2012) determined that stover removal could actually increase N_2O emissions by altering soil microbial communities and exacerbating temperature cycles. A detailed, region-specific analysis of soil effects due to stover removal may be necessary to accurately assess the GHG impacts of any stover-based biofuel.

Based on this LCA, the most important difference between corn stover and switchgrass as biofuel feedstock is the *potential* difference between SOC effects; corn stover harvest may risk significant SOC reductions, while switchgrass has the possibility of producing near-term SOC gains, assuming switchgrass cultivation does not induce iLUC. Some authors, notably Follett, *et al.* (2012), find that SOC gains can occur under sustained corn-stover harvest, however, these studies typically assume a conversion from conventional-tillage production to no-tillage, or production on marginal (low-SOC) land. In some situations, these assumptions may hold true, but there are at least two problems with assigning an SOC increase to stover. First, it is likely that the bulk of corn stover for future biofuel systems would be produced from existing corn acreage, so it is more appropriate to model likely changes from business-as-usual practices, which would not necessarily include a change in tillage. In addition, from a methodological standpoint it may not be defensible to assign increasing SOC to stover, since the business-as-usual comparison could arguably be corn cultivation without stover removal. In such a case removal of stover may be slowing SOC increases after a switch from till to no-till cultivation. Switchgrass, on the other hand, is seldom grown at present, so any cultivation of switchgrass would likely represent a change from business-as-usual and the SOC changes, whether gains or losses, could be assigned to the products of the cultivation system.

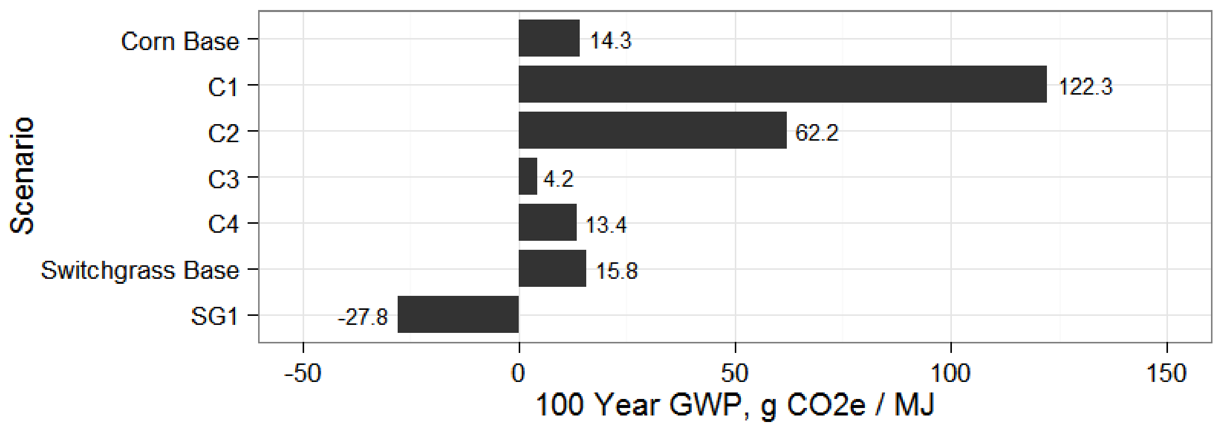


Figure 5-4 - GHG emissions from feedstock production for corn stover

The second greatest area of uncertainty in LCA results is the electricity deficit or surplus generated by the conversion facility. The baseline scenario predicts a substantial (~17 MW) surplus of electricity as well as some excess heat or low-pressure steam. The baseline scenario does not credit the produced ethanol for producing grid electricity due to the substantial uncertainty surrounding the recoverable energy from process byproducts as well as the total demand from the conversion facility. If the conversion facility could, in fact, produce surplus electricity as well as fuel, as described by Humbird *et al.* (2011) among others, displacement of conventional electricity could be credited towards the resulting biofuels.

Assuming that the credit for displaced electricity is equivalent to the GHG emissions from grid-average electricity, each MW of on-site electricity generation reduces the carbon intensity of produced fuels by approximately 2 g CO_2e per MJ, assuming 265 liter/tonne (63.5 gallon/ton) conversion efficiency. Under the most optimistic assumptions of facility energy balance, this could lead to biofuels that are nominally carbon-negative. Other researchers have raised the possibility of carbon-negative biofuels, e.g. Tillman *et al.* (2006), but significant uncertainty remains. One factor in carbon negative biofuels is the presumption that electricity generation displaces average or marginal electricity. Displacement is a consequential approach to assigning value to a co-product and only appropriate when exploring “what if” scenarios. If a facility is in operation and producing ethanol and electricity, then the environmental flows associated with the system should allocated (divided) among the two products – a so-called “attributional” approach.

5.4 Discussion

When SOC changes are omitted, and assuming no iLUC occurs, both corn stover and switchgrass biofuels, under the assumptions described in the base case scenario, have the potential to produce biofuels with substantial life-cycle GHG reductions compared to petroleum-based fuels. Under base case conditions, both fuels meet the 50% life-cycle GHG reduction target required to achieve the “Advanced” biofuel category of the RFS; in addition, both approach or may even meet the 60% reduction target for the “Cellulosic” designation. Either would represent a substantial milestone in sustainable transportation, if produced at commercial scale.The generally favorable GHG profile of these biofuels is due in part to the low-input conversion process. By drastically reducing the need for chemicals or enzymes in the hydrolysis steps, the impact of the conversion process becomes dominated by energy requirements. The conversion process produces energy-rich byproducts, including lignin cake and biogas, which can be utilized to meet the facility energy demand. In doing so, the conversion process approaches a closed-loop process, with the only additions beyond feedstock being a small quantity of inputs required for microbe propagation and flue gas cleanup. Even in cases where additional chemical-based steps are required, such as those reported in scenario C10 (the dilute-acid hydrolysis scenarios) and C11 (additional enzyme scenarios), the lifecycle GHG impacts are still dominated by feedstock production and processing. Under these scenarios, the resultant fuels mostly meet the RFS “Advanced” biofuel target, but would not meet the “Cellulosic” target without additional co-product credits or improvements to conversion efficiency.

With conversion process GHG impacts relatively small, SOC becomes the most important area of uncertainty in the cellulosic ethanol life cycle. It is critical that the SOC impacts of sustained corn stover harvest be better understood if this feedstock is to be a substantial element of future energy policy. This is especially important because stover’s SOC changes are likely to be losses under most conditions. There may be certain soil conditions, such as those with high clay content or very low initial SOC in which the assumption of SOC neutrality for partial corn stover harvest would hold true. Accurately estimating the SOC effects of stover collection on a site-specific basis may be required to accurately estimate the GHG impacts of stover-based biofuels. Under typical conditions, however, the consensus in literature is that routine stover collection would likely lead to some decrease in SOC, which imposes a substantial GHG penalty on the resultant fuels. If stover-based fuels are to meet the RFS targets, this penalty would have to be offset in some fashion; for example, by GHG credits from renewable electricity or reductions in N_2O from field emissions.

Switchgrass, on the other hand, appears likely to present an opportunity for reducing life-cycle GHG emissions by increasing SOC during cultivation. While the magnitude of this effect is uncertain, it is likely that it will offset the marginally higher GHG emissions from N fertilization than those of corn stover. It is important to note that the SOC sequestration by switchgrass may decline over time as SOC levels equilibrate at a higher level, and may be lost when switchgrass is replanted and soil is disturbed. Further research is required to determine the duration of SOC sequestration as well as the persistence of SOC in soils used for bioenergy crops after repeated harvest. Existing literature, along with the work described in Chapter 4, is fairly conclusive that corn stover removal leads to SOC decline. Even if the SOC effect of switchgrass or miscanthus is on the more conservative end of the range presented in current literature, it seems likely that its SOC effects are going to be significantly better than those of corn stover.

The importance of SOC in the biofuel life cycle highlights an inherent limitation in using large quantities of biomass for energy purposes: the embodied nutrients in the feedstock must, at some point, be replaced to avoid soil depletion. At present, the default method for replacing these nutrients is petrochemical fertilizers. More environmentally-friendly methods have been proposed to address nutrient replacement, such as compost or residual ash from biomass combustion, but it is unclear what impacts these methods might have when applied to corn production systems (Brown & Cotton, 2011; Pandey & Singh, 2010; Risse & Gaskin, 2010). Future research is required to better evaluate alternatives to petrochemical fertilization.

Acknowledgment: This material is based upon work supported by the Department of Energy under Award Number DE-EE0002881.

Chapter 6: Effects of Air Pollution Control Costs on Biofuel Production System Development

This study builds upon the Geospatial Bioenergy Systems Model (GBSM), a nationwide, spatially explicit techno-economic model of biofuel production (Parker, Hart, et al., 2010; Parker, Tittmann, et al., 2010). GBSM is an optimization model that uses county-level feedstock resource assessments, potential conversion facility locations, conversion technology models and fuel demand to model spatial distributions and supply curves of biofuel production under a variety of scenarios. The optimization chooses sites for production facilities based on the total cost of producing biomass and transporting it to the facility. At present, GBSM does not consider any environmental aspects of production, though energy and GHG footprints could be derived from the results with modest effort. Other environmental impacts could be derived by associating activity within the model (e.g. feedstock production, transport or conversion) with LCIs for that activity, as long as the LCIs were spatially explicit as well. Since insufficient spatial LCI data for constituent activities exists at present and models of conversion technology are speculative and immature, this work is likely to be dependent on the development of several critical datasets.

6.1 Introduction

The U.S. federal Renewable Fuel Standard (RFS2) mandates a significant increase in the supply of biofuels; 36 billion gallons (136 billion liters) of ethanol or 23.6 billion gallons (89 billion liters) of gasoline equivalent (GGe) must be brought to market by 2022. This represents an increase of 23 billion gallons (87 billion liters) of ethanol from 2012 production levels. Many analysts have begun to evaluate the implications this policy will have on U.S. energy, environmental and agricultural policies (Alfstad, 2008; Chen, Huang, Khanna, & Önal, 2011; Hoekman, 2009; Yaccobucci & Schnepf, 2007). While there is evidence that biofuels can help meet some energy security and greenhouse gas (GHG) reduction goals

(Farrell et al., 2006; M. Wang et al., 2007), there is still significant uncertainty regarding how policies to increase the supply of biofuels will affect other environmental objectives, such as improving air quality (Hill et al., 2009). Another concern is whether biofuel producers can meet the RFS2 goals; production targets for advanced and cellulosic biofuels have been repeatedly waived due to a lack of supply. The delayed development of advanced biofuels is typically attributed to problems in scaling up and optimizing production technology as well as unfavorable economic conditions within the sector. Permitting and environmental concerns are believed to be a secondary challenge; obtaining air pollutant emission permits for the combustion activity associated with biorefinery operation has been anecdotally described as an obstacle to building these facilities in some areas (Kaffka, Williams, & Murphy, 2013; Voegele, 2009; Youngs, 2011). This paper models the interaction between RFS2 biofuel production and air quality protection policies, by evaluating the degree to which current air quality regulations increase biofuel production costs and change the spatial distribution of production systems.

Previous work developed a spatially explicit bioenergy systems techno-economic optimization model, the Geospatial Bioenergy Systems Model (GBSM), to forecast the spatial layout, feedstock utilization and economic characteristics of a biofuel production industry that could meet the mandate (Parker, Tittmann, et al., 2010). The research described here extends this work by incorporating the costs of air quality regulation compliance in the existing techno-economic model. Cellulosic ethanol bio-refineries are typically large industrial facilities which obtain heat and electricity by on-site combustion; many burn process byproducts like lignin cake or biochar, others use raw biomass or fossil fuels. These facilities may have total electricity demands exceeding 25 megawatts (Humbird et al., 2011) (MW), as well as heat and steam requirements, which implies a need for substantial power generation capacity. In cases where solid fuels like lignin cake, coal or biomass meet this demand, there may be a high potential for air pollutant emissions. In addition to the facility's power system, bio-refineries may also contribute to air pollution through fugitive emissions from process vessels, exhaust emissions from associated mobile equipment, suspended dust from biomass handling and increased agricultural emissions from feedstock production.

Biofuels are likely to present a novel spatial distribution of air pollution sources. Rather than concentrating air pollutant emissions around industrial or extractive-industry centers, biofuel production will likely distribute itself across agricultural regions to minimize transport distances for biomass feedstock. This may cause a significant increase in air pollutant emissions in areas where such emissions have, historically, been low.

The U.S. has an air quality management policy which divides authority between Federal, State and local actors. The core of this policy is the Clean Air Act and subsequent amendments, which sets maximum allowable concentrations for several hazardous pollutants. These standards guide the regulatory, permitting and enforcement activity of state environmental quality departments and local Air Quality Management Districts (AQMDs). A region that exceeds a federal standard for pollutants is said to be in non-attainment of the Clean Air Act standards, or a "Non-Attainment Area" (NAA), which gives regulators greater leeway to enact strict pollution control policies, including restrictions on the issuance of permits and increased requirements for air pollution control devices.

Most existing research on biofuels has focused on the technological capabilities, feasibility, economics or GHG implications of biofuels (Hettinga et al., 2009; Sheehan et al., 2003; Spatari et al., 2005). Studies on air pollutant emissions have overwhelmingly focused on the effects of these fuels during combustion. Biofuels are generally thought to have, at worst, equivalent air pollution during combustion compared to the fossil fuels they displace and in some cases may reduce air pollution levels(Wagstrom & Hill, 2012). Comparatively less research exists on the air pollution implications of large-scale transition to biofuel production. Hill, *et al.* consider air pollutant emissions over the full fuel cycle of biofuels by monetizing the costs of health harms from gasoline and ethanol, to include them in an evaluation of total economic costs of different transportation fuels(Hill et al., 2009). In addition to life-cycle analyses, other authors focus on particular air pollutant effects, such as emissions from bio-refineries(Jones, 2010) or land-use change effects(Tsao et al., 2012). Tessum, *et al*. create a spatially explicit emissions inventory of the air pollutant emissions from current gasoline and ethanol production, but do not prospectively model future industry developments or the emergence of advanced technologies(Tessum, Marshall, & Hill, 2012). On the whole, the subject of air pollution effects from biofuel production has not been thoroughly explored, thus interactions between air quality policies and the existing biofuel mandate are not understood.

This paper advances research in this field by assessing how existing air quality policy could affect the spatial distribution of biofuel production and the available quantity and cost of biofuels. Permitting requirements could conceivably incentivize facilities to locate in areas with lower requirements. Since the economic and energy efficiency of biofuel production is strongly influenced by the location of the production facility, it is important to determine whether these factors need to be considered in future models of biofuel production.

6.2 Methods

This paper utilizes the GBSM, a mixed-integer, spatially explicit techno-economic optimization model; the development of GBSM has been described previously(Parker, Hart, et al., 2010; Parker, Tittmann, et al., 2010; Tittmann et al., 2010) and a detailed description of the model is available in the supplementary information associated with this paper. This model evaluates the optimal behavior of a biofuel industry given fuel demand, biofuel selling price, conversion costs and feedstock supply constraints. GBSM builds upon the concepts of previous biofuel modeling work by considering multiple conversion technologies, conversion facility scales, feedstock sources (including wastes, residues and purpose-grown energy crops) endogenously, whereas most previous work made fixed, exogenous assumptions for one or more of these parameters. The spatial layout of feedstocks and demand are developed from existing biomass supply (National Research Council, 2011; U.S. Department of Energy, 2011) and data for vehicle kilometers traveled (Hu, Reuscher, Schmoyer, & Chin, 2007) (VKT, a measure of travel activity which represents a motorized vehicle traveling one kilometer) respectively, to determine transportation costs and optimal biorefinery locations. Potential feedstocks include agricultural residues (e.g. corn stover), residue wood from forest product industries and thinning, municipal solid waste (MSW), herbaceous energy crops such a switchgrass or miscanthus, and pulpwood. While GBSM is computationally intensive, the endogenous consideration of so many variables maximizes the model's flexibility to incorporate changes in technology or market conditions.

For this analysis, the GBSM was modified to operate as a cost minimization model subject to meeting a demand for biofuel production. GBSM is considered a cost minimization model, rather than a profit maximization one, because revenue is fixed at the average selling price of fuels and production volumes are approximately RFS2 targets (some variation in total volume between scenarios is an artifact of the model's optimization process). Since revenues are fixed, all optimization occurs through cost minimization. The costs considered are the procurement of feedstock (PC_{ifc}), the transportation of feedstock to the biorefinery (DC_{ijf}), the transportation of the product fuel to the distribution terminals (TC_{jkp}) and the fixed (a_{jts}) and capacity-depenent (b_{jfts}) conversion costs, which are annualized to include capital and operating costs. Subscripts indicate the feedstock supply location (i), conversion facility location (j), fuel terminal location (k), feedstock type (f), feedstock cost (c), fuel type (p), conversion technology (t) and co-product type (e). The conversion cost is dependent on the size of the biorefinery. In this analysis, it is characterized as a binary-linear function with a fixed cost (a_t) if a facility is built and a variable cost (b_t) dependent on the capacity of the biorefinery expressed in terms of feedstock input (Yf_{jft}).

GBSM is formulated as a mixed integer linear program and implemented within the GAMS programming environment using the CPLEX optimization algorithm(GAMS Development Corporation, 2010; IBM, 2010). All capital costs are annualized at a 10% rate of return over a 20 year facility lifespan. The objective of the program for this analysis is to minimize annual cost.

$$Annual\ Cost = \sum_{ijfc}\left(PC_{ifc} + DC_{ijf}\right) \cdot F_{ijfc} + \sum_{jts} a_{jts} \cdot X_{jts} + \sum_{jfts} b_{jfts} \cdot Y_{jfts} + \sum_{jkp} TC_{jkp} \cdot T_{jkp} - \sum_{jtse} MP_e \cdot COP_{jtse} \qquad (6.1)$$

Revenue generated by coproducts is introduced as a negative cost based the quantities produced (COP_{jtse}) and selling prices of the products (MP_e).

The objective function is combined with a number of constraints representing the physical limitations or restrictions of the biomass industry in the mathematical model as well as appropriate non-negativity constraints (See supplementary material for a more complete description of core GBSM design). The RFS mandate is represented as a set of demand constraints that must be met for each of the categories of renewable fuels. The model includes the corn ethanol and biodiesel industries to account for their portion of both the mandate and the blending limits. Model runs were performed only at the 2022 mandated volumes.

Air pollution control costs are added to the model by determining which facilities would be subject to additional costs for air pollution control (APC) devices and assigning an extra cost to those facilities. EPA non-attainment areas are used to screen those facilities and determine which require extra APC (U.S. EPA, 2013b). If a facility is located in an EPA nonattainment area for particulate matter of < 2.5 micron aerodynamic diameter ($PM_{2.5}$), it is flagged as requiring additional $PM_{2.5}$ control devices. If a facility is located in an ozone nonattainment area, it is flagged as requiring additional nitrogen oxides (NO_x) control devices, since ozone is not directly emitted from the process but rather forms from atmospheric photochemical reactions between NO_x and volatile organic compounds(Seinfeld & Pandis, 2006). NO_x control is the default choice for reducing ozone concentrations because there are many natural sources of reactive VOCs and ozone forming reactions are most often limited by NO_x in most high-ozone areas. Additionally, VOC control is, in most cases, substantially less expensive than NO_x control, so adding APC technology for VOC control would have a comparatively minimal effect on the output of this model.

Air pollution control devices for $PM_{2.5}$ and NO_x are added to the total cost by modifying the fixed and capacity-dependent (a_{jt} and b_{jt}, respectively) facility costs as compared to the version described in previous reports.

$$a_{jt} = abase_{jt} + B_n(aG_{jnt}) \quad (6.2)$$

$$b_{jt} = bbase_{jt} + B_n(bH_{jnt}) \quad (6.3)$$

Where B_n is a binary operator which is 1 if the specified facility is in a NAA for pollutant n ($PM_{2.5}$ or Ozone), 0 otherwise, G_{jnt} are the fixed costs for adding pollution control devices to the facility and H_{jnt} are the capacity-dependent costs for adding pollution control devices to the facility.

There are multiple types of APC technology available for controlling each pollutant; in practice the most appropriate type would be selected on a case-by-case basis in order to best fit conditions specific to each conversion facility. This paper considers one representative type of APC for each technology and models cost based off of established values for that type. This is not intended to imply that the selected technology would always be deployed but rather to serve as a reasonable proxy for increased costs relating to emissions control devices.

GBSM models costs for two basic biofuel technological pathways, cellulosic ethanol and renewable diesel made by a Fischer-Tropsch (F-T) process. The ethanol pathway is based on the National Renewable Energy Laboratory (NREL) “Dilute-Acid Pretreatment, Enzymatic Hydrolysis and Fermentation process” (Humbird et al., 2011); other processes were considered but rejected because their reported costs were higher and therefore would not be selected by the cost-minimizing model (e.g. NREL’s thermochemical ethanol pathway (Dutta et al., 2011)). The F-T process was also based on an NREL design (Swanson, Satrio, Brown, Platon, & Hsu, 2010). The most notable difference between these two is a substantially lower yield of biofuels from the F-T diesel process, since much of the carbon in the feedstock is converted into a naptha-like co-product, which is too light to be used for fuel production and is instead sold into the chemicals market (U.S. EPA, 2010). Within the modeling framework of GBSM, conversion to F-T diesel is a higher-cost option to meet RFS2 targets, so the model preferentially chooses to meet RFS2 targets by production of cellulosic ethanol. F-T diesel conversion is used only sparingly, only for conversion of relatively uncontrolled “dirty” MSW, which cannot be used in the cellulosic ethanol process.

GBSM allows plant size to scale up or down to reflect the local conditions, to a minimum of 95 million liters per year (25 million gallons per year) and a maximum of 454 million liters per year (120 million gallons per year). Scaling of facility costs, including air pollution control devices is done by the method described in the cost estimates of the NREL reports(Humbird et al., 2011; Swanson et al., 2010).

$$Cost_{scaled} = \left(\frac{new\ size}{base\ size}\right)^{0.7} \cdot Direct\ Cost \cdot (1 + Indirect\ Cost\ Factor) \qquad (6.4)$$

Where the base size is that published in the NREL designs, 231 million liter/year (61 million gallon/year), for the biochemical pathway and 245 million liter/year (65 million gallon/year), for the F-T diesel pathway, the direct costs are as reported by NREL. Indirect costs were set at 60%, and include permitting, inventory management, administrative overhead and contingencies (Humbird et al., 2011). Both capital and operating costs were scaled with this method.

All conversion facilities are assumed to have a baghouse and/or cyclones as a primary PM control measure, these costs are built into the basic cost model for each appropriate technology. Additional $PM_{2.5}$ control, for facilities in PM nonattainment areas a dry electrostatic precipitator (ESP) (U.S. EPA, 2007) is used/modeled. NO_x control is modeled after a selective catalytic reduction (SCR) system (U.S. EPA, 2002). Cost parameters for the control technologies are provided in Table 6-1.

Conversion Technology	APC Type	Capital Cost ($ millions)	Operating Cost ($ 1000/year)
Cellulosic Ethanol – Base Facility		422.5	76,000
Cellulosic Ethanol	ESP	8.9	781
Cellulosic Ethanol	SCR	15.9	890
F-T Diesel - Base Facility		498	157,900
F-T Diesel	ESP	3.8	435
F-T Diesel	SCR	25.0	922

Table 6-1 - Cost factors for APC devices on a 61 million gallon/year Cellulosic Ethanol and a 64.7 million gallon/year Fischer-Tropsch Diesel Production Facilities

To better understand the sensitivity of this model to some key parameters, four air pollution control scenarios are modeled: “AQ_Off” reflects no consideration of air quality regulations or the cost of APC beyond the cyclones and baghouses included in the baseline conversion facility designs. AQ_Off is effectively the *status quo* of biofuel spatial models. “AQ_On” applies the additional cost factors described in Table 6-1, scaled as described in Equation 5, to any facility that locates in a non-attainment area. This tends to reduce the number of facilities which locate inside NA areas; the model seeks to locate equivalent capacity outside of NA areas instead. Where feedstock and demand conditions are sufficiently favorable, facilities inside NA areas are subject to this additional cost increment. It is expected that the AQ_On scenario will therefore differ from AQ_Off in both spatial distribution and costs.

The “AQ_Prohibit” scenario prevents any facilities from being constructed in non-attainment areas. This is a proxy for a more strict air quality control policy under which instead of conversion facilities in NA areas being subject to additional pollution control requirements, a complete ban on construction of facilities in NA areas exists instead. The “AQ_Added” scenario reflects the same spatial distribution of facilities as in the AQ_Off scenario, with APC costs added to any facilities within NA areas. This reflects a scenario under which facilities were unable to select sites which avoid APC costs. This scenario is not intended to reflect a likely course of action in practice, rather it is a tool to explore the relative importance of transportation and feedstock costs (which are dependent on the facility’s location) and the costs of air quality compliance.

All scenarios assume that the total RFS2 mandate can be met with ethanol. In practice, this would require the relaxation of the current restriction on gasoline-ethanol blends to 10% ethanol content or less (the “E10 blend wall”) or a substantial increase in higher-blend ethanol fuel consumption, such as E85. Other scenarios, which considered increased production of non-ethanol fuels such as F-T Diesel were modeled; results from these scenarios showed a very similar spatial distribution and higher costs than those presented in the following section. Since they do not substantially contribute to the discussion at the core of this study, they will not be discussed further.

6.3 Results

GBSM modeling showed a difference in average ethanol production cost between AQ_Off and AQ_On scenarios of less than one cent per gallon; in fact both scenarios have a production weighted average cost of $3.04, when rounded to the nearest cent (See Table 6-2). Shifting from the AQ_Off scenario to the AQ_Prohibit scenario, in which no facilities are allowed to be constructed in nonattainment areas, increases average ethanol price by around 4 cents per GGe. Simply adding APC costs to facilities which locate in non-attainment areas in the AQ_Off scenario added around $247 million in total, system-wide annualized costs.

Scenario	Volume (MGGe / year)	Annual Cost (billion $)	Difference from AQ_Off (million $)	Weighted Average Cost ($/gal)	Freight Ton-Miles (million /yr)	Facilities in $PM_{2.5}$ NA areas	Facilities in Ozone NA areas
AQ_Off	12,345	37.48	-	$ 3.036	9,680	23	52
AQ_On	12,346	37.54	57.0	$ 3.040	10,100	17	36
AQ_Prohibit	12,347	38.0	557.1	$ 3.081	12,170	0	0
AQ_Added	12,345	37.7	247.3	$ 3.056	9,680	23	52

Table 6-2 Summary of results from Scenario Modeling. All costs are in 2008 dollars.

Facilities which located in NAA in the AQ_On scenario typically responded to the increased costs by reducing scale and ceasing to accept the most economically marginal feedstocks. GBSM optimization allocates feedstocks to facilities on a marginal basis. Each dry tonne of feedstock has its own procurement and transportation cost; facility scale is determined largely by the cost of local feedstock. The facility optimization seeks the balance point at which the benefits of increased scale balance the costs associated with getting less preferred feedstock. Under the AQ_On scenario, facilities which locate in a NAA and thus, have higher costs, cannot accept as costly feedstocks as those which do have APC costs as well. As a result, the average facility size inside NAA is 51.5 million gallons/year, as compared to 54.1 million gallons/year outside of NAAs.

Figure 6-1 shows a map of the differences between the AP_Off and AP_On scenarios for the Ethanol-Centric scenario. The results of this analysis generally conform to intuitive expectations of such a scenario. In many places, facilities that had located inside non-attainment areas in the AQ_Off scenario, were either downsized or absent in the AQ_On scenario; in their place, there was an approximately equivalent increase in capacity outside of non-attainment areas. Downsizing typically involved facilities ceasing to accept their most marginally profitable feedstocks, usually those farthest away, and reducing their overall size. In areas where production used all available feedstock, such as in the main corn production regions of the U.S., Iowa and eastern Nebraska, relatively little change was observed, since no non-attainment areas were present.

The net system impact of air quality control regulations is small because most facilities do not locate in non-attainment areas, even in the AQ_Off scenario. Two-thirds of all conversion facilities, including many maximum-size facilities in the mid-west and southern U.S., are unaffected by air quality regulation in this model. Additionally, the APC devices themselves represent a relatively small fraction of total conversion costs, when present. The cellulosic ethanol facility in this model requires a capital investment of over $420 million for a base-size (61 MGY) facility(Humbird et al., 2011). This compares to capital costs of $9 million for additional PM control and $16 million for additional NO_x control or about 2% and 4%, respectively. Operating costs for this facility are predicted to be $76 million per year; APC operating costs are estimated to be less than $1 million for each pollutant. The relatively small effect of APC costs explains to a large degree why the spatial distribution and scale of production changes little between the AQ_Off and AQ_On scenarios.

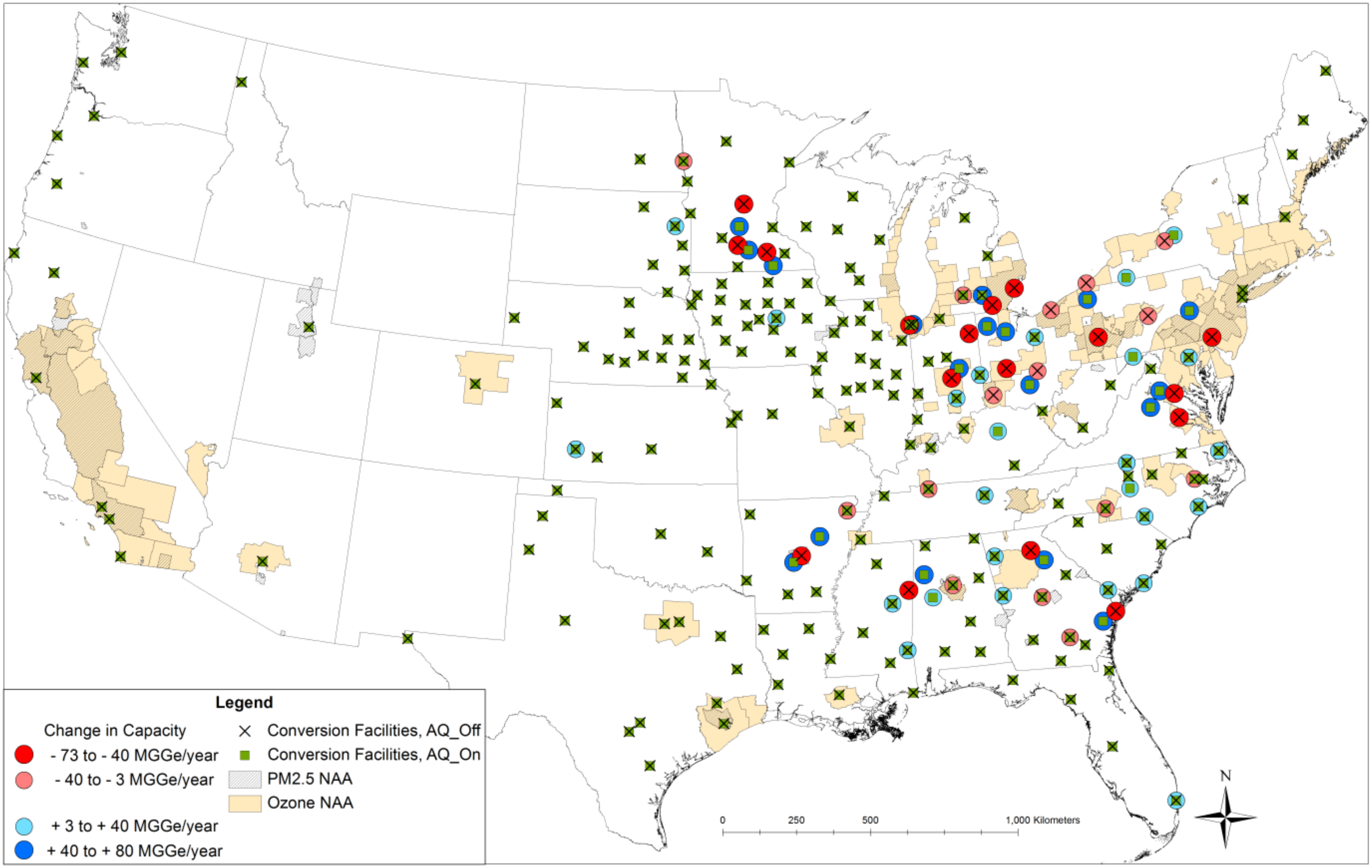


Figure 6-1 - Map of RFS2 biofuel production with and without AQ costs. Most of the conversion facilities predicted by the AQ_Off scenario are unchanged in the AQ_On scenario.

Generally, the cost advantages of locating near preferred feedstocks outweighed the cost detriments of having to install additional emissions control equipment. Costs for freight transport vary by region and contract terms, but an average value from 2007 is 16.5 cents per ton-mile (Research and Innovative Technology Administration, 2011). The difference in truck freight transport between the AQ_On and AQ_Off scenario is approximately 120 million ton-miles, which implies a cost of approximately $20 million, or one-third of the cost difference between the two scenarios. Conversely, transport costs dramatically increased in the AQ_Prohibit scenarios, under which facilities could not locate in non-attainment areas and were forced to locate elsewhere. The costs in the AQ_Prohibit scenarios were greater than those in the AQ_Added scenarios, which did not consider air quality restrictions when selecting sites and just added APC to all facilities in NA areas. This implies that the biofuel production gains greater cost savings from choosing preferred locations than from avoiding the need for APC.

The importance of feedstock choice in minimizing cost is further illustrated by Figure 6-2. Both scenarios get their lowest-cost feedstock largely from waste wood sources, which include construction and demolition residue and wood removed from landfill input streams; only half this supply is assumed to be recoverable due to cost and contamination issues, but that which remains is a very low-cost feedstock. These easily accessible sources can supply no more than the first billion GGe and once exploited, costs increase rapidly. MSW sources are typically the next to be exploited due to low, or even negative procurement costs, however the feedstock cost advantage is offset to some degree by higher conversion costs due to the need to remove potential contaminants. The bulk of biofuel production, and the middle parts of the average cost curves in Figure 6-2 are made up predominantly of agricultural and forestry residues, which have higher costs due to their spatially distributed nature and, in the case of agriculture residue, costs associated with collection and replacing soil nutrients lost when residues are removed(Sawyer & Mallarino, 2007). Energy crops are scarcely used; in some situations, facilities using herbaceous feedstocks used up to 40% energy crop when insufficient residues were available to supply a large-scale plant within a reasonable transport distance.

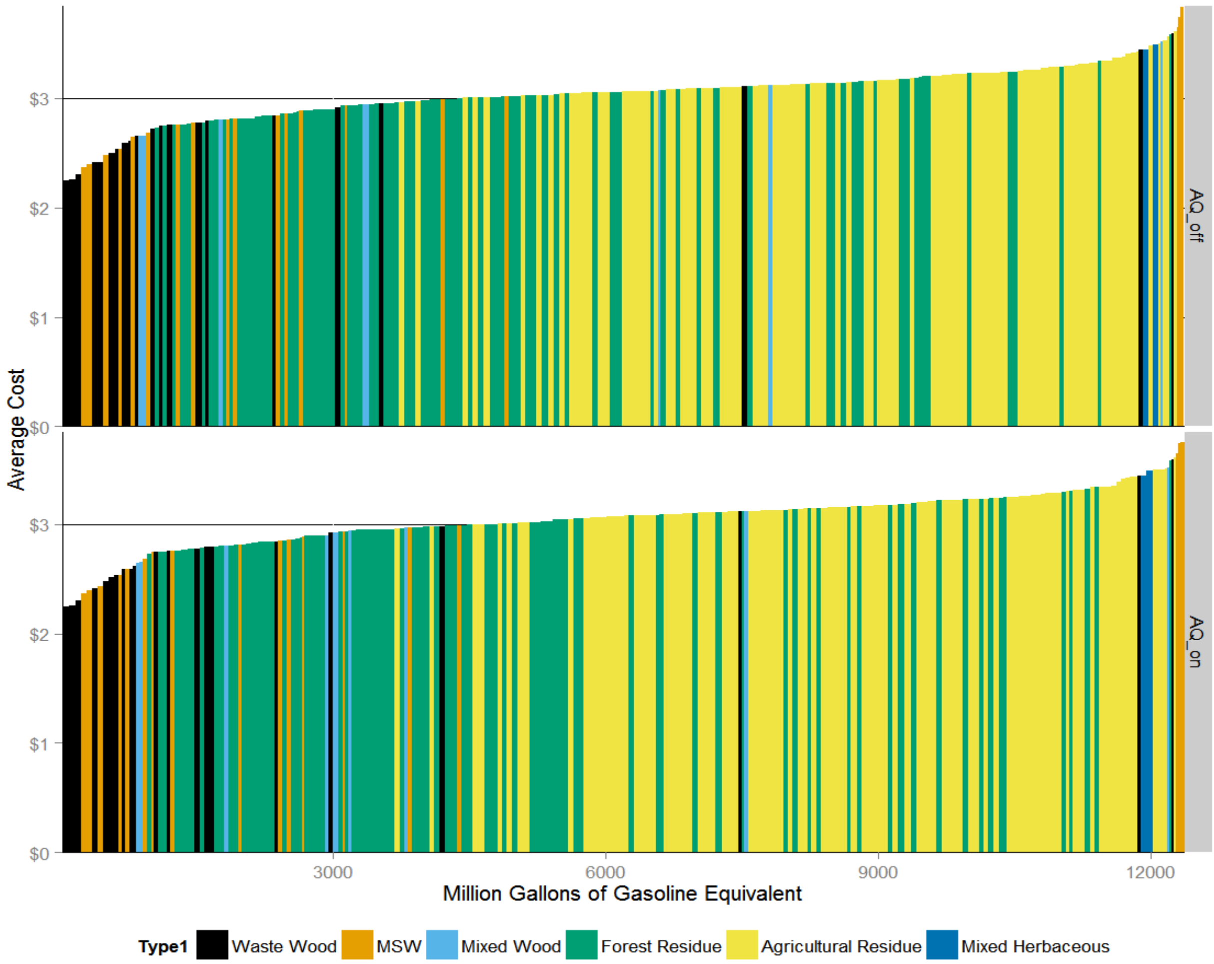


Figure 6-2 Cost curve for RFS2 biofuel production, under the AQ_Off (Top) and AQ_On (Bottom) scenarios with feedstocks indicated. Each bar represents the average costs for one conversion facility. Waste woods and MSW are typically used for the lowest-cost fuels, and energy crops for the highest. Agricultural and forest residues comprise the greatest share of production, at moderate cost.

6.4 Discussion

Air quality regulation exerts a comparatively small effect on the *net system* costs, production volume and spatial arrangement. The relatively small effect of air pollution regulations makes sense when the costs of APC are considered relative to the cost of conversion facilities. A cellulosic ethanol facility as modeled by GBSM which needed both $PM_{2.5}$ and NO_x control devices would cost approximately $25 million more than a facility without additional controls. This additional cost is measured against the over $400 million total capital cost for this facility. Even when interest and capital recovery is considered, this implies less than a 10% increase in annualized costs for these facilities. Because much of the feedstock for biofuel production is located in rural areas, which tend not to be in NAAs, many facilities preferentially locate outside of NAAs areas even when air pollution regulations are not considered during site selection. A minority of facilities are sited by the model in NAAs in the AQ_Off scenario, 60 out of 231. Since only a few facilities are subject to this small increase in costs, the total effects on the system would be expected to be comparatively small. Still, the capital and operating costs of APC in this paper reflect conservative estimates made in consultation with industry experts (Carlson, 2012) and seek to err on the side of over-design for the required level of pollution control.

The costs of feedstock procurement and transport tend to dominate the cost profile for most facilities, so GBSM typically indicates a priority for locating near feedstock supplies rather than avoiding NAAs, even in the AQ_On scenario. Transport is particularly important when considering air pollutant impacts since the overwhelming majority of feedstock transport in GBSM is predicted to be by heavy-duty diesel truck. These trucks can be significant sources of air pollutants, including $PM_{2.5}$ and NO_x, however they are not always considered during the air permit issuance process (they are often considered during local land-use and zoning decisions however). Accurate estimation of air pollutant emissions from biofuel production will require consideration of the freight transport elements of the biofuel production process.

There is also a GHG penalty associated with increasing transport distance. Every ton mile freight transport implies fuel consumption and associated GHG emissions. The AQ_On scenario includes 120 million more miles of feedstock transport by freight truck than AQ_Off. Assuming 187 g CO_2 emission per ton-mile of truck transport(Facanha & Horvath, 2007), the additional 120 million ton-miles result in 22.4 million metric tons of additional CO_2 emission per year.

The question for modelers is whether air quality regulation costs should be included in models of biofuel production systems at all? Models whose purpose is to estimate national-level biofuel supply or costs and which constrain themselves to meet certain production targets (e.g. RFS2) can probably omit air pollution control costs without unduly sacrificing accuracy. Specific locations, however, are still highly uncertain. These results suggest at present that the effect of air pollution control costs on site selection decisions or system-wide costs is likely to be small. Since the net difference in cost between the AQ_On and AQ_Off scenarios is less than 1%, 0.16% in this analysis, it is probably safe to omit air quality regulation costs in national scale models if the model uncertainty is significantly greater than 1%.

While air pollution control costs are not a major factor at the national level, they clearly have a strong influence on local-level decisions. In practice, site selection is typically a lengthy, involved process of negotiation with multiple stakeholders. GBSM cannot monetize the uncertainty associated with seeking permits in areas with strict air pollutant emission regulations. GBSM includes indirect costs, which are intended to model the costs of obtaining permitting and contingencies. However the approach used may not reflect a realistic risk premium for the possibility of a permit application being rejected. Large-scale modeling, such as GBSM which does not model atmospheric transport of pollutants, may be subject to edge effects around the borders of non-attainment areas; it is unlikely that state or local regulators would let a major pollution source open just outside the border of a nonattainment area without requiring some sort of additional pollution control.

Future research is required to better understand how to characterize the indirect and risk-based effects of air pollution regulation on conversion facility costs. While the indirect cost factor included in this version of GBSM ostensibly reflects the costs of the permitting process, a simple ratio based on direct installed costs cannot hope to accurately represent the complexity and uncertainty of the permitting process. More research is also required to understand at what scale site selection and local regulations, such as those governing air quality, become important.

GBSM, like all technoeconomic models, is limited by the sub-models which describe constituent elements. At present, several technoeconomic models of conversion processes are available, but none have been validated against operational, commercial-scale facilities. Current research also suggests that certain technologies are best matched with particular feedstocks. The models used by GBSM assume that each process is essentially feedstock-agnostic, with the exception of F-T diesel which is the only technology that claims to be compatible with dirty MSW feedstock. Without better models of conversion facility operation, large-scale models like GBSM view each technology as a generic black box, with only cost and yield affecting results.

Recent research suggests that ethanol may not be the preferred pathway for biofuel production. Rather, liquid hydrocarbons which are compatible with existing refinery and engine technology may better utilize existing fuel infrastructure(Regalbuto, 2009; Rye, Blakey, & Wilson, 2010). Accurately modeling this pathway would likely require the inclusion of a secondary refining step in which hydrocarbons from a biofuel conversion facility would be added to an existing petroleum refinery. This would likely shift the spatial distribution of biofuels, by creating an incentive to locate near existing petroleum pipelines or refineries. By treating biofuels according to their characteristics, rather than as fungible units which interchangeably contribute to a fixed target, a more nuanced understanding of future biofuel markets can be developed.

Chapter 7: Discussion and Conclusions

The studies described in this dissertation underscore some of the potential benefits and risks of large-scale biofuel production. The biofuel production process can be divided into two distinct parts, the feedstock production process, and the process of conversion to liquid fuels. For biofuel feedstocks like corn stover, the most significant risks arise from uncertainty in their effect on soil organic carbon (SOC) levels. This parallels the findings of many other studies on feedstocks which have found land use cover and change to be a dominant source of GHG emissions and uncertainty.

Conversion technologies face a different source of uncertainty and risks. Cellulosic conversion technologies are relatively immature and uncertainty exists regarding their performance at commercial scale. Nevertheless, biochemical methods for converting lignocellulosic feedstock may yield liquid fuels with substantially lower GHG emissions than equivalent petroleum-based fuels. Thermochemical conversion processes, which share most elements of their life cycle with biochemical ones, also share the potential for low GHG transport fuels, though these pathways were not examined in this dissertation. This conclusion rests on several critical assumptions, including the ability of conversion facilities to meet their energy demand using byproducts and feedstock production processes that do not lead to significant losses in SOC. Published literature suggests that cellulosic ethanol conversion facilities can achieve energy neutrality, including recent NREL designs, many LCA studies, and the modeling described in this dissertation (Chapter 5).

Analysis described in Chapter 5 confirms that there is sufficient potential energy in byproducts (lignin cake and biogas) to not only meet the energy needs of a theoretical conversion facility, but also allow for some excess electricity to be exported to the grid (C. W. Murphy, 2012). If energy neutrality (or surplus) is actually possible, then the balance of conversion facility impacts, from facility construction and chemical inputs, is small. This finding illustrates the importance of better understanding the effects of feedstock production, since when energy-neutral conversion facilities are possible, the feedstock production phase dominates energy use and GHG emissions in the biofuel feedstock.

Because the studies in this dissertation rely on engineering models which predict the characteristics of technologies that have never been deployed at commercial scale, their results require caveats. In fact, a decade of work has predicted very promising results, and yet only one full-scale cellulosic ethanol plant was constructed, and it closed very soon after opening (Chapman, 2012). More than 15 early commercial-scale conversion facilities are currently in some phase of planning, engineering or construction. The history of cellulosic ethanol argues against the likelihood of all of these plants actually coming into operation, but within the next few years some of them will operate at capacities between a few million to 30 million gallons per year (Advanced Ethanol Council, 2013). It is important that early models of conversion efficiency, mass/energy balance and life-cycle impact be validated against these pilot facilities as soon as possible.

Concern over negative GHG impacts from the biofuel life cycle is largely focused on the feedstock production phase, with good reason. Chapter 5 showed that even in scenarios where no SOC changes are considered, fertilization and agricultural equipment activity often contributes around one-third of total GHG impact to the biofuel production system. There may be some incremental increases in efficiency of feedstock production; however, fertilization and harvest equipment activity is likely to be a necessary element of agriculture for the foreseeable future. Future research should identify the optimal balance of nutrients and harvest management for minimizing net system GHG footprint and compare these optimal practices to industry standards.

Another phase of the life cycle which deserves further study is feedstock processing and storage. The constituent papers in this dissertation use a feedstock production rate that is adjusted for approximately 5% of dry matter to be lost during storage and processing, which is common in baled feedstock systems due to weather and mechanical handling (Hess et al., 2009a). Actual loss is highly uncertain; in unusually rainy or humid years, biomass degradation from microbial damage could be substantial. Finding a denser, more stable form, such as pellets or torrefied biomass may reduce the risk of supply disruption during bad weather years (Hess et al., 2009a). Converting feedstock into these intermediate forms has substantial energy costs, however (Mani et al., 2006; Morey, 2012). Preliminary analysis done as part of the LCA modeling described in Chapter 5, but not included in this dissertation, indicated that pelletizing was likely to significantly increase life cycle GHGs from the biofuel system, unless resulting in a substantial increase in conversion efficiency (Theerarattananoon et al., 2011). This conclusion should be revisited with additional consideration given to the benefits of a more durable storage medium and reduced risk from weather since pellets would presumably be kept in an enclosed facility, as opposed to in a field.

Of the factors examined in this dissertation, SOC changes may be both the most uncertain and the most impactful. The results of Chapter 4 are similar to those produced by Anderson-Teixeira (2009), which reported a marginal effect of residue removal around 0.22% SOC loss for every percent of residue removed, as compared to the 0.13% reported in Chapter 4. This level of SOC loss represents a CO_2 equivalent of hundreds to thousands of kilograms. When applied to the biofuel conversion process modeled in Chapter 5, this can mean that SOC loss is not only the largest single GHG impact in the biofuel life cycle, but that unless stover is harvested in a way that preserves SOC, stover-based biofuels can easily have a greater GHG footprint than petroleum gasoline, at least until SOC levels reach a new equilibrium. Even at the more optimistic end of the range for SOC changes, stover-based biofuels may struggle to achieve the RFS targets for advanced or cellulosic biofuels and present only a slight improvement over first generation biofuels.

SOC changes from switchgrass were not examined in this dissertation, however existing literature suggests it has a similarly broad range, from no change to gains of 500 kg SOC/ha, and substantial uncertainty (Anderson-Teixeira et al., 2009; Follett et al., 2012; Liebig, Schmer, Vogel, & Mitchell, 2008). Unlike corn stover, however, the SOC range spans from approximate carbon-neutrality to substantial increases in SOC. This implies that purpose-grown energy crops can have superior GHG characteristics than agricultural residues. This relies on two key assumptions, that removal of residues causes GHG emissions, compared to a situation in which they are not removed, and that the purpose grown energy crops can sequester carbon through their root mass, as grassy crops like switchgrass or miscanthus do. These assumptions may not hold true in all cases, but as Chapter 4 demonstrates, there is strong evidence that removal of stover causes SOC loss under most conditions. Follet, *et al.* (2012) found that corn cultivation could increase SOC in soils that had very little SOC to start, however these soils would likely be better suited for crops other than corn. Similarly, the possibility of deep-rooted grassy energy crops has been well demonstrated to have, at least, the potential to sequester carbon. This challenges the commonly held belief that purpose-grown energy crops are inevitably worse for the environment than agricultural residues. The analyses presented in this dissertation do not address every environmental impact pathway, instead focusing on GHGs.

The analysis presented in Chapter 4 is limited by a lack of variation within the likely stover removal rates; many of the studies considered only full removal or none at all. There is a marked need for further research into the effects of sustained biomass harvest on SOC. More test plots are needed, to better cover the range of soil and climatic conditions in likely growing areas, since those factors may influence biomass production and thereby, SOC. In addition to better data collection practices through randomized trials, there may be opportunities to find meaningful data from older experiments or "natural experiments" in fields traditionally used for silage production or from which stover was collected for other reasons.

Since it appears that SOC changes are unacceptably high except at low rates of stover removal, particular focus should be paid to the effect of conservative removal regimes (<40%). Corn cobs may be an especially promising potential feedstock; the cob is a relatively small fraction of the total stover mass and typically has a lower N, P and K content then stem or leaves, which reduces the amount of fertilizer required to replace soil nutrients. Since corn grain is typically harvested by mechanically removing the ears from the plant then stripping grain from the cob, it is possible to configure a process that retains the cob for biofuel production without necessitating additional passes by harvest equipment for stover recovery. The cob could simply be ejected into an accompanying trailer and hauled directly to the conversion facility or intermediate storage locations in a bulk trailer, eliminating the need for baling. This model may strike an appropriate balance between utilizing a large and economically preferable source of feedstock in a method that causes few environmental impacts. Further analysis is needed to better characterize SOC changes when only cobs are harvested; only one of the 22 studies in included in Chapter 4's dataset examined this condition.

Producing feedstock also adds uncertainty beyond that of SOC changes. Farming is inevitably uncertain; yields vary widely on a year-to-year basis due to climate, disease, water availability and economics. Additionally, there are uncertainties that are difficult to model without stochastic analysis, such as crop or equipment failures, fire, drought or policy action. Economics and market behavior also add uncertainty; adding a second product (stover) to the corn production system would expose producers to market mediated economic effects through two different markets (food and fuel). Research is currently evaluating how better to integrate uncertainty into life-cycle analysis and decision-making (Ebadian et al., 2012). Integrating these methods into biofuel LCA models may be a critical step in improving their ability to prospectively model biofuel production systems.

This dissertation also exposed a major limitation in the data. One of the main purposes of this model was to give future analysts a complete LCI to use as input data for other environmental impacts studies. Many air and water quality studies, for example, would benefit from knowing how much of a given pollutant is emitted during the production of feedstock. The LCIs described in this study can give a rough estimate, but fall short of their original goal in two key areas. First, several of the constituent LCIs, notably for fertilizers and pesticides, are dated and developed based on European production practices. LCIs for enzymes, such as cellulase, are based on lab-bench data since actual production practices are often proprietary.

This LCA has also shown that a substantial fraction of total environmental impact is generated during the production of fertilizers or other agrochemicals and the refining of petroleum products for the transport and materials handling equipment. These activities occur at some distance from the biofuel production process. For example, in the stover production module described in Chapter 5, almost 40% of GHG impacts were due to production of agrochemicals and fuel. The emissions associated with this activity would not happen in the corn field, but rather at refineries and chemical production plants some distance away from where the products are used. Insofar as the health impacts of these emissions depend on their spatial location, simply knowing that they are produced is insufficient to thoroughly understand their environmental impacts. The location of production and distribution infrastructure is a necessary, but often un-reported, component.

7.1 Implications for Biofuel Policy

In the near future, it is unlikely that second-generation biofuels will become cost-competitive with petroleum transportation fuels; policy action will be required to drive their adoption. Policy actions to force new technologies onto the market can have perverse outcomes; the EU biodiesel mandate is a prime example of this. EU policy forced palm-oil biodiesel onto the market, the feedstock for this supply was grown on tropical lands that were converted from rainforests and peat bogs, and this conversion led to substantial emissions of GHGs. The carbon debt from this conversion is greater than what would have been saved by decades of using the biodiesel in place of petroleum fuels (Fargione et al., 2008; Reijnders & Huijbregts, 2008).

Future biofuel policies must be designed with protections against negative outcomes, such as food market disruption or GHG emissions from LUC. There are three broad categories of SOC change to consider when assigning GHG impacts to biofuels: same-crop management changes (e.g. removing corn stover from existing corn field), dLUC (e.g. converting unused land to energy crop production), iLUC (e.g. market-mediated conversion of lands to replace production lost due to biofuel feedstock, which can have domestic and international components). While environmental impacts of conversion facilities and feedstock and fuel transport can be regulated using comparatively simple performance standards, protecting against LUC effects and SOC change is a much more complicated task.

The LCFS calls for modeling dLUC and assigns a carbon penalty for feedstocks that cause iLUC (Farrell, Sperling, et al., 2007; Farrell, Berkeley, et al., 2007; Marr, 2009). RFS2 prohibits a fuel made from non-waste feedstocks grown on land that was not used for agriculture prior to 2007 from qualifying for a Renewable Identification Number (RIN). Possessing a RIN qualifies a fuel to count towards RFS compliance and is therefore more valuable than a similar fuel without a RIN.

In the U.S. the RFS2 renewable feedstock requirements make farmers document the historical usage of any land used to produce biomass, so that they can document that the land was in use in 2007, implying that no direct LUC arises from using this biomass. There is also an aggregate compliance option, under which all biomass is assumed to be renewable as long as the total cropped acreage in the U.S. is no greater than that in December, 2007. While the two compliance pathways are useful for preventing dLUC within the U.S., they may inadvertently cause iLUC; by limiting biomass production to lands that were cropped in 2007, all renewable biomass production within the U.S. is obligated to come from a limited pool of land on which food agriculture has historically dominated. This increases the chance that any energy crops will displace food crops, which could lead to cropland elsewhere in the world being brought into production to make up the lost food production.

A focus on LUC also misses important SOC effects that occur even when land use is not directly modified. As discussed in Chapter 4, when sustained biomass removal is added to existing crop management practices, SOC may decline. Corn stover meets the criteria for renewable feedstock, as described by RFS, but it has the potential to cause SOC losses of sufficient magnitude to counteract the GHG benefits from using biofuels in the first place. Future policy should attempt to more specifically address SOC changes, where possible.

Direct LUC can generally be addressed through simple policy levers, such as the provisions governing renewable biomass in the RFS2. By simply requiring that all farmed biomass come from lands that are historically used for agriculture, the opportunity for SOC loss by conversion of high-SOC lands to agriculture is minimized. There may be some circumstances where this provision should be relaxed, however, such as the cultivation of warm-season native grasses, which typically increase SOC when cultivated, or cultivation of severely degraded or marginal lands, which can have very low SOC prior to planting. Even though this conversion would technically be considered dLUC from biomass production, the net SOC impact may be beneficial, since native grasses can increase SOC. Similarly, several concepts have been proposed for using plants to bio-remediate saline or contaminated soils and to use the resulting biomass for energy or fuels.

iLUC is much more complicated to model than dLUC, since establishing a direct causal relationship between a biomass harvested from a given field and land conversion in another region is fraught with confounding factors. While one-size-fits-all GHG equivalencies, such as those used by the LCFS, are highly uncertain, they may represent the best available tool for making policy based on life-cycle modeling at this time. More sophisticated monitoring and modeling of agricultural commodity markets can help improve understanding of price fluctuations and the conversion of land to agricultural use. If GHG equivalencies for iLUC are based off of economic modeling, there may be a problem with fluctuations in agricultural commodity markets causing fluctuations in the GHG intensity of fuels from existing production pathways. This phenomenon must be further evaluated by researchers and considered as iLUC policies are designed. The international nature of agricultural markets further complicates quantifying the impacts of iLUC. It may be possible for sufficiently powerful models to accurately estimate the effects of a given biofuel project, but unless the countries in which the LUC actually manifests have policies to limit SOC loss through LUC, there may be little that can be done. An ideal solution would be a global land-use change policy, however this is unlikely in the foreseeable future, though the Reduction of Emissions from Deforestation and Degradation (REDD) initiative is a promising step in this direction (Agrawal, Nepstad, & Chhatre, 2011; Angelsen, Brown, & Loisel, 2009). In absence of effective global LUC policy, it is important that each nation's bioenergy policies attempt to minimize the drivers of iLUC by including it in GHG accounting for domestic and imported biofuels wherever possible.

Even though research on LUC is still rapidly evolving, this dissertation highlights a few general principles:

- Lands with high amounts of stored carbon, such as forests or peat bogs, should not be converted to cultivation for biofuel feedstock.
- When converting lands to biofuel use, evaluate the direct carbon changes as well as how any lost productivity will be replaced.
- Regularly monitor soil carbon levels and fluxes; ensure that there are policy or contractual options available to facilitate changes in management (e.g. tillage, residue removal rate, cover crops, etc) if necessary.

7.2 Directions for future research

This dissertation is not intended to end discussion on any of the subjects covered. For some papers, notably Chapter 3, the primary utility of the work completed is as an input for future studies. The studies discussed earlier open many questions for future examination. Two, in particular, will be briefly discussed.

7.2.1 Opportunities for Carbon-Negative Biofuels

The work described in Chapters 4 and 5 indicates that second-generation biofuels can yield life-cycle GHG reductions compared to petroleum fuels; however, they are generally still net emitters of GHGs. Some of the scenarios analyzed in Chapter 4, indicate that there may be circumstances under which these fuels could be carbon-neutral or even carbon-negative (every MJ of fuel burned sequesters or displaces more GHGs than it releases during combustion). This concept has been proposed previously, such as in Tilman, *et al.* (2006). Tilman *et al.* focused on using warm-season native grasses as feedstock, since these plants sequester carbon in their root systems. Coproduct credits, typically from generation of renewable electricity from biomass at the conversion facility, also help reduce the net GHG footprint.

An ongoing study, which was presented in preliminary form in Murphy & Kendall (2013), will build upon the LCA of Chapter 4 to propose a production system which could produce ethanol that is actually carbon-negative. This system would use a novel approach of carbon management at the conversion facility. Instead of using lignin cake to generate electricity and heat, the facility would bury the solid byproduct to geologically sequester its embodied carbon. The facility would instead burn natural gas and biogas from its wastewater treatment plant to meet internal energy demand. Lignin is generally stable under anaerobic conditions, especially if it is relatively dry when buried. Preliminary work indicates that even under relatively conservative assumptions regarding the rate of lignin decay once buried, the amount of carbon durably sequestered as lignin exceeds the amount of carbon emitted, in the form of exhaust from natural gas combustion.

Natural Gas Replacement Lignin Cake Energy

	Data Source	**Value**
Facility Electricity Requirement	NREL (2011) + 25%	35 MW
Bio-methane Production Rate	NREL (2011)	5378 kg/hr
Biogas Boiler Thermal Efficiency	Pierce (1997)	31%
Additional Natural Gas Required	Calculated	5,060 kg/hr
Life Cycle CO_2 from Natural Gas	**Calculated, GaBi**	**15.6 Mg/hr**

Composition and Degradation of Lignin Cake

	Data Source	**Value**
Lignin Production Rate	NREL (2011)	12,226 kg/hr
Lignin Carbon Content	Domalski et al. (1987)	60%
Lignin Degradation Rate	Richard (1996)	40%
CO_2 Sequestration from Lignin	**Calculated**	**16.1 Mg/hr**

Table 7-1 - Carbon Flow Analysis for Burying Lignin and Burning Natural Gas at a Biochemical Cellulosic Ethanol Production Facility. Assuming that the lignin cake is 60% carbon and 40% of that biodegrades and is emitted as carbon dioxide, 500kg per hour of CO2e would be sequestered.

Table 7-1 demonstrates the balance between carbon entering the atmosphere (top) and carbon sequestered as buried lignin. When adding an additional margin of error to the predicted energy consumption of the NREL biochemical process design, lifecycle CO_2 emissions are estimated at 15.6 tonnes per hour. The same facility produces 12.2 dry tonnes of lignin cake per hour, which is approximately 60% carbon by mass. When conservatively assuming that 40% of the carbon decomposes and is emitted as CO_2, this results in an effective CO_2 sequestration rate of over 16 tonnes per hour.

There are additional carbon sequestration or carbon credits that might be attained in lignocellulosic ethanol pathways. For example, carbon may be sequestered in the deep root systems of warm-season grasses, or if lignin is buried in a landfill which captures and combusts LFG, additional carbon credits could be generated from the fraction of lignin that does degrade. When all sequestration pathways and carbon credits are considered, the total system could be carbon negative. More importantly, the carbon balance is not entirely reliant on displacement credits for fossil fuels or electricity. Displacement is a well-accepted method of calculating carbon impacts of renewable fuels, but it is subject to uncertainty due to rebound effects, market failures and other phenomena. The model above does not just rely on displacing fuels elsewhere in the market; a substantial amount of carbon is actually going into the ground in solid form, where it might stay for a climatologically significant period of time. The cost of burying lignin in this way may even be lower than the cost of other carbon sequestration schemes.

7.2.2 Comparison of Measured and Modeled SOC Changes

The paper described in Chapter 4 explored the effects of stover harvest on SOC though a meta-analysis of existing experimental studies on the subject. There is another substantial branch of literature which evaluates SOC changes from biomass harvest: modeled studies. In preliminary examination of modeled studies it appears that they tend to estimate smaller SOC losses from stover harvest. This impression should be tested by conducting a meta-analysis of modeled studies of SOC changes from stover removal, using similar methods as described in Chapter 4, and comparing the results against those from the meta-analysis of experimental studies.

Each soil model is calibrated and validated against a set of experimental data; however most validations do not have the temporal or spatial scale covered by the experimental studies in the meta-analysis. Since soil modeling is the most likely way in which SOC changes will be prospectively evaluated it is important to know whether there are systematic biases in SOC models.

Similarly, warm-season herbaceous crops, such as switchgrass or miscanthus, are thought to have potential SOC benefits. A meta-analysis of all available studies, using similar methodology as was used in Chapter 4, would help test the reliability and magnitude of these effects. At this point in time there are less data available on these crops, most likely because they are not commercially cultivated, and so a meta-analysis with a statistically significant sample size is not possible.

Chapter 8: Appendices

8.1 Extended Acknowledgements and Status of Papers

8.1.1 Developing a Life-Cycle Inventory for Corn Stover under Different Allocation Conditions (Chapter 3)

The work described in this paper was conducted during mid-to-late 2011. Colin Murphy performed most of the quantitative analysis and drafted the report. Alissa Kendall was the PI, made substantial contributions to the design and execution of the study and contributed to the writing of the paper. First authorship was decided by mutual consent. Initial submission of the paper to *Biomass and Bioenergy* (Submission number JBB-12-00293) was in March, 2012. The paper was returned with an invitation to revise and resubmit in November, 2012. The revisions were completed and resubmitted in January, 2013 and was accepted for publication in June, 2013.

8.1.2 Evaluating the SOC Impacts of Corn Stover: Aggregated Analysis of Multiple Studies (Chapter 4)

Colin Murphy responsible for most of the conceptual design of the study, all of the data clean-up, validation and reformatting, most of the literature review and was responsible for writing the largest share of this preliminary report. Gabriel Lade designed and implemented the econometric analysis. Boon-Ling Yeo did some of the literature search. Lindsay Price quality-controlled the data and also assisted on conceptual design of the study and revisions to the report. Alissa Kendall was the PI in charge, contributing to the conceptual design of the study and writing the report.

Submission to the Proceedings of the National Academy of Sciences expected Fall, 2013.

8.1.3 Life Cycle Inventory Development for a Low-Input Cellulosic Ethanol Production System

Colin Murphy was responsible for most of the data collection and implementation of the study. Alissa Kendall was the PI in charge, directing the design and execution of the study, as well as to the resulting reports and papers. Special acknowledgement to Daniel Derr, or Logos Technologies for his assistance over the duration of this project.

Submission to GCB Bioenergy is expected in Fall, 2013

8.1.4 Effects of Air Pollution Control Costs on Biofuel System Development

Colin Murphy was largely responsible for developing the conceptual framework of this analysis, developing the cost factors for air pollution control devices, obtaining necessary cost data and nonattainment area maps, developing the list of NAICS classifications which could serve as potential sites for a conversion facility and consulting with outside experts regarding the appropriateness of modeling assumptions. Nathan Parker was responsible for much of the prior development of GBSM, implemented the changes to GBSM within the General Algebraic Modeling System (GAMS) framework, ran the scenarios, debugged the code and produced maps based on the output. Colin Murphy wrote the majority of the manuscript, which was edited and revised collaboratively. By mutual decision of the authors, it was decided that Colin would be the lead author.

Submission to Environmental Science & Technology expected, Fall 2013

8.2 Table of Studies Included in Chapter 4

Study	# of Fields?	Replicates	Clay Percent	Removal Levels	Initial SOC	N Levels	CC	Tillage Levels	Duration (years)	Sampling depth (cm)	Notes
(Larson, Clapp, Pierre, & Morachan, 1972)	1	4	+	3	+	3	-	CT	11	15	
(Barber, 1979)	1	4	-	2	-	1	-	CT	6,11	15	
(Bloom & Schuh, 1982)	1	4	-	2	+	2	-	CT	13	20	
(Maskina, Power, Doran, & Wilhelm, 1993)	1	4	+	3	-	1	+	NT	5	7.5	
(Robinson, Cruse, & Ghaffarzadeh, 1996)	2	3*	+	2	+*	3	+	CT	12, 34	15	
(Dick et al., 1998)	1	3	-	2	+	4	-	X	4, 10	20	Some treatments include manure
(Clapp et al., 2000)	1	4	-	2	+	2	-	NT, RT, CT	13	30	

(Reicosky & Evans, 2002)	1	4	-	2	+*	2	+	CT	30	20, 50[ǂ]	
(Wilts et al., 2004)	1	4	-	2	+	3	+	CT	29	30	
(Hooker et al., 2005)	1	3	-	2	-	1	+	NT, CT	28	15	
(Dolan et al., 2006)	1	2	-	2	-	1	-	NT, RT, CT	23	45	
(Humberto Blanco-Canqui, Lal, Post, & Owens, 2006)	1	3	+	5	+	1	+	NT	2	10	
(Moebius-Clune et al., 2008)	1	4	+	2	-	X	+	NT, CT	32	15	
(Humberto Blanco-Canqui & Lal, 2009)	3	3	+	5	+	1	+	NT	4	20	
(D. L. Karlen, Birell, et al., 2011)	1	3	-	4	+*	4	+	RT	5	15	
(Kenney, 2011)	3	3	+	5	+	1	+	NT, RT	2	5	Master’s Thesis
(Stetson et al., 2012)	1	3	-	3	+	1	-	NT	8	5	1 Trtmt. Included Winter Cover Crop

(Guzman, 2013)	2	3	-	3	+	3	+	NT, CT	3	15, 45[ǂ]	PhD Dissertation
(J. Johnson et al., 2013)	1	4	+	3	+	1	-	NT, CT	5,6	10	
(J. Johnson et al., 2013)	1	4	+	4	+	1	-	NT, CT	6	20, 60	Unpublished Data
(Stott et al., n.d.)	1	X	+	4	+	1	+	NT	6	30, 60	Unpublished Data

8.3 Data and Parameters for Base Case Model, Chapter 5

Material or Energy Flow	Source
Ammonia, Liquid, (US)	GaBi PE (2006)
Ammonium Nitrate Phosphate (EU)	Ecoinvent (1999)
Diesel Fuel (US)	GaBi PE (2006)
Potassium Chloride (EU)	Ecoinvent (1999)
Lime Flour (US)	GaBi PE (2006)
Irrigation Water (US)	GaBi PE (2006)
Electricity, US Grid Mix	Ecoinvent (2008)
Sulfuric Acid, 96% (US)	GaBi (2005)
Urea, Stami Process (US)	GaBi (2005)
Molasses, sugar beet (Switzerland)	GaBi PE (2006)
Vancomycin	Ponder & Overcash (2009)
Water, Decarbonized (EU)	Ecoinvent (2008)
Natural Gas, US Mix	GaBi PE (2006)
Steel, Hot-Dip Galvanized, 80% Recycled (US)	World Steel Association (2011)
Steel, Welded Pipe 80% Recycled (US)	World Steel Association (2011)
Concrete, #5 Mix	Marceau, *et al.* (2007)
Diammonium Phosphate (EU)	Ecoinvent (1999)
Glyphosate (herbicide, EU)	Ecoinvent (1999)
2, 4 D (herbicide, EU)	Ecoinvent (1999)

8.4 Crop production and Processing Parameters, Chapter 5

Corn Cultivation Parameters

Yield (dry tonne/ha*yr)	3.95
Moisture Content (at collection)	12%
Total Tonnes Feedstock Per Day	1481.12
Irrigation water (m^3)	0.00
Fertilizers Used (kg / ha*yr)	
N, as Ammonium Phosphate Nitrate	4.68
P2O5, as Ammonium Phosphate Nitrate	7.91
Potassium Chloride	45.37
Ammonia, liquid, 30% (weight is as pure ammonia)	32.47
Limestone Flour (1 um)	0.00
Fluxes to Air and Water	
N2O Flux (% of applied N)	1.06%
N2O Flux to Air (kg/ha*yr)	0.53
Phsophorus Flux to Water (kg/ha*yr)	0.12
Methane Flux to Air (kg/ha*yr)	0.00
Total N to Water (kg/ha*yr)	9.99
NO to Air (kg/ha*yr)	4.02

Pretreatment Parameters

Electricity Consumption (kW)	6774
Diesel Consumption (kg / hr)	181

Process Parameters

Makeup Water (lb/hr)	607,647
Electricity (kW)	21,777
Steam Burden (MMBTU/hr)	200

Switchgrass Cultivation Parameters

Yield (dry tonne/ha*yr)	7.8
Moisture Content (at collection)	0.12
Total Tonnes Feedstock Per Day	1658.857
Irrigation water (m^3)	0
Fertilizers Used (kg / ha*yr)	
N, as DAP	17.04
P2O5, as DAP	75.10
Potassium Chloride	0.00
Ammonia	0.00
Fluxes to Air and Water	
N2O Flux (% of applied N)	1.06%
N2O Flux to Air (kg/ha*yr)	1.12
Phsophorus Flux to Water (kg/ha*yr)	0.23
Methane Flux to Air (kg/ha*yr)	0
Total N to Water (kg/ha*yr)	21.24
NO to Air (kg/ha*yr)	4.02

Transportation Parameters

Unloaded Truck Fuel Economy (mpg)	5.00
Bale Transport, Average miles (one-way)	25
Bulk Transport, Average miles (one-way)	75
Ethanol Transport, Average miles (one-way)	150.00
Loaded vs. Unloaded Fuel Economy	0.69

8.5 Life-Cycle Inventory Model for Biochemical Cellulosic Ethanol Production – Detailed Development Report

8.5.1 Foreword

This appendix documents the development of a LCA model for biochemical cellulosic ethanol. At the time of writing, the model had been named *EthCycle*, though this name has been dropped in subsequent writings, it is retained here to help distinguish the developed LCA model from other models used to generate information and data used in the LCA model.

Included in this report is a summary of the EthCycle model design, preliminary results, and a user guide. It was submitted to Logos, EdeniQ and the Department of Energy in completion of project number DE-EE0002881. This report also originally included a results section, which has been superseded by the results described in Chapter 5. Some of the discussion of model development, literature review and design concepts are simply more in-depth versions of discussions in Chapter 5.

8.5.2 Introduction

This document describes the development of a life cycle assessment (LCA) model of a biochemical cellulosic ethanol production process (EthCycle) in a 40 million gallon per day facility. The biochemical conversion process represented in the model is based on data and assumptions drawn from previous cellulosic ethanol LCAs and academic literature within several relevant sub-disciplines (e.g. agronomy, soil science, power system operations, cellulosic conversion), engineering calculations, and information from collaborators at Logos Inc. and EdeniQ.

This model has three primary purposes:

1. To characterize the environmental impacts associated with the production of cellulosic ethanol by the proposed process on a field-to-blending terminal basis.
2. To assist in quantification of life cycle greenhouse gas (GHG) intensity for cellulosic ethanol to provide guidance relevant to California's Low Carbon Fuel Standard (LCFS).

3. To develop a general LCA model of advanced biochemical cellulosic ethanol production for future use.

The model is developed within the Microsoft Excel environment, using Visual Basic (VBA) scripts where appropriate to automate tasks and improve user friendliness (Microsoft, 2006).

The model currently reflects the process outlined by EdeniQ and Logos staff based on the proforma provided in June of 2012; these basic conceptual relationships are still reflected in the model discussed in Chapter 5, but some numbers have been subsequently changed. Figure 8-1 provides a flow diagram of the EdeniQ process. Areas where design parameters are unspecified are estimated using current literature, primarily the most recent National Renewable Energy Laboratory (NREL) Biochemical Process Design report (Humbird et al., 2011). As new data are made available, the model can be updated to reflect the specific characteristics of the EdeniQ process. Once these data are obtained, EthCycle will be able to produce a reliable accounting of life cycle environmental impacts, including but not limited to GHGs, of ethanol produced at the simulated facility.

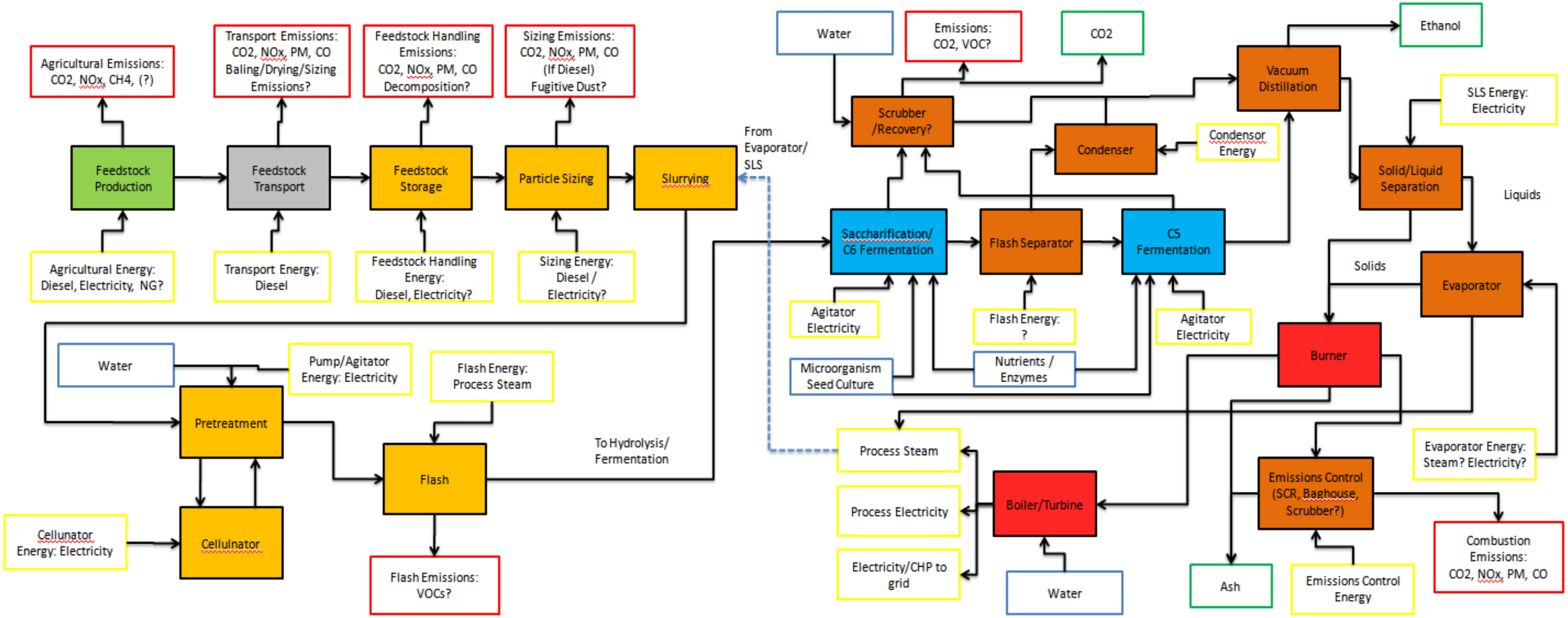
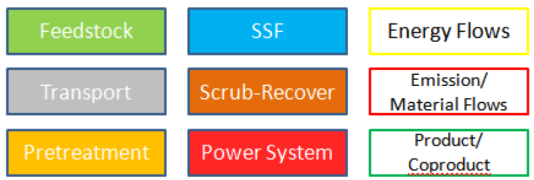


Figure 8-1 - Facility Process Flow Diagram of EdeniQ Biochemical Cellulosic Ethanol Production Process. Note this this figure reflects conversion facility operations, not data or process flow within the EthCycle model



8.5.3 Model Scope and System Definition

This model evaluates the environmental flows consumed and generated during the production of biochemical cellulosic ethanol on a field-to-blending-terminal basis, using a process-based LCA approach. This means that cultivation, harvest and transport of feedstocks; processing and conversion of feedstocks into ethanol; and transport to a fuel blending terminal are included in the study's system boundaries. Terminating the analysis at the blending facility, as opposed to terminating it at the use-phase (combustion in a motor vehicle), reflects the reality that once ethanol enters the retail market, it is indistinguishable from other ethanol gasoline blends. Analysis of impacts at the use phase would also require characterization of vehicle technologies and fuel markets, which are beyond the scope of this project, but similar questions have been addressed by other authors [e.g. (Poulopoulos, Samaras, & Philippopoulos, 2001; Spatari et al., 2005)].

Other system boundary considerations in this model include simplified modeling of the ethanol production facility's construction, namely assessment of major construction materials only (concrete, steel, and aggregate), and no consideration of facility decommissioning. Previous studies have shown that the decommissioning of buildings has negligible life cycle impacts (Scheuer et al., 2003). Production of mobile equipment, including farm equipment, is also excluded on similar grounds. The fate of waste streams from the facility is assumed to have minimal impact on life cycle performance of the ethanol; most of the solid waste from the process is combusted to generate energy for the process. The facility has an on-site wastewater treatment plant with an anaerobic digester, which produces methane that is also combusted on site for energy production. Treated water is recycled into the process, water losses are assumed to be primarily through evaporation leading to a minimal amount of wastewater discharged into the municipal wastewater system. Residual ash from biomass combustion and other un-recycled materials are assumed to be disposed of as appropriate with minimal environmental impact because they are not produced in large quantities (minimizing transport-related burdens) and are largely inert when disposed of in landfills.

8.5.3.1 Functional Unit

The LCA model uses different functional units depending on the process. Feedstock production is modeled on a per-hectare basis, since relevant fertilizer and mobile equipment activity data is almost universally provided in this form. A per-hectare feedstock modeling basis also permits sensitivity analysis for yield assumptions and soil related emissions. The functional unit of the facility model is one operational hour. This allows easy coordination with mass-balance and engineering process models. Per -hectare values are converted to a per-operational-hour basis by multiplying by the ratio of facility feedstock consumption to per-hectare feedstock yield.

One operational hour is not an appropriate functional unit for comparing results with other ethanol production processes, however. The final reported functional unit for the study is one MJ of ethanol, though this is directly proportional to any other volumetric or energy-based unit.

8.5.3.2 Life Cycle Inventory Data

Life cycle inventories (LCIs) for material and energy inputs to EthCycle are derived from LCI databases such as *Ecoinvent* and *GaBi* Professional (PE International & LBP, 2008). LCI datasets characterize the environmental flows associated with a particular product or process throughout its supply chain. For example, during the life cycle of cellulosic ethanol production, electricity is consumed by processes such as lighting and climate control. A LCI database will provide a dataset for electricity that includes all the upstream processes for production and delivery of electricity for a particular region, such as the continental U.S. or the U.S.'s Western electricity grid. This dataset is then used in the LCA model for cellulosic ethanol to characterize the life cycle environmental flows attributable to electricity consumed during the ethanol production life cycle.

While using LCI databases is critical for completing comprehensive and timely LCAs, one challenge of using such databases is that inventory datasets may not be geographically or temporally appropriate, resulting in potential inaccuracies. These shortcomings in LCI data are well-documented and widely discussed in the LCA literature, for example (Björklund, 2002; Huijbregts et al., 2001). Recent, comprehensive LCIs of chemical inputs to the biofuel system, including pesticides, fertilizers, antibiotics and propagation nutrients are notably scarce. Wherever possible the most appropriate LCI datasets were selected that best represent the likely production conditions, though in some cases the use of European data or data more than ten years old was required. In general, the input flows for which there was significant uncertainty about the quality of LCI information were of relatively low impact, however LCI data is a source of uncertainty in this type of analysis.

This report overwhelmingly focuses on GHG impacts of ethanol production, however EthCycle is flexible enough to assist in a wide variety of future analyses, such as toxicity analyses, natural resource consumption, or water-quality impacts. To engage in analyses of flows other than GHGs, EthCycle tracks LCI data as exhaustively as is possible. The Ecoinvent and Gabi Professional databases typically track several hundred flows for any production process. EthCycle's preserves the exhaustive set of flows from each LCI used in the model and can report hundreds of input or output flows for the ethanol fuel produced, or even for each sub-module. Visual Basic (VBA) scripts were developed in Microsoft Excel to assist in adding LCI data from a wide variety of sources to EthCycle because environmental flows are tracked differently in each database.

8.5.3.3 Allocation Methods

Co-product allocation is required when a production system includes multifunction processes. For cellulosic ethanol co-product allocation may be required to model inputs to the production system, such as feedstocks; and outputs from the system where ethanol is produced along with other valuable products, such as surplus electricity from lignin combustion.

EthCycle is largely based on an attributional approach, meaning that changes in markets and supply chain activities caused by the production facility are not accounted for. The biochemical cellulosic ethanol processes which are the focus of EthCycle currently do not project significant co-product streams other than electricity. The ash from combustion may have value as a soil additive (Risse & Gaskin, 2010), however is value in this usage is uncertain and is excluded from this analysis (Pandey & Singh, 2010). Treatment of co-products was done using consequential displacement of calculations, but did not include economic systems modeling (Phillips et al., 2007).

EthCycle will model two cellulosic ethanol feedstocks: corn stover (the non-grain parts of the corn plant remaining after grain harvest, including the cob) and grassy energy crops (such as switchgrass or miscanthus). The use of stover requires an allocation step, since it is a co-product (or residue) of corn production. Grassy energy crops require no allocation since the biomass is dedicated entirely to biofuel production.

Corn stover presents several allocation challenges. Stover has traditionally been considered a waste product and is often left on corn fields to protect top soil from erosion, and naturally decompose and return carbon and nutrients to the soil. Systematic removal of stover will require application of additional nutrients and may also contribute to soil degradation (erosion or decreased soil organic carbon levels). In addition, corn is most commonly grown in rotation with soybeans or other nitrogen-fixing plants to reduce demand for nitrogen fertilizer. Crop rotation requires allocation of impacts between all products. The current model uses a simplified assumption that attributes only the replacement of nutrients removed in stover by synthetic and mineral fertilizer to the stover used as feedstock. Chapter 3 examines the effect of alternative allocation assumptions on the performance of the stover ethanol production pathway.

8.5.3.4 Impact Assessment

The primary impact categories modeled in EthCycle include criteria pollutant emissions, acidification potential (AP), eutrophication potential (EP) and 20 and 100 year global warming potentials (GWP_{20} and GWP_{100} , respectively). Pollutants tracked in the LCI are automatically assigned to these categories and then characterized with the appropriate potentials (Guinee et al., 2002; IPCC, 2007). Other indicators or summary statistics can be added to the model if desired.

8.5.3.5 Assumptions and Limitations

LCI data from existing databases, such as GaBi Professional and Ecoinvent, are a source of uncertainty in the model. These databases generate LCI datasets using a variety of models, empirical measurements and literature sources and include assumptions regarding supply chains, production technology and environmental impacts that may not be applicable to the production system modeled in EthCycle. For example, pesticide datasets are only available for European conditions and are at least ten years old, so they are both temporally and spatially unsuitable to characterize current U.S. conditions. Nevertheless, these LCI datasets represent the best available data as well as the state of practice within the LCA community. In other cases, LCIs from literature may track only a few types of energy or material, they are included on an equivalent basis to more comprehensive LCI datasets, however future work should attempt to standardize assumptions, analytic practices and modeling conditions across all LCIs.

8.5.4 Life Cycle Inventory Development

EthCycle breaks the biofuel production process into a series of stages, or *modules*, roughly analogous to the different color codes in **Error! Reference source not found.**. Each color code is treated as a single module and in general, each module is represented in its own worksheet in MS Excel. In order to maintain transparency and facilitate future sensitivity analyses, the model has been designed to function as simply as possible; minimizing the use of lengthy in-cell formulas wherever possible and providing in-source documentation for any VBA scripts.

8.5.4.1 Life Cycle Database Operations

The model uses LCI datasets from existing databases to characterize inputs and emissions across the system boundary. Each module (worksheet) yields its own life cycle inventory, so that outputs can be reported with enough detail to highlight emissions hot-spots in the production system.

Each material that is used in a particular module is represented by a columnar LCI entry consisting of data from Ecoinvent, GaBi PE, or other literature. These data represent the input or output flows for a unit of material or activity. The sum of all module LCIs is the total life cycle flow of energy and materials for a particular module. Each LCI is converted to a per-operational-hour functional unit to allow all LCIs to be summed into a field-to-blending-terminal total or converted to other units, such as per-gallon of delivered ethanol.

8.5.4.2 Feedstock Module

The current version of the model includes a biomass production module for corn stover and switchgrass. In addition, there is a calculation tool for soil carbon change and another for non-continuous farming practices, in which inputs and harvest parameters vary substantially over time, such as switchgrass or *miscanthus* cultivation. Other feedstocks could be substituted using similar methodology, or by directly inputting an externally-produced LCI.

8.5.4.2.1 Cultivation Modules – Common Elements

Corn stover and grassy energy crop cultivation share many common agronomic practices, so the fundamental design of their modules share many common features. Both require some measure of fertilization, may require additional chemical inputs and are harvested primarily by diesel-powered field equipment.

Both corn and grassy crops require fertilizer to achieve high yields. The amounts of fertilizer required are determined in different ways for each crop, discussed below. Once fertilizer needs have been determined, there are multiple fertilizer compositions which could be used. The choice of which compound to apply may be determined largely by local supply and economic conditions. Many articles that discuss the effect of fertilization regimes do not specifically identify the compound added, but instead quantify the total amount of elemental nutrient (typically N, P and K) added (Conant, Paustian, Del Grosso, & Parton, 2005; Wortmann & Klein, 2008). Many functions that estimate the losses to air or water also quantify fertilizer additions in terms of the mass of N, P or K, so EthCycle considers fertilizer as on a per-nutrient-mass basis, until converting to a particular composition to match an LCI entry for production impact.

Emissions from fields through volatilization or runoff of fertilizer are also an important consideration. High-intensity corn production requires high levels of nitrogen (N) fertilization, even when in rotation with a nitrogen-fixing plant such as soy. Emission factors for these flows are difficult to obtain, and where available are developed by fitting functions to empirical data tied to the specific geographical and climate conditions of the site where data were collected. Most studies caution that results are applicable only to the study area, making extrapolation of these data and relationships uncertain.

In the EthCycle model, emission and runoff factors were selected for their relevance to climate and soil conditions similar to those of the U.S. Corn Belt and southern plains; however, these emissions factors are at best approximations and future research will be needed to develop more values specific to anticipated feedstock production regions.

Nitrogen fertilization can result in volatilization of N as N_2, NH_4, N_2O or nitrogen oxides (NO_x). EthCycle tracks the latter two pathways, omitting the former because N_2 is inert and harmless and NH_4 is either quickly removed, by dry or wet deposition, or atmospheric reactions (Seinfeld & Pandis, 2006).

Nutrient leaching into groundwater was not considered in this model, but run-off to surface water was. This was judged to be an acceptable assumption due to the wide use of tile drainage systems in U.S. corn production (Powers, 2005). The most common N_2O volatilization rate, 1.25% of added N, comes from the IPCC (2007), though this study uses a more recent value, 1.06% of applied N, from Linquist et al. (2012), which is based on calculations from cereal crops. A NO_x volatilization rate of 238 mg/m^2 was taken from Akiyama et al. (2000). This rate reflects a Japanese study, but provides the most direct function for converting applied N to NO_x emissions.

N loss to surface water came from Powers (Powers, 2005), a definitive study on water-related life cycle impacts from corn. Powers found that 31.6% of applied N ended up in surface water in Iowa and was based off an extensive database of N concentration measurements in local waterways. Since precipitation in Iowa generally exceeds the needs of corn, a significant amount of runoff is likely to occur, carrying with it a large fraction of applied N. Most of the Corn Belt requires no irrigation, but not all areas receive the excess of precipitation of Iowa. Accordingly, the runoff rates of Iowa probably reflect a relatively high-bound estimate of runoff losses.

Phosphorous loss to surface water, 4.66% of applied P, also came from the Powers study. Powers concluded that potassium loss to water was minimal due to soil microbial activity and the relatively low solubility of potassium salts under conditions found in the soil.

There are several potential loss pathways for carbon compounds from fields as well. Urea application to soil has been demonstrated to cause a significant transient emission of CO_2; the IPCC estimates this to be equal to 20% of the C applied in the form of Urea. Applications of organic fertilizer, such as mulch, compost or manure, also result in the emission of CO_2, methane or volatile organic compounds (VOCs) due to microbial activity and lime, which is often added to increase soil pH also promotes CO_2 emission. Modeling these systems is extremely complicated due to the nonlinear interactions between these substances and soil. They are additionally complicated by the fact that many are waste flows from other systems and would emit carbon compounds if they were not applied to fields. The current version of EthCycle does not attempt to estimate emissions due to organic fertilization, but the model is designed to accept these values if generated externally.

The environmental impacts of diesel production, from oil field up to distribution, are estimated using GaBi PE data according to the LCI methodology discussed earlier. Combustion emissions of criteria pollutants are calculated using the Tier III emission factors applied to the power output of the engine. Emissions of sulfur (as SO_2) and CO_2 are calculated by determining the mass of fuel consumed and typical carbon and sulfur content of diesel fuel. All combustion emissions are put in a column in the LCI output section and incorporated into the sum for this module.

The corn stover cultivation module is very similar to the one presented in Chapter 3; figure 8-2 shows how data flows within the module. EthCycle's default allocation methodology assumes that the *status quo* is repeated no-till corn cultivation with grain harvested and stover left on the field. Therefore, the only environmental burdens assigned to stover are those that arise from its addition to the existing corn cultivation practices: replacement of embodied N, P and K by chemical fertilizer, changes in soil organic carbon content from stover removal and additional field equipment activity for harvesting and baling. Fertilization practices are highly dependent on local soil, climatic and economic conditions as well as a farmer's past experience. Most guidance on the subject encourages farmers to test their soil for nutrient availability, carbon content and other factors, so that fertilization regimes can be tailored to local conditions (Nutrient Stewardship, 2011). The default model calculates the mass of N, P and K removed from the field by using stover composition values from Wortmann & Klein (2008). EthCycle can accommodate other allocation methods, such a economic or energy-content apportionment, using the methodology described in (C. Murphy & Kendall, 2013).

8.5.4.2.2 Stover Cultivation Module – Unique Elements

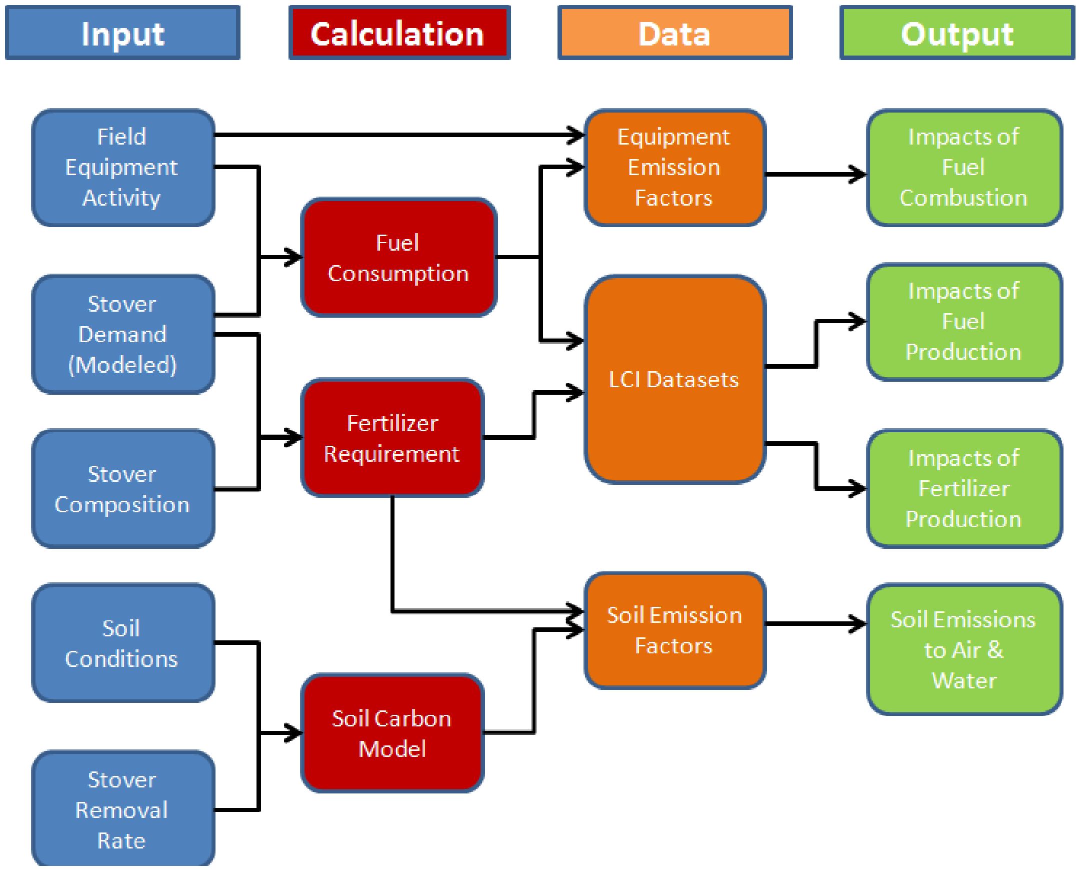


Figure 8-2- Data flow diagram for Corn Stover Production Module

Agricultural equipment activity generally follows the feedstock harvest and processing system described by the *Pioneer Scenario* from the Idaho National Laboratories (INL) Uniform feedstock model (See Pretreatment Section) (Hess et al., 2009a). The *Pioneer Scenario* calls for a two-pass harvesting system in which corn grain is removed by a standard grain combine, after which a flail shredder cuts down the remaining stover and arranges it in windrows. After a suitable period to allow for drying, typically about three days, a fraction of the biomass is baled and stored at field-side, using plastic wrap or tarps if necessary to protect the stored against rain. The shredding, windrowing, baling and stacking of bales represent activity that would likely not occur in absence of the need for biomass, so they must be modeled and attributed to feedstock production. This module allows for the activities that take place before field-side to be modeled as part of the feedstock production operations. All of the activities described are performed by mobile agricultural equipment which is overwhelmingly diesel powered in North America.

8.5.4.2.3 Switchgrass Cultivation Module – Unique Elements

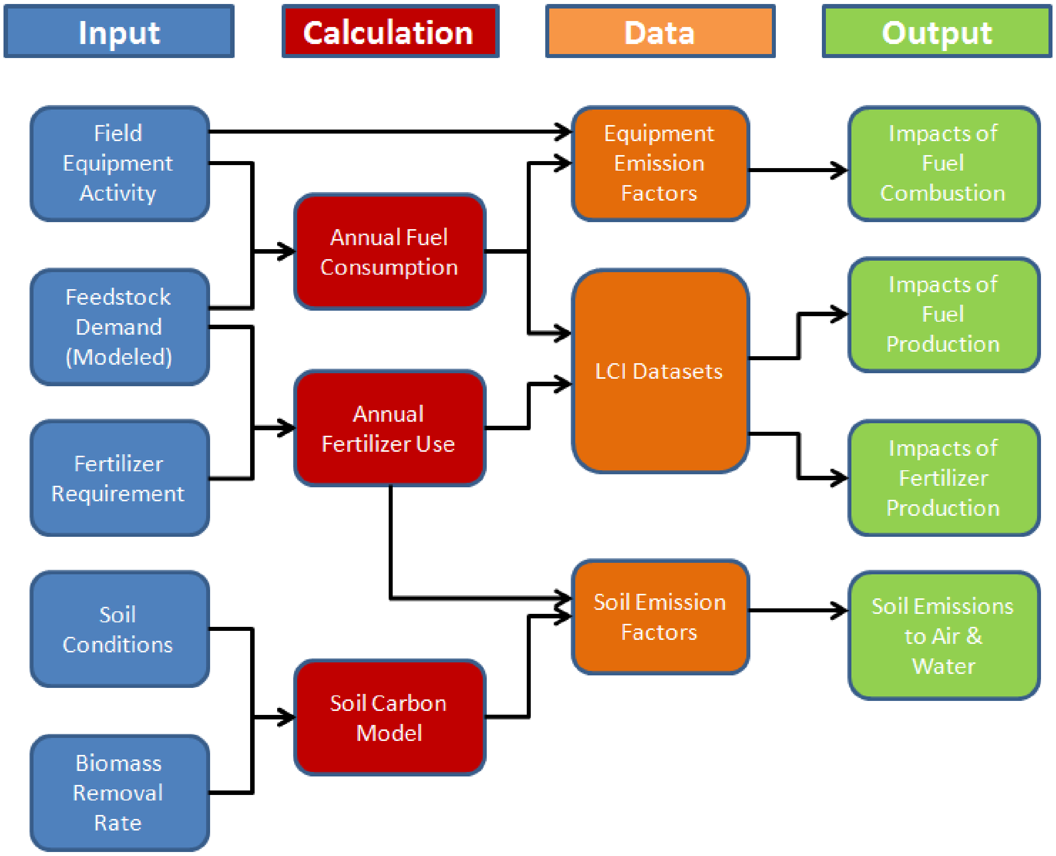


Figure 8-3 - Data Flow Diagram for Switchgrass Production Module

Switchgrass harvesting, in contrast to corn, has not been routinely done in commercial quantities, so comparatively fewer data exist on harvest practices and equipment. Figure 8-3 shows how data are handled within the module. The switchgrass cultivation data used in this study were provided by Ceres Inc., a company that has extensively researched grassy crop cultivation. The data rely on the University of Nebraska crop budgets for agricultural equipment work rates and energy consumption as well as their own research into fertilization parameters (Klein & Wilson, 2013). The fuel consumption values provided approximately agree with similar values elsewhere in literature, including the INL Advanced Uniform feedstock model. Switchgrass and *miscanthus* differ from corn in that there may be predictable and significant differences in activity on a year-to-year basis due to the growing cycle. Both crops have an establishment phase, in which harvests are limited and agronomic practices are tailored to maximize the growth of young plants. After a year or two of establishment, there is a 6-10 year period of maturity, in which substantial amounts of biomass are harvested each year and the plant regrows in a manner similar to coppicing. After this maturity period, the plot must be re-seeded to maintain high yields. Most standard life-cycle analysis models, including the default version of EthCycle, cannot easily accommodate variable emission rates and so average emissions and materials use across the lifespan of the plot. Future work from the UC Davis group will re-examine this system using tools capable of accounting for activity that varies over time. An additional area where existing data may be insufficient and variability high, is feedstock production. Environmental flows associated with feedstock production depend on agricultural yields, fertilizer requirements, soil emissions, irrigation requirements, and harvest practices. All of these factors depend on climate and soil conditions, which in turn are dependent on geography. Data are usually only available in a highly aggregated (national, state or county-averages) or highly disaggregated (one particular field) form. Accurate estimation of feedstock production impacts may require site-specific experimental work. The EthCycle model uses U.S. national averages as its default values for corn production. For switchgrass, production practices described by Ceres Inc. (confidential communication) are modeled in combination with crop budgets from the University of Nebraska (Klein & Wilson, 2013).

8.5.4.3 Soil Organic Carbon Module

Removing large amounts of biomass from a field can significantly impact the reservoirs of carbon contained within soil. If the soil contained high amounts of organic carbon, disrupting it through tillage or mechanical activity can promote microbial metabolic activity and release significant amounts of methane and carbon dioxide. These relationships are highly dependent on local biogeochemical conditions and a significant amount of uncertainty exists regarding their magnitude (Lal, 2006).

Feedstock modeling is particularly challenging due to many complex interactions between different nutrient pools within biologically active soil. Nitrogen and carbon pools both have multiple in and out flows, which can affect emissions to air and water. These complex biogeochemical processes are simplified within EthCycle, using national or regional average data. Emissions of nitrogen-based compounds are estimated using simple emissions factors (IPCC, 2007; Kim et al., 2009; Linquist et al., 2012). Soil carbon effects are subdivided into two categories, direct and indirect.

SOC changes can result from feedstock production and harvest activity and, depending on the feedstock and agronomic conditions, can be positive or negative. In this study we report baseline results for fuel carbon intensity assuming no changes to soil carbon. Chapter 4 evaluates SOC response to stover harvest in more depth and Chapter 5 includes in scenario analyses which examine changes to soil organic carbon levels in soils used for switchgrass production and for corn fields where stover is harvested. The soil organic carbon changes are derived from a statistical regression developed from a meta-analysis of many field trials (Anderson-Teixeira et al., 2009).

Indirect changes are those mediated by market or policy activity; for example, when corn acreage which was previously used to supply human consumption is used for biofuel, the unmet demand will be satisfied with corn or substitute grains grown elsewhere, there may also be price signals that reverberate through markets if prices for corn and corn substitutes rise when demand is unmet. The land use change caused by replacing this grain is iLUC; Smith (2007), conceptualizes iLUC as dLUC that is temporally or spatially shifted from its cause. This conception of iLUC highlights the importance of having specific data about both the crop that is directly affected by a proposed biofuel system and the land affected indirectly. Since neither corn stover nor grassy energy crops such as switchgrass or miscanthus have been collected on large scale at present, no such data exists. iLUC changes from stover and grassy crop utilization may be relatively small, since stover is currently a residual product and grassy crops can be grown on marginal agricultural land, but it is too early in the development of large-scale biofuel production capacity to reach a firm conclusion on this subject. EthCycle ignores iLUC effects due to this uncertainty.

8.5.4.4 Annual Agricultural Activity Calculator

Switchgrass production has variable activity depending on the stage in the plant's growth cycle. The first year is an establishment phase, with high levels of fertilization and no harvest. The second year has a reduced harvest and unique fertilization regime. Subsequent years reflect mature, productive plants and management does not vary significantly until the field is removed and re-seeded. This module simplifies averaging fuel, fertilizer and agro-chemical use over variable time scales and use rates. The current rates come from Ceres Inc and the Nebraska Crop Budgets, as above. At present, EthCycle assumes an 8 year planting cycle for switchgrass and averages all emissions out over that time frame.

8.5.4.5 Pretreatment Module

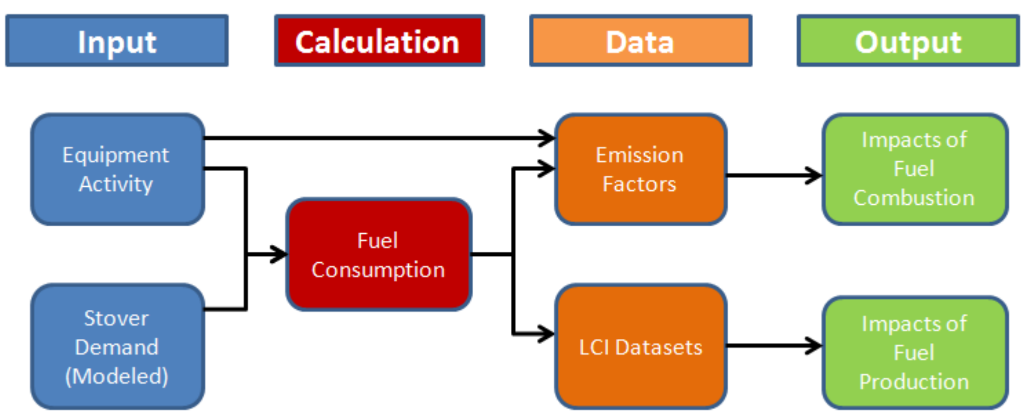


Figure 8-4 - Data Flow Diagram for Pretreatment Module

EthCycle pretreatment operations are defined to include everything from the point at which baled biomass is removed from field-side storage until it is inserted into the conversion process. The EthCycle model labels this as “Off-Site Pretreatment” in order to distinguish it from operations also labeled as pretreatment in the facility flow diagram, however this step could happen at any number of locations, including at the conversion facility. Pretreatment operations are modeled on those described in the *Pioneer Scenario*, and described in Figure 8-4. This data source was selected for its readily available data on equipment activity and energy consumption as well as its forward-looking vision of future biomass harvesting and processing operations.

The INL model describes two methods for harvesting, processing and transporting lignocellulosic feedstock. One method is based on the current state of practice, in which feedstock is baled and transported directly to a conversion facility, where it is shredded and processed. The *Pioneer Scenario* describes a likely future of the U.S. bioenergy sector, in which feedstocks are ground into and stored as a uniform-format feedstock that can be used for a wide variety of bioenergy processes. The uniform feedstock concept has two significant advantages over conventional baling. The first is that the ground feedstock has a higher bulk density than bales, which allows for truck and rail transport to carry more mass per trip, reducing the cost and environmental impacts of transportation. The second advantage is that a uniform feedstock becomes a commodity, which can be traded across regions or supply chains, helping insulate bioenergy producers from supply disruptions by facilitating spot market transactions. It also helps producers by allowing them to sell any excess biomass without worrying about compatibility with unfamiliar processes.

EthCycle generates LCI values for the pretreatment module by calculating the required energy from the mass-based energy consumption data for each step in the pretreatment process. Diesel combustion emissions are estimated using the same methodology as used for agricultural equipment and, similarly, assume EPA Offroad Tier III compliant engines. Criteria pollutant emissions are calculated based on the engine output, CO_2 and SO_2 emissions are calculated based on the fuel consumption.

Since the *Pioneer Scenario* envisions processing operations occurring at a dedicated facility near biomass suppliers, the model assumes that any equipment that is not required to be mobile (e.g. grinders and bulk handlers) is powered by grid electricity instead of diesel. This is a lower-cost and lower-emission solution than diesel. This assumption can easily be changed by the user.

Many processing techniques have been suggested to facilitate efficient transport and handling of biomass once harvested. The density of baled cellulosic material is typically too low to fully utilize the maximum weight capacity of most heavy-duty diesel trucks. Densification near or at the field side may improve the efficiency of feedstock transportation and may also disrupt cellular structure, thereby improving the efficiency of biochemical conversion (Kaliyan & Morey, 2010; Theerarattananoon et al., 2011). Pelletization is an extreme form of densification, in which biomass is extruded through metal dies at high pressure, which disrupts cell walls and fuses biomass into a dense, stable form. This maximizes the density for efficient transport and protects it from losses in storage, but it is the most intensive of densification options; the increase in logistical energy efficiency may be smaller than the input energy, unless rail or barge transport is anticipated. Many laboratory scale studies on pelletization have been conducted but the energy demand of full-scale field equipment may be significantly greater, on a per-tonne basis, than that of laboratory studies (Morey, personal communication, 2012).

8.5.4.6 Process Module

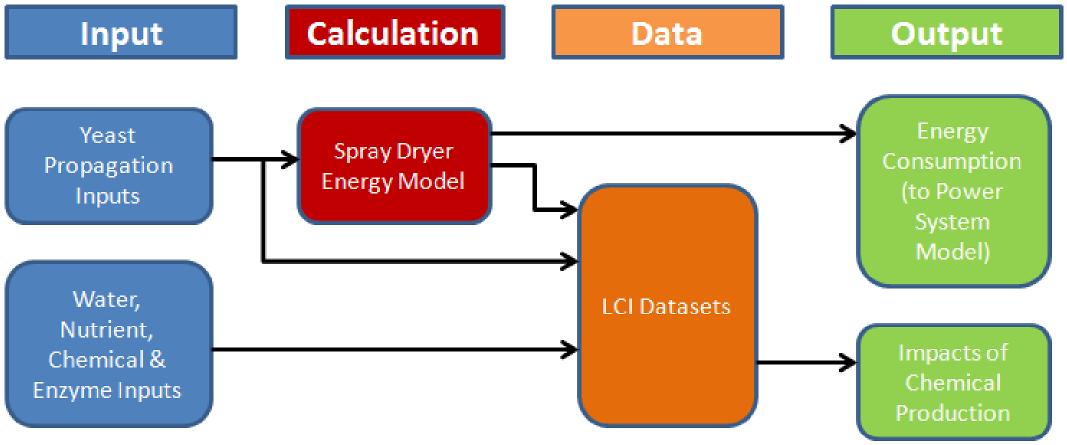


Figure 8-5 - Data Flow Diagram for Process Module. Note that energy flows are tracked in the Power System Module

In this model the term "process" refers to all of the material conversion activities, excluding energy generation and exhaust scrubbing that occurs in the conversion facility. Figure 8-5 describes the information and data flow in the process module and connections to other modules. This section of the model reflects current understanding of lignocellulosic process design, which is a rapidly developing field and has not yet been successfully commercialized.

A primary obstacle to using lignocellulosic feedstocks for liquid fuel production is the reluctance of cellulose to break down into its constituent sugars, which can then be fermented into ethanol. Most processes require significant additions of enzymes, such as cellulase, to liberate sugars from lignocellulosic materials. EthCycle currently estimates CO_2-equivalents for enzymes based on the values of Maclean and Spatari (2009), which are in turn developed from a study of energy and material inputs to enzyme production (Zhuang, Marchant, Nokes, & Strobel, 2007). Unfortunately, these estimates do not include a complete LCI dataset (MacLean & Spatari, 2009). The current EdeniQ process design calls for enzymes to be produced by the microorganisms which are also responsible for fermentation. This eliminates the need for external enzymes, but further research is required to determine whether this process will work at commercial scale.

The model currently includes some of the energy and material demands for a large propagation train for cultivating the strains of yeast which drive fermentation. These values are proprietary to EdeniQ and not reported in this dissertation.

The demand for steam and electricity dominates environmental flows associated with the facility. While the user can set the total amount of demand for each within this module, most of the relevant calculations happen in the power system module, which is discussed later in this document.

8.5.4.7 Scrubber-Recovery Module

The processes for distillation, exhaust scrubbing, including ethanol recovery from gaseous and liquid waste streams, are comparatively well understood, and they can represent a significant impact on net life cycle emissions and energy usage. The module for these processes asks the user for steam and electricity utilization in order to calculate power demand. The module then allows modeling of several exhaust streams with associated scrubbing devices. The user inputs the mass flow of any components of interest (e.g. criteria pollutants in the boiler exhaust or ethanol in the headspace vent from fermentation) as well as the scrubbing efficiency, power demand and any materials required for the scrubber (e.g. activated charcoal, water or lime). This allows the user to evaluate tradeoffs between increased demand for power or materials and scrubbing efficiency. At present, the model assumes no significant fugitive emissions of VOCs or other pollutants, though they can be added if this assumption is incorrect.

8.5.4.8 Energy Potential of Process Byproducts

Since the energy balance and GHG intensity of cellulosic ethanol is critically tied to the ability of a conversion facility to supply its energy needs by utilizing process byproducts, the model includes a module to estimate the electricity and steam potential from process byproducts such as lignin cake, cell mass, uncoverted sugars, etc. Since EthCycle is not a mass/energy balance model, this module is not intended to provide accurate quantification of real-world experience, but rather to inform user decisions about input parameters for the Power System Module.

The process proposed by EdeniQ produces two streams with significant energy value. Partially-dried lignin cake and biogas from the wastewater treatment digester. There is also a stream of sludge from the wastewater clarifier, but the energy content of this stream is likely to be minimal. While this will be fed into the boiler and several literature sources indicate that there will be net energy production as a result, we assume that its energy value is negligible and its inclusion in the boiler feed stream is to reduce its mass prior to waste disposal.

The Energy Potential module accepts user input of the total amount of solid byproduct available for combustion, either as a raw number or as a fraction of feedstock input. The solid byproduct composition (lignin, protein, cell mass, cellulose, sugars, water) can either be calculated based on the assumption that its composition will be approximately the same as that of the NREL process design, or the composition can be modified by the user. Each component is assigned a specific heat, based on values from literature (Blunk & Jenkins, 2000; Energy Research Center of the Netherlands, 2012; EngineeringToolbox.com, 2012; McKinney, 2004). Mass flow rates of these byproducts are assumed to be the same as the NREL design as well. The composition of the solid byproduct from the EdeniQ process has not been fully analyzed, nor has the methane generation potential of its wastewater. The NREL design produces approximately the same amount of fuel, with a higher net yield. Since the EdeniQ plant has more feedstock consumed, but produces the same amount of fuel, the NREL design was felt to provide a conservative estimate of the solid byproducts from EdeniQ's process. Since the solid byproduct will enter the boiler with a substantial water content, this module subtracts the energy needed to heat and vaporize water from the potential energy of the inputs.

The calculated specific heats reflect the chemical energy embodied within the process byproducts. An estimate of actual electricity generation is made using thermal conversion efficiency factors for fluidized bed biomass boilers (22.9%), as reported by Grass and Jenkins (1994). This estimate is from 1994 and probably does not reflect the state of the art technology, so an additional range of results is generated for other generally well-accepted efficiency values. The facility uses some of the reject heat from electricity generation for other uses. A common rule of thumb is that half of the reject heat from such processes can be economically recovered at a range of temperature points. The proposed EdeniQ facility has substantial heat demands, but utilizes only about two-thirds of this available waste heat. Further research is necessary to confirm these estimates.

In addition to the solid byproducts, many process designs, including the current NREL design, call for process wastewater to be treated in an anaerobic digester. Since the wastewater will likely contain a high level of organic material and residual sugars and other nutrients from the fermentation process, it appears to have a high potential for methane generation. This methane can either be combusted in a biogas engine, or mixed with the facility's boiler air intake and combusted along with the solid byproduct. Methane generation is highly dependent on the specific composition of digester inputs as well as operating conditions and it is left to the user to define the methane potential of any wastewater treatment stream. The energy potential of the biogas is added to the total generation potential for the factory. The residual sludge from the digester can also be combusted, but due to its water content and high concentration on non-flammable components, it is assumed to add a negligible amount of energy to the process.

This module's purpose is to give an order-of-magnitude estimate of how much energy can be generated by combusting process byproducts. A more accurate estimate should be generated using specific operational parameters for the type of combustor used in any facility as well as the actual composition and methane generation potential of any process byproducts.

8.5.4.9 Power System Module

A major source of environmental impacts during the production of cellulosic biofuels is the demand for heat and electricity for the conversion process. Preliminary work indicated that if facility energy demands were not met by utilizing byproducts, life-cycle GHG emissions for the resulting fuel might increase by a factor of four or five.

Conversion and distillation both typically require significant amounts of heat. EthCycle must be able to attribute energy demands to their respective processes in order to analyze which elements of production are responsible for environmental impacts. Accordingly, the model sums the demands for heat and steam, then assigns a proportion of total demand to each module in the process (if desired, energy demands can be further subdivided within modules).

EthCycle also allows for the use of grid electricity and natural gas to make up any energy demand not supplied by combustion of process byproducts. The model can accommodate any fuel source that has available LCI data or alternatively, can burn supplemental biomass from the same source as the biomass being used as feedstock. Alternatively, if surplus electricity is available, EthCycle can model returning it to the grid for a credit against displaced generation elsewhere.

In addition to heat demand, there are significant cooling burdens associated with several phases of production. Some of this cooling will be accomplished with water from the external supply while some will require powered chilling. This element of the process needs significant further evaluation and currently is not included in EthCycle.

The mass and energy balance models used to develop the current version of EthCycle reflect an early vision of a future facility. As thermal and process optimization continues, the energy demands of the facility are likely to drop. Users of EthCycle are advised to carefully interpret the quantitative values supplied by the current model, since they do not represent an optimal facility design.

The production process envisioned by EdeniQ is likely to be highly energy-intensive; the default model calls for almost 30 MW of power consumption and while this is comparable to the estimated power consumption from the similarly-sized facility of the 2011 NREL design. This energy demand must be met by renewable energy for the resultant fuel to yield a net reduction in life-cycle GHG emissions compared to petroleum fuels. There will be a significant amount of solid residue, primarily lignin, remaining after ethanol production. This can be combusted, along with biogas from the wastewater treatment digester to meet this demand and emit only biogenic carbon, however the actual amount of energy produced has significant uncertainty. Under conservative assumptions, it appears that there is sufficient, even excess, energy within these waste streams to meet the heat and electricity demands of the proposed facility, however better data regarding the properties of the solid coproduct and the methane generation potential of wastewater streams is needed to confirm this conclusion.

8.5.4.10 Construction Module

In most energy production systems, facility and infrastructure construction typically contributes only a small portion of life cycle environmental impacts when compared to operational impacts. Because of this, only a simplified treatment is included in EthCycle.

The two largest elements of environmental impact from construction are the production of concrete and steel, which represent the greatest mass of material within the proposed conversion facility. The life cycle inventories for these materials were obtained from the Portland Cement Association and the World Steel Association, respectively (Marceau et al., 2007; World Steel Association, 2011). Facility lifespan was, upon recommendation from industry partners, assumed to be 20 years and no building decommissioning was considered. Impacts were distributed over the facility lifetime by simple straight-line amortization.

This analysis indicated that these two construction materials accounted for only 0.022 g of GHG equivalent for every MJ of ethanol produced; less than 0.01% of life cycle GHG emissions. This result supports the assumption that construction impacts are generally small compared to operating emissions, and suggests it is not necessary to model facility construction in greater detail.

8.5.4.11 Transport Module

EthCycle estimates transport emissions and energy consumption based on standard assumptions for freight logistics in its default scenario (Winebrake et al., 2008). Previous work at UC Davis in the area of geospatial modeling of biofuel systems has indicated that average transport distances between field and processing facility are around 50 miles (Parker, Hart, et al., 2010). The *Pioneer scenario* envisions processing and storage facilities located relatively near to fields in order to minimize the distance across which bale transport, which is less efficient than bulk, must be utilized. EthCycle assumes an average bale transport distance of 15 miles and an average bulk transport distance of 35 miles. Further research will be required to test the validity of these assumptions.

Feedstock transport was modeled as described in the uniform feedstock model (26 bales per 53 foot trailer, or 21.8 metric tons of minimally compressed bulk feedstock). Agricultural transport trucks are typically older than the fleet average, since they travel shorter distances and haul lower value goods. EthCycle assumes trucks with California 2002 model year compliant engines with 120,000 engine hours per truck. These assumptions can be modified by the user.

Using representative values for fuel economy and assuming empty back haul at 1.4 times the fuel economy of loaded trucks (Frey et al., 2008), estimates of diesel consumption were generated and entered into the LCI section. Emission factors for the criteria pollutants were derived from EMFAC and entered into the module LCI section, along with carbon and sulfur emissions from fuel combustion.

8.5.4.12 Impact Assessment

Air pollutant emissions, including GHGs, are the principal interest of the current EthCycle model. These also have significant implications for the commercial and environmental feasibility of the modeled production pathway. GHG emissions will determine whether the fuel achieves the targets set out by the Low Carbon Fuel Standard or the advanced biofuel mandates of the Federal Renewable Fuel Standard. Air pollutant emissions will play a role in determining where production facilities can locate.

Accordingly, the impact categories produced by the current version of the model tend to focus on GHG and air pollutants. At present, all criteria pollutants are tracked as well as CO_2, methane, nitrous oxide and sulfur hexafluoride, which are all GHGs. Based on tracked GHG data, CO_2-equivalent emission are calculated using both 20 and 100 year global warming potential (GWPs). Several other environmental indicators are provided, including acidification and eutrophication potential. It is important to remember, however, that the LCI section of each module tracks a comprehensive list of material and energy flows, if the user desires information on a different flow or different environmental impact category, these can be provided.

8.5.5 Areas of Uncertainty

The EthCycle model currently represents the best available information from a wide variety of sources in literature as well as from partners in industry. Biochemical cellulosic ethanol production has not yet reached commercial scale, however, so substantial uncertainty still exists. The following section will attempt to define existing areas of uncertainty as well as suggest how this might be reduced.

8.5.5.1 Feedstock Production

Feedstock production may represent the single largest source of uncertainty within the cellulosic biofuel life cycle. Feedstock production is also responsible for the majority of GHG emissions in this LCA and many others. Several authors have noted that soil carbon is very responsive to human activity, such as cultivation, and may represent a very large potential source or sink for atmospheric carbon (P. Smith, 2007; W W Wilhelm et al., 2007).

8.5.5.1.1 Agricultural Yield Uncertainty

Farming is inevitably uncertain; yields vary widely on a year-to-year basis due to climate, disease patterns, surface water availability and economics. Farmers regularly change the specific cultivars planted and agronomic practices to match transient economic conditions. This complicates forecasting feedstock availability, which is of critical importance when constructing biorefineries with 30+ year operational lifespans. Additionally, there are uncertainties that are difficult to model without stochastic analysis, such as crop failures, fire, drought or policy action. Some infrequent conditions could reduce feedstock production to almost zero for one or more seasons. Spot market transactions can reduce some of this risk, but most conversion facilities in the near-term will be specialized towards one particular feedstock and conversion efficiency or plant uptime may suffer if alternative feedstocks are used. The INL uniform feedstock model attempts to address this problem by standardizing the physical format of feedstock in such a way to maximize its transferability between biorefineries. Pelletization, torrefaction or fast pyrolysis may offer similar options for standardizing feedstock, but all are still limited by the inherent uncertainty of agriculture.

Research is currently evaluating how better to integrate uncertainty into life-cycle analysis and decision-making (Ebadian et al., 2012; Huijbregts et al., 2001). Integrating these methods into biofuel LCA models may be a critical step in improving their ability to prospectively model biofuel production systems.

8.5.5.1.2 Soil Carbon Uncertainty

Cellulosic biofuels, by their very nature, entail removing substantial amounts of carbon-containing compounds from fields. Almost every feedstock production process involves some measure of fertilization and soil disturbance, which can promote microbial activity and reduce SOC stocks. As demonstrated in the sensitivity analysis, there is significant potential for massive GHG emissions from soil carbon loss, as in the case of corn stover. Similarly, there is significant potential for carbon sequestration with some grassy crops under appropriate conditions in the short term; over the long term, soil carbon in these crops may reach a new equilibrium (Anderson-Teixeira et al., 2009).

GHG emissions from iLUC can be difficult to model and even more difficult to prevent through policy. Accurate modeling of iLUC typically requires economic equilibrium modeling, which struggles to accommodate immature markets. Policy can limit iLUC within borders, however the globalized nature of agricultural product markets means that iLUC effects often cross borders. U.S. corn ethanol policies have been widely regarded as responsible for significant price fluctuations in foreign markets and crowding out of traditional crops. In absence of effective global LUC policy, it is important that U.S. policy attempt to minimize the drivers of iLUC by including it in GHG accounting for domestic biofuels wherever possible. Smith's contextualization of iLUC as temporally or spatially-shifted dLUC (2007) helps explain why; you cannot accurately estimate dLUC changes without knowing about the soils and crops being directly affected. Determining this across distance and time is necessarily difficult. Even though research on this subject is still rapidly evolving, a few general principles are clear:

1. Do not convert lands with high amounts of stored carbon, such as forests or peat lands to biofuel use.
2. When converting "marginal" lands to biofuel use, evaluate the direct carbon changes as well as how any lost productivity will be replaced.
3. Regularly monitor soil carbon levels and fluxes; ensure that there are policy or contractual options available to facilitate changes in management (e.g. tillage, residue removal rate, cover crops, etc) if necessary.

There is a small, but expanding body of literature on the subject of estimating SOC change due to dLUC for biofuel crops. Anderson-Teixeira's paper attempts to consolidate them into a single average estimate and in doing so, highlights the high variability between different studies. Standardizing measurement practices including soil depth, treatment of litter and moisture conditions may help reduce this uncertainty and establish clear rules to exclude the most egregious cases of SOC loss.

It seems clear from the various papers on the subject that corn stover is a risky bioenergy feedstock due to the possibility of rapid SOC loss when stover is routinely removed. If stover is to be used, no till practices and other SOC conservation measures will be necessary. Further research into nitrogen cycles and emissions of N_2O or other GHGs is necessary; Kim & Dale conclude that stover removal significantly reduces N_2O emissions from the field by removing the nitrogen embodied in stover (2009), but few other studies report similar changes. If N_2O fluxes are really as significant as Kim & Dale posit, then stover's potential as a bioenergy feedstock is greatly improved.

Grassy crops such as switchgrass and miscanthus may have greater potential than previously realized as a biomass feedstock due to their tendency to sequester carbon in root mass. While the sequestration effect may reach equilibrate over the long term, the near-term potential of grassy crops to sequester carbon deserves careful consideration. It has even been proposed that certain mixtures of grasses could yield a biofuel product that was carbon-negative over its life cycle (Tilman et al., 2006). To put it succinctly, corn stover seems to have significant downside risk from SOC changes while grasses seem to have significant upside potential from the same source. Further research is required to confirm this.

8.5.5.2 Preprocessing and Transportation Uncertainty

At present, most spatial models of biofuel production anticipate that heavy-duty freight trucks will dominate the transportation of feedstock. Rail and barge transport are more efficient, but are tied to fixed infrastructure. Within truck transport there are two primary options for transport: as bales, or as a bulk product, such as shredded, torrefied or pelletized biomass or pyrolysis oil. Transport in bales minimizes cost and allows facilities to grind to their own specifications. Bulk biomass is likely to be more dense and therefore more efficient to transport. Converting biomass to bulk form requires energy, with pelletization and pyrolysis requiring more than shredding or torrefaction. The energy requirements of all of these processes are uncertain and need to be tested under real-world conditions. There are likely some conditions under which the energy involved in densifying the biomass is outweighed by the efficiency improvements gained, but this cannot be determined without case-by-case analysis.

Pelletization may have the potential to increase yields from biochemical cellulosic ethanol production by disrupting the cell walls and allowing better enzymatic access to cell contents. It also produces a very stable, high-density product. The energy required to pelletize biomass at large scale is not well studied in available literature; the overwhelming majority of studies are on laboratory-scale equipment which may dramatically underestimate the energy required to pelletize large quantities of biomass (Morey, 2012). Future research should attempt to quantify both the yield benefits of pelletization and the energy required to create the pellets. If biorefineries ultimately achieve some of the more optimistic levels of excess electricity production, it’s possibly that pelletization could be powered by the facility’s renewable generation.

Finally, there is uncertainty regarding the quality of feedstock itself. Some early projects have been plagued by the presence of dirt and fines in feedstock from test fields. This is likely due to the novelty of stover collection for some producers and could be solved by better harvest and collection practices and equipment. Some degree of dirt and fines are almost unavoidable, since most storage concepts require dry feedstock, necessitating a period of field drying in a windrow prior to baling or shredding. Several alternative feedstock collection practices have been proposed but not adequately modeled. Wet storage of biomass, in a fashion similar to silage, has also been proposed (Shinners & Binversie, 2007). In theory, fermentation would break down some of the cell walls, improving efficiency enough to offset fermentation losses. Other concepts call for only the cob and husk of the corn to be collected, since these, particularly the cob, have a composition well suited for biofuel production. They can also be harvested in a single pass, with the grain and the baling step omitted. Further research is necessary to determine whether one of these, or another alternate feedstock collection method yield superior life-cycle GHG performance.

8.5.5.3 Conversion Uncertainty

The EthCycle model reflects the current state of the art, however there is still substantial development remaining before this technology is deployed at commercial scale. Accordingly, the model reflects several assumptions regarding how biochemical cellulosic ethanol production is likely to occur in the future and also includes several gaps were data are still missing.

8.5.5.3.1 Enzyme Requirements

Hydrolysis of cellulose into fermentable sugars requires substantial amounts of energy, and in most cases, specialized enzymes. EdeniQ's model anticipates that their microbes will produce their own hydrolysis enzymes, however this has not been tested at scale. When commercial enzymes must be added, they can have a significant effect on life-cycle energy consumption and GHG emissions, since their production process is energy and chemical intensive (MacLean & Spatari, 2009). While the non-enzyme chemical additions modeled under EthCycle's default conditions do not drastically affect the final GHG or energy balance, it is important that a comprehensive understanding of all chemical inputs be developed, to both account for their life-cycle GHG impact and track potential emissions of pollutants. Modeling the effect of enzymes is further complicated by the lack of transparency in their production. Most enzyme makers regard the manufacturing process to be a trade secret, so developing a life-cycle inventory requires many approximations and assumptions. As enzymatic chemistry becomes a more important industrial tool, it will become imperative that LCIs for industrial enzymes be developed.

8.5.5.3.2 Facility Power Requirement Uncertainty

EthCycle estimates the available energy from process byproducts and concludes that it is plausible that the modeled facility would be able to meet its heat, cooling and electricity needs by combusting these byproducts in a fluidized bed boiler. NREL's 2011 biochemical process design arrives at the same conclusion. Both EthCycle and NREL's model conclude that biochemical facilities may be able to export a substantial amount of electricity as well. This electricity, which is entirely produced by biogenic carbon, could represent a significant carbon credit from displacing conventional grid-mix electricity, which could be applied towards the fuel's GHG intensity. In addition, this electricity could qualify as renewable under many states' Renewable Portfolio standards. While fluidized bed boilers are a fairly well-understood technology, they have not been combined with biofuel production in the way envisioned by EthCycle or NREL. Before any carbon credits for renewable generation are created, the ability of biochemical facilities to produce electricity in excess of their own demand needs to be convincingly demonstrated. A substantial fraction of the potential energy from waste streams comes from anaerobic digestion of wastewater. This technology needs to be demonstrated in conjunction with the wastewater streams from cellulosic ethanol production.

When external fuel is required to operate the facility, the life-cycle GHG impacts of the resulting fuel rapidly exceed EPA mandated levels to qualify for Renewable Identification Numbers under the Renewable Fuel Standard, which reduces the value of such fuels. Purchasing external energy also represents a substantial cost for an already low-margin business to bear. The ability of facilities to power themselves by combusting byproducts is perhaps the single greatest area of uncertainty for biochemical cellulosic ethanol.

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Chapter 9: References

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