

Manuscript Title: Impact of aviation non-CO₂ combustion effects on the environmental feasibility of alternative jet fuels

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1 Procedural Overview of Life Cycle Analysis of GHG Emissions

The life cycle analysis of alternative jet fuels encompasses emissions from the complete fuel cycle. This includes recovery and transportation of the feedstock from the well, field, or mine to the production facility, processing of these materials into fuels, transportation and distribution of the fuel to the aircraft tank, and finally, the combustion of the fuel in the aircraft. The steps of such a well-to-wake life cycle analysis are shown schematically in Figure S1. These “well-to-wake” (WtW) steps can be broadly grouped into fuel production and distribution, “well-to-tank” (WtT), and fuel combustion, “tank-to-wake” (TtW). The interested reader is directed to a recent guidance document created by a consortium that was assembled by the US Air Force (AFLCAWG, 2009) to learn more about the details of creating a life cycle GHG inventory for transportation fuels.

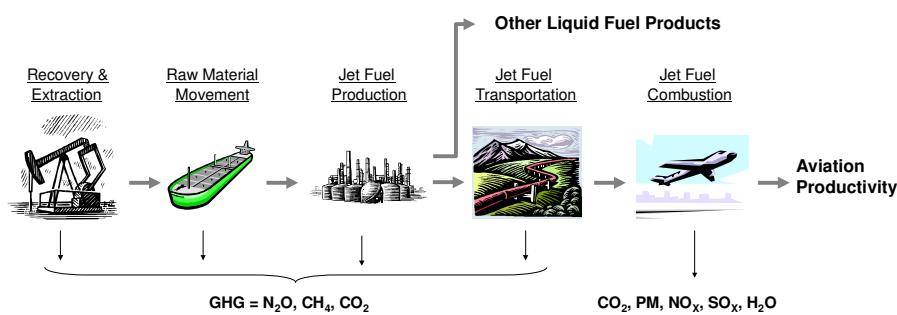


Figure S1: Steps considered, in the well-to-wake, life cycle GHG inventory of conventional jet fuel

For each step of the life cycle, GHG emissions are assessed and reported on the basis of per-unit energy consumed by the aircraft (per megajoule). The GHG covered are carbon dioxide, methane and nitrous oxide. The results herein do not account for energy or GHG emissions associated with the initial creation of infrastructure such as extraction equipment, transportation vehicles, farming machinery, processing facilities, etc. The impact of such emissions on the total life cycle GHG emissions of the pathway is usually relatively small, and within the uncertainty range of the analysis. (Hill et al., 2006, Edwards et al., 2007).

1.1 Analysis Procedure

Analyses of life cycle GHG emissions for several jet fuel production pathways were carried out based on available information in the scholarly and technical literature. The Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) framework (versions 1.8b and 1.8a) and its supporting data, both developed and maintained by Argonne National Laboratory, was the primary tool used in the well-to-wake life cycle GHG analysis.¹ A simulation year of 2015 was used and default GREET assumptions were used in the analysis of the pathways, except where more recent data were obtained.

A key limitation of the GREET framework is that it is designed for ground transportation fuels and vehicle systems and does not include jet fuel production pathways. Also, not all the feedstocks analyzed are available in GREET. Hence, this work utilized data from the literature on jet fuel and jet fuel alternatives where available (e.g. fuel properties, refining efficiency) and incorporated them into the GREET framework to derive life cycle GHG emissions. Where supporting data are presented, mixed units are used for consistency with GREET version 1.8a/1.8b.

The GREET framework was primarily used as a database and calculation platform, where the quality of results depends on the quality of input assumptions such as energy efficiencies, fuel properties and emission allocation method for co-products. Hence, a de novo approach was taken in identifying and

¹ The specific version of GREET used for each pathway within a section is stated at the beginning of the section; however, the impact on the results of this work of using GREET version 1.8a or 1.8b is negligible compared to the inherent uncertainties of life cycle analysis.

reviewing key inputs and assumptions for each pathway. Specifically, default GREET input assumptions were examined for the fuel pathways available in GREET. Key parameters with a significant impact on the life cycle GHG emissions of the pathway were identified. Default GREET values for these key parameters were updated wherever necessary using reviews of recent information available in the literature. Where a specific pathway was not available in GREET, the pathway was built within the GREET framework with all relevant input parameters gathered from the open literature.

1.2 Characterization of SPK Combustion Emissions and Effects

In maintaining the *lens* framework from the main text, the percentage reductions in soot and NO_x emissions attributed to the use of SPK fuel, as compared to conventional jet fuel, are given by distributions with functional forms and bounds shown in Figure S2. Results with the low and high lenses reflect deterministic use of the low and high values while the mid-range lens reflects the results of Monte Carlo simulations using random variables drawn from the distributions of Figure S2.



Figure S2: Input distributions for NO_x and soot reductions resulting from the use of SPK fuel

The upper and lower bounds of NO_x reduction were based on experimental results from Bester and Yates (2009), Bulzan et al. (2010), Dewitt et al. (2008), and (Timko et al. 2010).. The functional form of the distribution was chosen to reflect a conservative estimate within the bounds of experimental data. NO_x emissions are strongly dependent on engine throttle setting, specific engine/combustor technology and ambient temperature; hence, it is little surprise that results of the aforementioned research efforts do not conclusively indicate a single value.

The upper and lower bounds of SPK induced soot reduction were based on experimental measurements from PW308 and CFM56 gas turbines. Mass-based soot reductions from SPK use in the PW308 varied from 98% at 7% power, which is representative of idle, to 58% at 65% power, which is representative of cruise conditions (Timko et al. 2010). Similarly, SPK fuel in the CFM56-7 led to a 67% reduction in soot at 7% power and a 79% reduction at 65% of full throttle (Lobo 2011). The mode of the distribution is consistent with measurements from Bester and Yates (2009) and Bulzan et al. (2010), who measured average reductions of 85% and 90% in soot emissions over the throttle range of a CFM-56-2C1 engine using coal based F-T jet fuel from Sasol and natural gas based F-T jet fuel from Shell, respectively.

SPK fuel was assumed to cause no change to the radiative forcing from aircraft contrails and contrail cirrus per unit of fuel mass relative to conventional jet fuel because no data has provided quantifiable evidence otherwise. Qualitatively, the magnitude of the atmospheric impact from contrails and contrail cirrus depends on details of plume evolution and the relative ability of aerosol particles to act as ice-forming nuclei (Wuebbles et al., 2007). The presence of ice-forming nuclei may trigger the formation of contrail cirrus much later than the original emission if the background atmosphere has changed to a state allowing for cloud formation (Sausen et al., 2005). Hence, the complete elimination of sulfate aerosols and the significant reduction of soot emissions caused by SPK fuel might serve to reduce contrail and contrail cirrus formation. Conversely, the increase in water vapor from SPK fuel may serve to stimulate additional contrails and contrail cirrus if their formation is more strongly dependent on background atmospheric aerosol concentrations rather than local concentrations in the exhaust jet. Wuebbles et al. (2007) emphasize that improving the understanding of contrails and contrail cirrus formation requires coordinated regional-scale measurements to correlate the growth, decay, and trajectories of contrail ice particles with the ambient aerosols and gaseous aerosol precursor concentrations.

2 Jet Fuel from Conventional Petroleum

The conventional jet fuel production pathway forms the baseline against which the life cycle GHG emissions of alternative jet fuels are compared. Jet fuel could represent JP-8, Jet A, or Jet A-1, which are the fuels in use by the US Air Force, commercial aviation in the US, and commercial aviation in Europe as well as much of the rest of the world, respectively. Section 2.1 considers the extraction of conventional crude oil while Section 2.2 considers petroleum refining to produce jet fuel.

The steps involved in the production of jet fuel from conventional petroleum sources include crude oil extraction, transportation of crude oil to US refineries, refining of crude oil to jet fuel, and the transportation of jet fuel to the aircraft tank. The GHG emissions resulting from crude oil extraction, crude oil transportation and jet fuel transportation were obtained using data from two recently published National Energy Technology Laboratory (NETL) studies on the life cycle GHG emissions of petroleum-based transportation fuels (Skone and Gerdes, 2008; Skone and Gerdes, 2009). The emissions that result from crude oil refining were calculated using both a top-down and a bottoms-up perspective. This work differs from that of Skone and Gerdes (2008, 2009) in that the jet fuel pathway considers only jet fuel refined within the US and excludes jet fuel made from unconventional petroleum sources, such as oil sands, from the final result. Jet fuel refined within the US comprised 88.7% of all domestic jet fuel consumption in 2005 (Skone and Gerdes, 2008).

2.1 Crude Oil Recovery and Transportation

The source of crude oil is important in order to properly represent the range of resulting GHG emissions. The GHG emissions from crude oil recovery and crude oil transportation are designated origin specific GHG emissions. The variation in these emissions by crude oil source is primarily due to specific hydrocarbon flaring and venting practices during extraction, the emissions resulting from local electricity production, equipment efficiency and the transportation distance of crude oil to a US port.

Imported crude oils are on average heavier (lower API gravity²) and contain higher levels of sulfur than domestic products (Skone and Gerdes, 2009). The changes in crude oil properties as well as processing technique drive a variation in processing emissions of converting crude oil into finished fuel products. The GHG emissions associated with the processing of crude oil to jet fuel were developed using the GREET framework. These results are presented in conjunction with the origin specific GHG emissions and finished fuel transportation emissions derived from Skone and Gerdes (2008 and 2009) to establish GHG inventories for conventional jet fuel produced at US refineries.

Of the crude oil mix fed into US refineries in 2005, only 34% was domestically produced. The other 66% was imported from other countries located around the world. When including domestic production, over 90% of the crude oil mix came from only 11 countries (Skone and Gerdes, 2008). The remaining fraction of imported crude is designated 'other' and corresponds to the weighted average of all imported crude (excluding Canadian oil sands).

² API gravity is a measure of the density of a petroleum liquid relative to water. An API gravity greater than 10 indicates lighter than water while an API gravity less than 10 indicates heavier than water. $API\ gravity = 141.5/SG - 131.5$, where SG = specific gravity

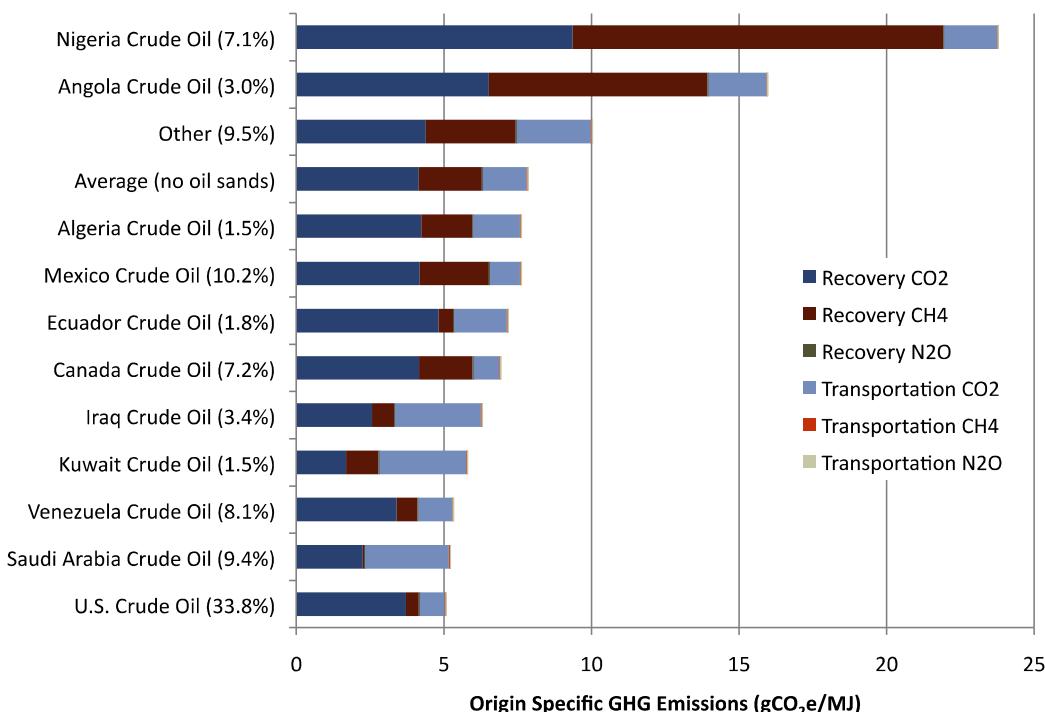


Figure S3: Origin specific GHG emissions by species of crude oil entering US refineries in 2005 (fraction of total imports in parentheses). Based on country profiles published in Skone and Gerdes (2008, 2009)

In their 2008 life cycle GHG analysis of petroleum based fuels, Skone and Gerdes developed crude oil extraction profiles, including methane flaring and venting data, for each of these 11 countries. They also developed a transportation profile for each country by accounting for the transport of imported crude oil from its point of extraction to foreign ports, ocean tanker transport of waterborne imported crude oil to domestic ports and crude oil transport within the US. The significance of examining the transportation profile of crude oil is that importing crude oil from Saudi Arabia and Kuwait results in more GHG emissions from transportation than crude from other sources. The recovery and total transportation GHG emissions (by species) from 2005 are given for crude oil from each source in Figure S3. Beside the label for each source, the volumetric fraction of total crude fed into US refineries imported from that country is given in parentheses. The volumetric fractions do not add up to 100% because Canadian oil sands are not listed.

These data highlight that domestically produced crude oil results in lower GHG emissions than any other source because of reduced transportation emissions. Even though CO₂ emissions resulting from domestic oil extraction are higher than Iraq, Kuwait, Venezuela and Saudi Arabia, the combination of transportation emissions and methane venting causes these regions to have higher origin specific GHG emissions than the US. In the cases of Iraq, Kuwait and Saudi Arabia, transportation emissions (primarily ocean transport emissions) represent 47%, 51% and 55% of the total origin specific GHG emissions.

The primary driver for countries with excessive origin-specific GHG emissions is methane venting. Methane emissions from Nigerian and Angolan crude extraction exceed all other origin specific GHG emissions. Mexican and Canadian crude also have non-negligible methane emissions from venting.

The variation in profiles shown in Figure S3 was used to establish the low emissions, baseline and high emissions scenarios for jet fuel from conventional crude. The low emissions scenario was composed of purely domestic crude oil, the baseline scenario adopted the weighted average of all crude oil fed into US refineries, excluding Canadian oil sands, and the high emissions scenario used only Nigerian crude. The transportation of jet fuel from US refineries to the aircraft tank are independent of the source of crude oil; hence, a single result was used for all three emissions scenarios.

2.2 Conventional Jet Fuel Production from Crude Oil

The properties of conventional crude oil were based on the projected average crude oil received by US refineries in 2015, obtained using historical data provided by the EIA. There is a definite trend for crudes to become heavier and more sour (more sulfur) in the future; therefore, a business as usual scenario would likely see jet fuel production becoming more energy intensive as more hydroprocessing is required to maintain current product quality. This means that the energy intensity of refining may increase beyond the values used in this study.³

The key parameter in analyzing the GHG emissions associated with the production of jet fuel from crude oil is fuel-refining efficiency. Two methods were employed in the derivation of jet fuel refining efficiency. The first method was a top-down approach, which derived the jet fuel refining energy efficiency from the overall US refining energy efficiency. This formed the baseline case. The second method was a bottom-up approach, which estimated jet fuel-refining efficiency by summing the energy requirements for the individual refining processes. Specifically, two extreme cases were examined: straight-run fuel production and hydroprocessing of crude oil. The refining efficiencies obtained using the bottom-up approach were used for the low and high emissions cases, respectively, providing a bound on the range of possible values.

2.2.1 Top-Down Approach (Baseline Case)

The overall US refinery efficiency as estimated by Wang (2008)⁴ was 90.1% (LHV), based on statistics of process fuel use in US refineries, and 2006 refinery fuel inputs and outputs provided by the EIA. Overall refinery efficiency is defined as (Wang, 2008):

$$\eta_0 = \frac{E_{products}}{E_{inputs}} \quad \text{Equation 1}$$

where η_0 = petroleum refinery energy efficiency,
 $E_{products}$ = energy of all petroleum products,
 E_{inputs} = energy in crude input, other feedstock inputs, and process fuels.

The jet fuel-specific refining efficiency was calculated from the overall refinery efficiency using the kerosene relative energy intensity⁵ and Equation 2, developed by Wang et al. (2004). The relative energy intensity of the production of kerosene (jet fuel), X_s , based on an energy-content process allocation method, is 62.4%, and the overall refining efficiency, η_0 , is 90.1%.

$$\eta_s = \frac{\eta_0}{\eta_0 + X_s(1 - \eta_0)} \quad \text{Equation 2}$$

From Equation 2, the refining energy efficiency of jet fuel is 93.5% (LHV). This refining efficiency was used in the baseline case for the life cycle analysis of GHG emissions from the production of jet fuel from conventional petroleum.

Based on 2006 US refinery data published by the EIA, Wang (2008) calculated the shares of process fuel used in US petroleum refineries (see Table S1). These shares were used as inputs to the GREET model for the baseline case of jet fuel production.

³ From data on sulfur content and API gravity of average crude oil input to US refineries from 1995 to 2006 given by EIA (EIA, 2008a), it was estimated that there was approximately a 2% annual increase in sulfur content and 0.25% annual decrease in API gravity. From these trends, the average crude oil quality received by US refineries in 2015 was estimated.

⁴ This work was used to update the refining efficiency of gasoline, diesel, LPG, residual oil and naphtha in GREET (version 1.8b). (GREET, 2008)

⁵ Relative energy intensity was defined as “the ratio of total energy use share to the mass share of a given fuel.” It provides a measure of how energy intensive the production of a particular fuel is relative to the mass share of that fuel produced. A relative energy intensity of more than 100% for a particular fuel means that the production of that fuel consumes a greater share of overall process energy than the mass share of that fuel produced. The energy intensity of the overall refinery is 100%.

Table S1: Type of process fuel and fuel share in the refining of jet fuel and ULS jet fuel

Type of process fuel	Process energy share (%)
Electricity	3.5
Natural Gas	41.3
Refinery Gas	39.6
Coke	14.3
Residual Oil	1.3
Total	100

2.2.2 Bottom-up Approach (Low and High Emissions Cases)

The jet fuel produced by a refinery may be straight-run, produced from hydroprocessed stocks, or a blend of both. The refining efficiency of each production method was estimated by summing the energy inputs of individual processes. These two cases formed the low and high emissions scenarios, respectively, for the life cycle analysis of GHG emissions in the production of jet fuel from conventional petroleum.

The energy for the processes involved in refining jet fuel was taken from a 2007 Department of Energy sponsored report (Pellegrino et al., 2007). The report provided both a range of refining process energy use, as well as average energy use. The average energy use data for the relevant refining processes were used to calculate the jet fuel refining efficiency.

Straight-Run Jet Fuel

The main processes involved in the production of straight-run jet fuel are crude desalting and atmospheric distillation, followed by chemical treatments (such as the Merox process) to remove contaminants like mercaptans and organic acids, etc. The estimated process energy in crude desalting and atmospheric distillation is shown in Table S2. As no data were found in the literature regarding the energy needed for chemical treatment, it was assumed that the energy needed for this process was negligible by comparison.

Table S2: Energy requirement in the production of straight-run jet fuel

Refining process	Energy required (J/MJ product)
Crude desalting and atmospheric distillation	20,055
Chemical treatment	Assumed to be negligible
Total	20,055
Overall refining efficiency (LHV)	98%

Under these assumptions, the refining efficiency of straight-run jet fuel is about 98% (LHV). This refining efficiency likely represents the maximum efficiency for the production of jet fuel from conventional crude and was used in the low emissions scenario. The corresponding process fuel and fuel shares for the production of straight-run jet fuel are shown in Table S3.

Table S3: Process fuel and fuel shares for the production of straight-run jet fuel

Type of process fuel	J/MJ of jet fuel	Process fuel share (%)
Electricity	423	2.1
Natural Gas	5,772	28.8
Refinery Gas	9,669	48.2
Coke	3,548	17.7
Residual Oil	643	3.2
Total	20,055	100

Hydroprocessed Jet Fuel

The refining processes involved in producing jet fuel from hydroprocessing include crude desalting, atmospheric and vacuum distillation, hydrotreating and/or hydrocracking. Since the production of this hydroprocessed jet fuel was considered as the high emissions scenario, it was assumed that all the above

processes were required (including both hydrotreating and hydrocracking). The energy needed for the refining processes to produce hydroprocessed jet fuel is shown in Table S4.

Table S4: Energy requirement in the production of jet fuel from hydroprocessing

Refining process	Energy required (J/MJ product)
Crude desalting and atmospheric distillation	20,055
Vacuum distillation	16,379
Hydrotreating (to S content of ~500ppm)	24,368
Hydrocracking	75,092
Total	135,894
Overall refining efficiency (LHV)	88%

The refining efficiency of hydroprocessed jet fuel is approximately 88% (LHV). As mentioned earlier, this refining efficiency was assumed in the high emissions scenario. The corresponding process fuel shares for the production of hydroprocessed jet fuel are shown in Table S5.

Table S5: Process fuel and fuel shares for the production of jet fuel from hydroprocessing

Type of process fuel	J/MJ of jet fuel	Process fuel share (%)
Electricity	9,137	6.7
Natural Gas	82,683	60.9
Refinery Gas	30,713	22.6
Coke	11,294	8.3
Residual Oil	2,067	1.5
Total	135,894	100

2.2.3 Conventional Jet Fuel Results

The life cycle GHG emissions from the production of jet fuel from conventional crude are shown in Table S6. These results incorporate the recovery (crude extraction) and transportation results discussed in Section 2.1 to complete the life cycle GHG inventory. A comparison of the domestic results from this study with the average results presented by Skone and Gerdes (2008) is shown in the far right column of the table. Despite using a different approach to derive the GHG emissions in the processing of feedstock in the baseline case (top-down) from that used in the NETL study (bottom-up approach), similar results were obtained. The combustion CO₂ equivalent emissions used by Skone and Gerdes are slightly higher than those calculated in this study. This is due to their estimates of CH₄ and N₂O emissions from jet fuel combustion. These emissions were excluded in this study due to the high level of uncertainty associated with their estimation. Overall, the life cycle GHG emissions of jet fuel from conventional crude obtained by NETL (88.0 gCO₂e/MJ) are about 0.7% higher than the baseline results (87.5 gCO₂e/MJ) developed herein.

Table S6: Summary of results for jet fuel from conventional crude and a comparison of results to the NETL petroleum baseline study

	Conventional Jet Fuel			NETL
	Low	Baseline	High	Baseline
Key Assumptions				
Crude oil origin	US	Average	Nigeria	n/a
Processing Technique	Straight Run	Average	Hydro-processed	n/a
Refining efficiency (LHV)	98.0%	93.5%	88.0%	n/a
Life Cycle CO₂ Emissions by Stage				
Recovery of feedstock (gCO ₂ /MJ)	3.7	4.2	9.4	4.3
Transportation of feedstock (gCO ₂ /MJ)	0.8	1.5	1.8	1.3
Processing of feedstock to fuel (gCO ₂ /MJ)	1.6	5.5	11.0	5.5
Transportation of jet fuel (gCO ₂ /MJ)	0.8	0.8	0.8	0.9
Combustion CO ₂ (gCO ₂ /MJ)	73.2	73.2	73.2	73.7
WTT GHG Emissions by Species				
WTT CO ₂ emissions (gCO ₂ /MJ)	7.0	11.9	22.9	12.0
WTT CH ₄ emissions (gCO ₂ e/MJ)	0.5	2.3	13.0	2.3
WTT N ₂ O emissions (gCO ₂ e/MJ)	0.1	0.1	0.1	0.1
Total WTW GHG Emissions (gCO₂e/MJ)	80.7	87.5	109.3	88.0
Life Cycle GHG Emissions Relative to Baseline Conventional Jet Fuel	0.92	1.00	1.25	1.01

3 Fischer-Tropsch Jet Fuel

The Fischer Tropsch (F-T) process first involves the steam reforming or gasification of any carbon containing feedstock (e.g. natural gas, coal or biomass) to synthesis gas (syngas), which is a mixture of hydrogen and carbon monoxide. The syngas is subsequently converted to paraffinic hydrocarbons in the presence of an iron- or cobalt-based catalyst (Fischer-Tropsch synthesis). A third upgrading step cracks the longer hydrocarbon chains to maximize the production of synthetic paraffinic liquid fuels like diesel and jet fuel. Syngas must be cleaned before Fischer-Tropsch synthesis step to remove contaminants, particularly sulfur, to avoid poisoning the catalyst. Hence, the resultant Fischer-Tropsch liquid fuels are virtually free of contaminants and the jet fuel fraction of the product slate falls into the category of synthetic paraffinic fuels.

All jet fuels produced using F-T synthesis have similar characteristics, independent of feedstock type. Any small variations in fuel properties are primarily associated with the operating conditions (e.g., catalyst, temperature, and pressure) within the synthesis reactors and how the direct products of the synthesis are treated and processed. All jet fuels produced using the F-T process share common characteristics with regard to compatibility with existing infrastructure and aircraft, combustion emissions, and their relative merit for use in aviation. Feedstock choice, however, does have a strong influence on fuel production capacity, production cost, life cycle greenhouse gas emissions, and technology readiness (Hileman et al., 2009).

3.1 Fischer-Tropsch Fuel from Coal

This examination of life cycle GHG performance of F-T jet fuel production from coal without carbon capture and sequestration was conducted. A stand-alone F-T liquid fuels plant designed to maximize liquid fuels production with no excess electricity was examined. Sufficient electrical energy was produced to fuel all internal processes, with negligible excess electricity produced for export. The process included the upgrading (hydroprocessing) of long-chain liquids to a final product slate of diesel (C₁₈), jet fuel (C₁₂) and naphtha (C₄-C₆). The energy allocation method was adopted for assigning energy and emissions to various liquid products.

Most studies in the literature focus on F-T reactor designs and conditions that produce diesel and naphtha. To produce jet fuel instead of diesel, additional hydrocracking and greater syngas recycle are needed, resulting in a small increase in hydrogen and power requirements for the plant. Furthermore, a moderate decrease in the CO₂ associated to jet fuel compared to diesel would ensue due to changes in the allocation fractions. As these additional energy requirements do not lead to substantial increases in CO₂ emissions from the facility (Gray et al., 2007), they were ignored in this analysis, (i.e. the production of F-T jet fuel is assumed to have the same emissions as the production of F-T diesel). Although F-T jet fuel can be made without added burdens, it is not possible to have a product slate of 100% F-T jet fuel⁶ (a value of 25% is taken as the preferred value in these studies, and a sensitivity study is shown for a co-fed coal and biomass F-T facility).

Process efficiency and coal type were judged to be key parameters having a significant impact on the overall GHG emissions of the Coal to Liquids (CTL) pathway. Equation 3 defines process efficiency for a general F-T facility.

$$\text{Process Efficiency} = \frac{1 \text{ MJ}_{\text{fuel}}}{1 \text{ MJ}_{\text{feedstock}} + \text{Process Energy}} \quad \text{Equation 3}$$

Both bituminous and sub-bituminous coal based processes were examined.⁷ In 2007, almost 65% of bituminous coal production in the US occurred via underground mining while the remainder was surface-mined. On the other hand, sub-bituminous coals are almost exclusively surface-mined (EIA, 2008b). Underground mining results in substantially greater methane emissions compared to surface mining processes. Methane emissions arising from the production of underground-mined and surface-mined coals were estimated using aggregate coal mining methane emissions data (EIA, 2007; Bartis et al., 2008).⁸

The low emissions case assumed a lower heating value process efficiency of 53% with surface-mined bituminous coal.⁹ In the baseline case, a process efficiency of 50% was used (Bartis et al., 2008; Deutch and Moniz, 2007; Van Bibber et al., 2007; Murano and Ciferno, 2002) with the 2007 average US coal mix of underground-mined and surface-mined bituminous coal and surface-mined sub-bituminous coal¹⁰; the use of anthracite or lignite coal was not considered in this analysis. The high emissions case assumed a process efficiency of 47% and underground-mined bituminous coal (based on case 1 of Southern States Energy Board CTL study, SSEB, 2006). For comparison, the first Sasol CTL plant built in the 1950s had process efficiencies under 40% (UK DTI, 1999; Gray and Tomlinson, 2001).

The inputs assumed for the three scenarios are summarized in Table S7.

⁶ An F-T plant configured to produce 70% diesel and 30% naphtha should theoretically be able to undergo modifications such that it could yield 60% jet fuel and 40% naphtha (Gray et al., 2007). Sasol is developing the ability to produce a joint Battlefield-Use Fuel of the Future (BUFF) using F-T synthesis. This fuel could be used in place of JP-8 in military aircraft and they report a yield of ~30% that conforms to the freezing point standards of JP-8. The rest of the product slate is composed of “heavy” diesel and naphtha (Lamprecht, 2007).

⁷ Lignite coal can possibly be used as a feedstock to CTL plants but lignite production in the US is much lower (~7% of total coal production in 2007, EIA 2008c) compared to bituminous and sub-bituminous coal production (46.7% and 46.3% of total coal production in 2007, respectively, EIA 2008c). Reliable data on methane emissions associated with the mining of lignite coal are not available. For these reasons, lignite coal is not analyzed in this work.

⁸ Bartis et al., 2008 estimated methane emissions of 338 pounds of carbon dioxide equivalent per ton of underground-mined coal and methane emissions of 42.4 pounds of carbon dioxide equivalent per ton of surface-mined coal based on EIA data (EIA, 2008b). The methane emissions per MJ of coal production were calculated from the lower heating values of bituminous coal and sub-bituminous coal.

⁹ Thomas Tarka, interview with David Ortiz, October 3, 2008.

¹⁰ Compared to 2007, the coal production mix in 2017 is projected to comprise a larger proportion of surface-mined sub-bituminous coal from Western coal production, particularly the Powder River Basin. (EIA, 2008d)

Table S7: Input assumptions for the production of F-T jet fuel from coal (without carbon capture) for low emissions, baseline and high emissions cases

	Low	Baseline	High
Process efficiency (LHV)	53%	50%	47%
Coal input	Surface-mined bituminous coal	Average bituminous and sub-bituminous coal mix ¹¹	Underground-mined bituminous coal
Coal mining methane emissions (g CO ₂ e/MJ coal)	0.80	2.8	6.4

The life cycle GHG emissions from the production and use of F-T jet fuel from a CTL plant without carbon capture and sequestration are shown in Table S8.

Table S8: Summary of results for F-T jet fuel from coal pathway (without carbon capture)

	Low	Baseline	High
Life Cycle CO₂ Emissions by Stage			
Recovery of feedstock (gCO ₂ /MJ)	0.8	0.8	0.8
Transportation of feedstock (gCO ₂ /MJ)	0.1	0.1	0.0
Processing of feedstock to fuel (gCO ₂ /MJ)	100.5	117.2	122.4
Transportation of jet fuel (gCO ₂ /MJ)	0.6	0.6	0.6
Combustion CO ₂ (gCO ₂ /MJ)	70.4	70.4	70.4
WTT GHG Emissions by Species			
WTT CO ₂ emissions (gCO ₂ /MJ)	102.1	118.8	123.9
WTT CH ₄ emissions (gCO ₂ e/MJ)	1.5	5.7	13.7
WTT N ₂ O emissions (gCO ₂ e/MJ)	0.0	0.0	0.0
Total WTW GHG Emissions (gCO₂e/MJ)	174.0	194.9	208.0
Life Cycle GHG Emissions Relative to Baseline Conventional Jet Fuel	1.99	2.23	2.38

3.2 Fischer-Tropsch Fuel from Switchgrass

A self-sufficient Biomass to Liquids (BTL) plant was assumed for the GHG analysis presented here. This assumes that biomass feedstock is used to meet internal process energy needs, with little or no excess electricity produced for export. Similar to the CTL plant analyzed above, the BTL plant was assumed to produce commercial quality liquid fuels like diesel and jet fuel, and the energy allocation method was adopted for assigning energy and emissions between liquid fuel products.

The biomass feedstock examined is switchgrass grown on land assumed to not incur adverse direct or indirect land use change emissions (e.g. idle or abandoned cropland). Switchgrass was considered because of its better yield and improved scalability relative to residues or waste products.

Switchgrass is a perennial warm season grass native to North America, found in remnant prairies, native grass pastures, and naturalized along roadsides. Other forms of herbaceous biomass include mixed prairie grasses, wheat, hay and leaves, among others. As a replacement for annual crops, warm season grasses have also been shown to provide important habitat for wildlife, including game birds and other species threatened by the loss of tall grass prairie habitat (McLaughlin et al., 2002). The assumptions regarding the yield, energy and emissions associated with switchgrass cultivation were based on a survey of existing cultivation data from the literature.

¹¹ From EIA (2008b) about 49% of total bituminous and sub-bituminous coal production in 2007 is made up of surface-mined sub-bituminous coal, 18% is made up of surface-mined bituminous coal, and the remaining 33% is made up of underground-mined bituminous coal. Coal methane emissions, lower heating value and carbon content of the average coal mix used in the baseline case are based on weighted average values.

3.2.1 Switchgrass Yield And Cultivation Trends

The approach used is similar to that taken by the National Academies in their 2009 report on Liquid Fuels from Coal and Biomass. Figure S4 shows a distribution of annual switchgrass yields taken from Gunderson et al. (2008) that were used to establish predictive maps of potential yields across the continental United States. The data set comprises approximately 1400 observations with a mean of approximately 4.9 tons/acre/yr. For each data point, the specific cultivar, crop management information, ecotype, precipitation and temperature in the long-term climate record were documented. Using their model, Gunderson et al. (2008) predicted yields in excess of 8.9 tons/acre/yr for lowland ecotypes¹² in the Appalachian region and 5.4-6.2 tons/acre/yr in the Nebraska/South Dakota region. Similarly, yields for upland ecotypes in the Appalachian region were predicted to be greater than 6.2 tons/acre/yr and 3.1-4.5 tons/acre/yr in the Nebraska/South Dakota region. Gunderson et al. (2008) openly discuss that their model predicts the theoretical maximum yield for a given set of input conditions; hence, experimental yields for these regions will most likely be lower in practice.

Other studies have focused on establishing estimates for a national average yield. Heaton et al. (2004) found an average switchgrass yield of 4.6 tons/acre/yr (+/- 0.3 tons/acre/yr) and McLaughlin et al. (2002) projected a national average annual yield of 4.2 tons/acre/yr. Vadas et al. (2008) adopted a nominal yield of 4.0 tons/acre/yr and an optimistic yield of 5.8 tons/acre/yr based on data from large field plots in southern Wisconsin while Adler et al. (2007) simulated switchgrass production in Pennsylvania as 4.3 tons/acre/yr using DAYCENT.¹³ Finally, the GREET herbaceous biomass production pathway assumes a yield of 6.0 tons/acre/yr.

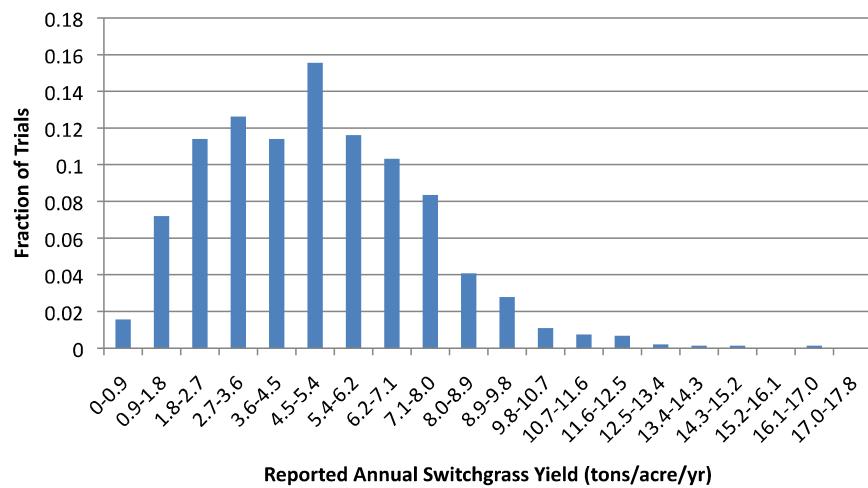


Figure S4: Distribution of reported switchgrass yields across the United States (data from Gunderson et al., 2008)

While numerous studies have estimated the potential yield of switchgrass, many of these results are based on small plots (less than 5m²) and the results are not necessarily indicative of what can be expected of farm-scale production (National Academies, 2009). Schmer et al. (2008) managed switchgrass as a biomass energy crop in field trials of 7.4 to 22.2 acres on marginal cropland from 10 farms across a wide precipitation and temperature gradient in the mid-continent US. The actual farm-scale production resulted in harvested yields about 35% to 50% lower than those of small-scale plots. It is possible that the lower yields from large-scale production can be attributed to farmers' inexperience with the cropping system or differences in cropland quality; however, farmers worked closely with the researchers in collecting this data and the land had been in active crop production before being converted to switchgrass production (National Academies, 2009). Actual yield data from Schmer et al. (2008) ranged from 2.3 to 5.0 tons/acre/yr with a mean of 3.2 tons/acre/yr.

¹² Lowland and upland ecotypes are defined by position relative to the level where water flows or where flooding occurs

¹³ DAYCENT is the daily time-step version of the CENTURY biogeochemical model. From weather (daily maximum and minimum air temperature, precipitation), soil-texture class, and land-use inputs, DAYCENT simulates fluxes of carbon (C) and nitrogen (N) between the atmosphere, vegetation, and soil while predicting crop production, soil organic-matter changes, and trace-gas fluxes.

In their analysis, Gunderson et al. (2008) concluded that switchgrass yield is most influenced by ecotype (upland or lowland) and the relationship of precipitation and temperature. Lower yields were attributed to factors that were not quantified across the data set, such as soil pH, inherent soil fertility, total solar radiation (vs. long periods of cloud cover) and others that are artifacts of each individual growing site and cannot be aggregated for a generalized result. The specific rate of nitrogen application was found not to have a significant influence on yield. Very high levels of fertilization certainly did not guarantee increased biomass production, and in many cases, the zero fertilizer plantings did as well as any fertilized stands. Based on these conclusions, the yields adopted for the low emissions, baseline and high emissions scenarios (as shown in Table S9) were assumed to be independent input parameters from other cultivation inputs (on a per ton basis).

Table S9: Switchgrass yields assumed in the low, baseline and high emissions scenarios

	Low¹	Baseline²	High³
Yield (tons/acre/yr)	5.8	4.6	3.2
Notes:			
1. Optimistic yield from Vadas et al. (2008) based on large field plots in southern Wisconsin			
2. Projected national average from McLaughlin et al. (2002)			
3. Average farm-scale yield from Schmer et al. (2008) based on mid-continental US			

3.2.2 Cultivation and Transportation of Switchgrass

The key inputs for switchgrass production are the process fuels and electricity used in farming, fertilizer inputs and herbicide usage. These parameters have been identified in several studies but are the subject of much uncertainty. Although it was determined that these inputs do not have a substantial impact on yield, they are essential for estimating the GHG emissions associated with switchgrass production. A summary of the available data is given in Table S10.

These data show considerable variation in the application rates of non-nitrogen fertilizers and herbicides. The phosphorous and potassium application rates quoted by Vadas et al. (2008) are an order of magnitude larger than those given by Adler, which are in turn an order of magnitude larger than the GREET default values.

Using the same arguments, which were previously made in considering yield as an independent parameter, the process fuel usage, nitrogen fertilizer application and other fertilizer and herbicide application were decoupled from their respective data sets. Hence, they were also considered as independent parameters for the purposes of the scenario analysis. The input parameters used for the low emissions, baseline and high emissions scenario are outlined in Table S11. The GREET default parameters were not used at all in this work because they are a decade older than the other results and they are not consistent with the 2015 timeframe of this study.

Default GREET transportation and distribution assumptions were adopted for switchgrass. Specifically that bailed switchgrass is transported 40 miles by truck from the field to an F-T processing facility in loads of 24 tons.

Table S10: Reported cultivation inputs for switchgrass

	Adler et al. (2007) ¹	Vadas et al. (2008) ²	Schmer et al. (2008) ³	GREET (2008) ⁴
Process Fuels (Btu/ton)				
Diesel	82874	113046	107533	201589
Gasoline	0	22609	0	0
Electricity	0	7536	0	15641
Crop Management (g/ton)				
Nitrogen	5218	11348	7701	10635
P ₂ O ₅	1236	10387	0	142
K ₂ O	2488	24607	0	226
Limestone	9491	0	0	0
Herbicides	6.4	0	185	28

Notes:

1. Actual fertilizer application rates were only given for nitrogen. All others were given in terms of CO₂e with application rates calculated using production emissions from GREET 1.8b.
2. Actual phosphorous and potassium usage was given in terms of elemental weight and converted to P₂O₅ and K₂O using molar mass fractions. Lube oil consumed is expressed in terms of diesel equivalent on an energy basis.
3. Data is the average of 10 field scale plots in Nebraska, North Dakota and South Dakota.
4. From Oak Ridge National Laboratory in 1998.

Table S11: Cultivation inputs for switchgrass in the low, baseline and high emissions scenarios

	Low	Baseline	High
Process Fuels (Btu/ton)			
Diesel	82874	107533	113046
Gasoline	0	0	22609
Electricity	0	0	7536
Nitrogen Fertilizer (g/ton)	5218	7701	11348
Other Fertilizers (g/ton)			
P ₂ O ₅	0	1236	10387
K ₂ O	0	2488	24607
Limestone	0	9491	0
Herbicides	185	6.4	0

3.2.3 Nitrous Oxide Emissions

Nitrous oxide emissions can either be estimated using specialty software or through simple IPCC emissions factors. Estimates from Adler et al. (2007) using DAYCENT included both direct emissions of N₂O through nitrification and denitrification processes in the soil and indirect emissions of N₂O through soil nitrogen losses in forms other than N₂O, (e.g., NO_x, NH₃, NO₃), which were subsequently converted to N₂O elsewhere. Conversely, the GREET method employs the IPCC 2006 conversion factor for direct and indirect N₂O emissions from switchgrass production, as shown in using Equation 4.

$$\text{N}_2\text{O Emissions} \left(\frac{\text{g}_{\text{N}_2\text{O}}}{\text{ton}} \right) = \left(\frac{\text{g}_{\text{nitrogen fertilizer}}}{\text{ton}} \right) \cdot 0.01325 \cdot \left(\frac{44\text{g}_{\text{N}_2\text{O}}}{28\text{g}_\text{N}} \right) \quad \text{Equation 4}$$

The N₂O emissions from Adler et al. (2007) were found to be 43% higher than those predicted by Equation 4 from the same application rate. The principle reason for this discrepancy is that annual nitrogen in crop residues (above-ground and below-ground) was not included. Estimates of the nitrogen deposited on the soil in the form of crop residues was obtained using the IPCC Tier 1 methodology for perennial grasses (De Klein et al., 2006) and implemented through Equation 5.

$$N_2O \text{ Emissions} \left(\frac{g_{N_2O}}{\text{ton}} \right) = \left(\left(\frac{g_{\text{nitrogen fertilizer}}}{\text{ton}} + 6025 \right) \cdot 0.01_{\text{direct}} + \left(\frac{g_{\text{nitrogen fertilizer}}}{\text{ton}} \right) \cdot 0.001_{\text{indirect}} \right) \cdot \left(\frac{44g_{N_2O}}{28g_N} \right) \quad \text{Equation 5}$$

where 6025 is the nitrogen in crop residues, 0.01_{direct} is the emissions factor for N_2O from nitrogen and 0.001_{indirect} is the emissions factor for volatilized NH_3 and NO_x from synthetic nitrogen converted to N_2O . The N_2O emissions as calculated using the new IPCC methodology are within 2% of those estimated by Adler et al. (2007) for the same nitrogen application rate. As such, Equation 5 was used for all N_2O calculations within the switchgrass production pathway.

For the low emissions case, a process efficiency of 52% was assumed, based on the analysis by Kreutz et al. (2008) of a 4400 bpd BTL plant. The baseline case assumes a process efficiency of 45% from the Choren process based on the “self-sufficient basis scenario” where all required process energy is provided by biomass feedstock (Baitz et al., 2004). Choren currently operates the only commercial-scale BTL plant in the world, producing 300 bpd of F-T liquids. This is further confirmed by estimates of roughly a 5% efficiency drop for BTL plants compared to CTL plants due to additional processing energy for biomass grinding and drying.¹⁴ The high emissions case directly applies a 5% drop in process efficiency compared to 47% assumed in the CTL case, resulting in a process efficiency of 42%.

The input assumptions and life cycle GHG emissions for the production and use of F-T jet fuel from switchgrass are shown in Table S12. The ‘biomass credit’ represents the CO_2 that is absorbed from the atmosphere during biomass growth. Note that the CO_2 emitted during the combustion of process fuels and the F-T fuel is approximately equal to the CO_2 absorbed from the atmosphere during growth of the biomass feedstock.

Table S12: Summary of results for F-T jet fuel from switchgrass with no soil carbon sequestration

	Low	Baseline	High
Key Assumptions			
Feedstock	Switchgrass	Switchgrass	Switchgrass
Process Efficiency (LHV)	0.52	0.45	0.42
Life Cycle CO_2 Emissions by Stage			
Biomass Credit (gCO_2/MJ)	-192.7	-222.7	-238.6
Recovery of feedstock (gCO_2/MJ)	3.8	6.4	11.4
Transportation of feedstock (gCO_2/MJ)	0.6	0.6	0.6
Processing of feedstock to fuel (gCO_2/MJ)	122.1	152.1	168.0
Transportation of jet fuel (gCO_2/MJ)	0.5	0.5	0.5
Combustion CO_2 (gCO_2/MJ)	70.4	70.4	70.4
WTT GHG Emissions by Species			
WTT CO_2 emissions (gCO_2/MJ)	-65.8	-63.1	-58.2
WTT CH_4 emissions (gCO_2e/MJ)	0.1	0.2	0.5
WTT N_2O emissions (gCO_2e/MJ)	7.2	10.3	13.3
Total WTW GHG Emissions (gCO_2e/MJ)	11.9	17.7	26.0
Life Cycle GHG Emissions Relative to Baseline Conventional Jet Fuel	0.14	0.20	0.30

The life cycle GHG emissions of the BTL pathway using switchgrass as a feedstock are 0.14 times to 0.3 times those of conventional jet fuel with no soil carbon sequestration. When the soil carbon sequestration credit is included, the emissions from the pathway range from -0.02 to -0.05 times those of conventional jet fuel. The larger value for land use change emissions in the high scenario occurs due to the lower assumed yield per acre.

Nitrous oxide emissions represent more than 50% of the total life cycle GHG emissions from the switchgrass to F-T jet pathway. As a result, life cycle GHG emissions for this pathway are strongly

¹⁴ Thomas Tarka, interview with David Ortiz, October 3, 2008.

influenced by any uncertainty associated with the IPCC correlations that were used in the nitrous oxide estimates.

4 Hydroprocessed Renewable Jet Fuel from Rapeseed

Renewable oils can be processed into a fuel that has properties similar to those of F-T fuels. The processing involves hydrotreatment to deoxygenate the oil with subsequent hydrocracking to create hydrocarbons that fill the distillation range of jet fuel (Hileman et al., 2009). This section deals only the production and use of Hydroprocessed Renewable Jet fuel (HRJ) from rapeseed oil.

4.1 HRJ from Rapeseed Oil

The production of HRJ from rapeseed oil was analyzed with the GREET framework using cultivation and processing data from the literature.¹⁵ Rapeseed has been grown for the production of animal feed and vegetable oils for both human consumption and biofuel production. The leading producers of rapeseed are currently China, Canada, India and the European Union (FAO, 2010). The use of rapeseed oil as a feedstock for biofuels is of particular interest in Europe, where Rapeseed Methyl Ester is one of the two main biofuels under consideration (CONCAWE, 2002). This analysis assumes that rapeseed oil is produced in Europe and subsequently imported to the United States to be hydroprocessed into HRJ. The key parameters used to form the low, baseline and high emissions scenario were the rapeseed yield, oil content, farming energy, fertilizer application, transportation distance and oilseed drying energy requirements. In addition to a scenario where land use change emissions were assumed zero, a scenario where rapeseed is grown on set-aside land¹⁶ was examined; the aforementioned key parameters were varied within each land use change scenario.

4.1.1 Cultivation of Rapeseed

Rapeseed cultivation was assumed to take place predominantly in the United Kingdom (UK) and France based on data from Mortimer and Elsayed (2006), Edwards et al. (2007), Richards (2000) and Prieur et al. (2008). The analysis was supplemented by additional data from Sweden and Denmark from Bernesson et al. (2004) and Schmidt (2007). This was deemed appropriate due to the relative similarity in climate among southern Sweden, Denmark, France and the UK.

Rapeseed yield was estimated using data for the UK and France from 1999 through 2009. The baseline scenario adopted a projected rapeseed yield in 2015 of 3.35 Mg/ha (Eurostat, 2010) using linear regression on the historical data. The low and high emissions scenarios were developed using the same method employed to estimate soybean and palm yields. Specifically, based on historical rapeseed yield data from 1999 through 2009 (Eurostat, 2010), the variation between the lowest yield and the line of best fit was -16.8% (UK in 2001) while that between the highest yield and the line of best fit was +15.7% (France in 2009). Based on these historical data, it was assumed that yield fluctuations in some future year could be 16.8% lower than in the baseline case, corresponding to the high emissions case of 2.79 Mg/ha. Similarly, a yield in some future ideal growing year could be 15.7% higher than in the baseline case, corresponding to the low emissions case of 3.89 Mg/acre.

Yearly data from both France and the UK is shown in Figure S5. The weighted average corresponds to the ratio of total harvested weight to total planted area from both countries. Although there is substantial fluctuation in yield from year to year, the underlying trend is increasing over time at a rate of 23.7 kg/ha/year.

¹⁵ Rapeseed oil is not a preexisting pathway within GREET. As such, a new pathway was built within the GREET framework using the soy oil to renewable diesel pathway as a guide.

¹⁶ From 1988 through 2009, the EU government compensated farmers to remove 10%-15% of their land from production to deliver some environmental benefits following considerable damage to agricultural ecosystems and wildlife as a result of the intensification of agriculture. The program has since changed such that the set aside system is on a voluntary basis with no compensation. Land that was set aside by farmers could be available for increased rapeseed cultivation (Gray, 2009).

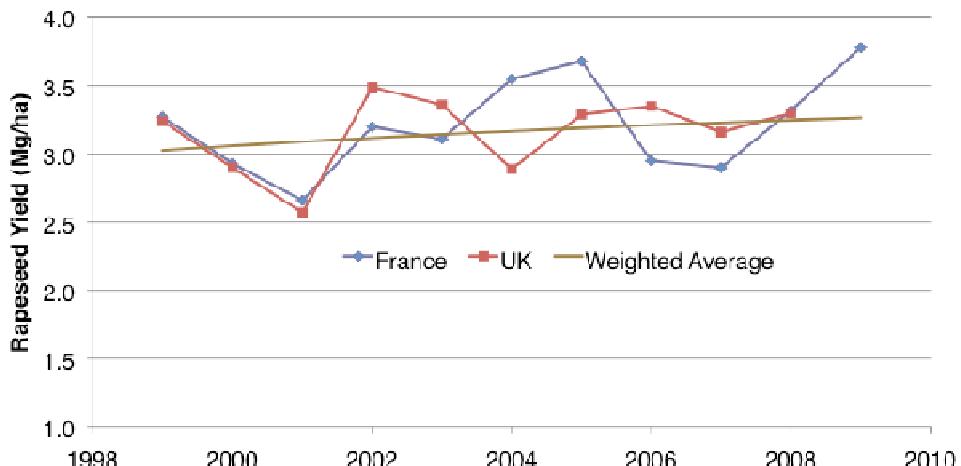


Figure S5: Yearly rapeseed yield for France and the UK between 1999 and 2009

The oil fraction of rapeseed ranges from 40% to 45% by mass based on the sources used to model cultivation. The oil yield per kilogram of rapeseed is higher than any other renewable oil feedstock considered in this work. In this analysis, oil fractions of 45% (Prieur et al., 2008; Bernesson et al., 2004), 44% (Schmidt, 2007) and 41% (Richards, 2000; Mortimer and Elsayed, 2006) were assumed in the low, baseline and high emissions scenarios.

Inputs to rapeseed cultivation are fuels for farming operations, nitrogen fertilizers, phosphate, potash and herbicides. The energy consumption of seed crop growth and processing of seeds is less than 1% of all energy used in cultivation and harvesting and was considered negligible for the purposes of this analysis (Richards, 2000). The usage per hectare of each of these resources in the low, baseline and high emissions scenario is given in Table S13. Nitrogen fertilizer application was assumed to occur in the form of 50% ammonia and nitrogen solutions and 50% ammonium nitrate and ammonium sulfate. Default GREET assumptions for soybeans were adopted regarding the types of herbicides applied during rapeseed cultivation. The largest variation was found in the use of diesel fuel on the farm. The low emissions scenario was based on data from Mortimer and Elsayed (2006) whose estimate for North East England was by far the most optimistic. The baseline scenario was based on French data from Prieur et al. (2008), although Bernesson (2004) gave a similar estimate in his analysis of rapeseed production in Sweden. The high emissions scenario employs data from Richards (2000) for arable lands in England, which is confirmed by Schmidt (2007) with his farming energy estimates of rapeseed production in Denmark.

The corresponding production inputs per Mg of rapeseed for each scenario were calculated by combining the production inputs and yields per hectare. The production of rapeseed oil results in straw biomass production. The average ratio of oilseed production to straw is approximately 0.96:1.¹⁷ This analysis assumed that the straw was ploughed back into the fields after harvest. This leads to minimized depletion of soil nutrients and fertilizer savings, which were accounted for in the cultivation inputs (Prieur et al., 2008). Where there is a nearby heat or power generation facility that is outfitted to accommodate biomass feedstocks, the straw represents a potential energy source (Richards, 2000); however, straw from rapeseed is rarely harvested because of burning problems with the newer varieties and lower yields than grasses or wheat. Lower yield makes rapeseed straw more expensive to harvest so it is simply tilled back into the soil by most farmers (Bernesson et al., 2004).

¹⁷ The straw and oilseed production from Richards (2000) were 4 Mg/ha and 4.08 Mg/ha, respectively (ratio of 0.98:1). The straw and oilseed production from Schmidt (2007) were 2.93 Mg/ha and 3.13 Mg/ha, respectively (ratio of 0.94:1).

Table S13: Farming energy, fertilizer and herbicide usage for the production of rapeseed in the low emissions, baseline and high emissions scenarios

	Low	Baseline	High
Rapeseed Yield (Mg/ha)	2.79	3.35	3.89
Rapeseed Oil Fraction (mass)	45%	44%	41%
Fuel Usage			
Diesel (MJ/ha) ¹	1857	2310	3934
Fertilizer Usage			
Nitrogen(kg-N/ha) ²	140	164	180
Phosphate (kg-P ₂ O ₅ /ha) ³	34	47	56
Potash (kg-K ₂ O/ha) ⁴	35	43	82
Herbicides⁵	1.8	2.3	2.8

Notes:

1. Mortimer and Elsayed (2006) – Low Case; Prieur et al. (2008) – Baseline Case; Richards (2000) – High Case
2. Bernesson et al. (2004) and Schmidt (2007) – Low Case; Prieur et al. (2008) – Baseline Case; Edwards et al. (2007) – High Case
3. Bernesson et al. (2004) – Low Case; Prieur et al. (2008) – Baseline Case; Mortimer and Elsayed (2006) and Schmidt (2007) – High Case
4. Prieur et al. (2008) – Low Case; Richards (2000) and Bernesson et al. (2004) – Baseline Case; Mortimer and Elsayed (2006) and Schmidt (2007) – High Case
5. Richards (2000) – Low Case; Prieur et al. (2008) – Baseline Case; Mortimer and Elsayed (2006) – High Case

Emissions from N₂O were estimated using IPCC Tier 1 methodology (De Klein et al., 2006). Nitrogen in above and below ground crop residues was estimated by applying the aforementioned crop residue production ratio to estimate the amount of straw tilled back into the soil. Rapeseed straw has been characterized as 0.75% nitrogen by mass (Karaosmanoglu et al., 1999) leading to 7125 g of nitrogen reapplied to the field in the form of straw biomass per megagram of oilseed production. The IPCC Tier 1 methodology estimates the combined direct and indirect conversion rate for nitrogen from synthetic fertilizers as 1.325% and nitrogen from crop residues as 1.225%. These rates include the atmospheric deposition of nitrogen volatilized from managed soils as well as nitrogen from leaching and runoff. The formula for calculating N₂O emissions from rapeseed cultivation is given by:

$$\text{N}_2\text{O Emissions} \left(\frac{\text{g}_{\text{N}_2\text{O}}}{\text{Mg}} \right) = \left(\left(\frac{\text{g}_{\text{nitrogen fertilizer}}}{\text{Mg}} \right) \cdot 0.01325 + \left(7125 \frac{\text{g}_{\text{N-crop residue}}}{\text{Mg}} \right) \cdot 0.01225 \right) \cdot \left(\frac{44\text{g}_{\text{N}_2\text{O}}}{28\text{g}_\text{N}} \right) \quad \text{Equation 6}$$

The least defined aspects of rapeseed production are the drying and storage practices. In practice, there is little consensus on the oilseed moisture content at harvest, which has implications for energy consumption during drying. A recent survey of current harvesting, drying and storage practices of oilseed rape in the UK found that most farmers harvest above 12% moisture content, which is the threshold for Ochratoxin B production (Armitage et al., 2005).¹⁸ After harvest the rapeseed must be dried to a moisture content of 9% for storage (Prieur et al., 2008; Richards, 2000; Schmidt, 2007). Most rapeseed is stored for about 3 months before being sold. This tendency is driven mainly by market strategy and cash flow. Longer storage periods may require lower moisture contents to minimize mite infestation and deterioration through rancidity. Mites are the greatest problem faced by rapeseed farmers and were observed on more than 25% of sites. From the perspective of seed crushers, moisture content (high or low) and admixture of stores were the most common reason for rejection or price reductions (Armitage et al., 2005). This analysis assumed moisture contents of 13%, 14% and 15% at harvest and 9% after drying in the low emissions, baseline and high emissions scenario, respectively. Losses due to mites, rancidity and admixture were neglected due to

¹⁸ Ochratoxin B is the most abundant food contaminating mycotoxin in the world. Human exposure occurs primarily through consumption of improperly stored food products (Armitage et al., 2005)

lack of quantitative data but these could become important for ill-maintained rapeseed stored over long periods of time.

Table S14: Rapeseed drying and storage assumptions in the low emissions, baseline and high emissions scenario

	Low	Baseline	High
Moisture Content			
Harvest ¹	13%	14%	15%
Storage ²	9%	9%	9%
Drying Energy Consumption³			
Diesel (MJ/L _{evaporated})	n/a	4.7652	6
Grid Electricity (MJ/L _{evaporated})	n/a	0	3.6
Diesel (MJ/Mg)	165.0	277.0	423.5
Grid Electricity (MJ/Mg)	0.0	0.0	254.1
Notes:			
1. Mortimer and Elsayed (2006) – Low Case; Average of low and high cases – Baseline case; Bernesson et al. (2004) – High Case			
2. Prieur et al. (2008), Richards (2000), Mortimer and Elsayed (2006), Schmidt (2007)			
3. Mortimer and Elsayed (2006) – Low Case; Bernesson et al. (2004) – Baseline case; Schmidt (2007) – High Case			

Approximately one third of farmers surveyed in the UK use ambient air drying to reduce the moisture content of their seed from the value at harvest to that required for storage. Drying using ambient air can take from 2 to 4 weeks, although 2 weeks is the most common. The other two thirds of farmers use hot air dryers to reduce drying times at the expense of increased energy consumption (Armitage et al., 2005). This work assumed the use of hot air drying according to energy consumption estimates from Mortimer and Elsayed (2006), Bernesson et al. (2004) and Schmidt (2007) in the low, baseline and high emissions scenarios, respectively. The assumptions regarding the drying and storage of rapeseed used in this work are summarized in Table S14.

4.1.2 Extraction of Oil from Rapeseed

A modified version of the process for oil extraction from soybeans established by Sheehan et al. (1998a), including only the processes relevant to rapeseed in an N-hexane extraction facility, was used to model the process inputs to extracting oil from rapeseed. Ozata et al. (2009) also used this approach in their analysis of biodiesel from rapeseed. The changes to the data from Sheehan et al. (1998a) were limited to removing the energy demands for drying as this has been explicitly quantified for rapeseed in Table S14. The process energies were converted from energy per unit mass of oilseed to energy per unit mass of oil using the oil fractions from the low emissions, baseline and high emissions scenarios. The outputs and energy consumption assumed in the extraction of oil from rapeseed are shown in Table S15.

Table S15: Process inputs for extracting oil from rapeseeds

	Low ¹	Baseline ¹	High ¹
Receiving and Storage			
Electricity	18.60	19.02	20.41
Rapeseed Preparation			
Electricity	68.76	70.32	75.46
Steam	153.35	156.83	168.31
Oil Extraction			
Electricity	11.46	11.73	12.58
N-hexane	94.15	96.29	103.34
Meal Processing			
Electricity	63.56	65.01	69.77
Steam	492.54	503.74	540.59
Oil Recovery			
Electricity	1.21	1.24	1.33
Steam	77.04	78.79	84.55
Solvent Recovery			
Electricity	1.66	1.69	1.82
Steam	0.00	0.00	0.00
Oil Degumming			
Electricity	5.38	5.50	5.91
Steam	60.53	61.91	66.44
Waste Treatment			
Electricity	1.82	1.86	1.99
Steam	32.56	33.30	35.74
Totals			
Electricity	172.45	176.37	189.27
Natural Gas ²	1020.03	1043.21	1119.54
N-hexane ³	94.15	96.29	103.34
Notes:			
1.	All values are in Btu per pound of oil		
2.	Steam is generated from natural gas with an efficiency of 80%.		
3.	GREET uses Liquefied Petroleum Gas (LPG) as a surrogate for N-hexane when calculating emissions		

4.1.3 Co-Product Usage and Allocation Methodology

In the extraction of oil from rapeseed, rapeseed meal is produced in large quantities as a co-product (1.22-1.44 kg of meal per kg of oil). Rapeseed meal is primarily used as an animal feed and could potentially displace barley, corn, and soybean meal. One kg of rapeseed meal is equivalent to 0.87 kg of soybean meal on a protein basis (Prieur et al., 2008).

The displacement method was determined to be inappropriate because of the large variation in life cycle GHG emissions that will result from the choice of displaced feedstock, (i.e., barley, corn, and soybean meal). The mass or energy allocation method may not be most appropriate as rapeseed meal is not valued based on its mass, or sold as a commercial energy product. The commercial value of the protein in rapeseed meal for animal feed resulted in market value allocation being adopted in this work. This is internally consistent with other pathways examined by Stratton et al (2010) as well as with Prieur et al. (2008), Mortimer and Elsayed (2006) and Ozata et al. (2009).

4.1.4 Transportation of Rapeseed Oil to HRJ Production Facilities

Rapeseed cultivation, harvesting and oil extraction were assumed to occur primarily in France and the UK. The one-way distance from the farm to the oil extraction facility was assumed to be 115 km (Prieur et al.,

2008).¹⁹ It was then assumed that the United States imports this oil to a domestic hydroprocessing facility where it is converted to jet fuel. This transportation profile is not available in GREET and was created using the data from Table S16. Default GREET assumptions were used for the details of each transportation mode.

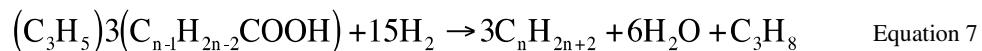
Table S16: Transportation profile of Rapeseed Oil from Europe to the United States

Transportation of Rapeseed Oil to European Shipping Ports¹	
Mode (%)	
Truck	100
Distance (kilometers)	150
Transportation of Rapeseed Oil from European Ports to US ports²	
Mode (%)	
Ocean tanker	100
Distance (kilometers)	
Western UK to Eastern US (50%)	5520
Western France to Eastern US (25%)	5780
Southern France to Western US (25%)	7170
Average	6000
Transportation of Rapeseed Oil from US ports to HRJ production facilities¹	
Mode (%)	
Truck	50
Rail	50
Distance (miles)	
By truck	160
By rail	800
Notes:	
1. Author's own estimates	
2. Shipping distances from http://www.searates.com/reference/portdistance/	

4.1.5 Energy Requirements for HRJ from Renewable Oils

The hydrotreatment process for the production of HRJ from renewable oils was based on the UOP hydrodeoxygenation process, which primarily produces “green diesel” (Marker et al., 2005; Huo et al., 2008). Other techniques are available to produce hydrocarbon fuels from renewable oils beyond the approach developed by UOP; however, the UOP process is currently the most established for jet fuel production. Similar to F-T fuels, additional hydroprocessing is needed for the production of jet fuel instead of diesel, resulting in increased hydrogen and power requirements. The assumption that additional processing requirements for F-T jet fuel relative to diesel are negligible is justified in the literature (Gray et al., 2007); however, in the case of HRJ, using diesel as a surrogate for jet is only appropriate for crude estimates.

The UOP process used for the creation of Hydroprocessed Renewable Diesel (HRD) is described by the following chemical reaction:



where n is the carbon chain length of the fatty acids within the triglyceride molecules used as a feedstock for the process. Triglycerides are formed from a single molecule of glycerol acting as a backbone to three fatty acids. This simplified analysis assumed that rapeseed oil contains only fatty acids with a carbon chain length of 18. The error introduced by this assumption is likely small compared to the uncertainty in quantifying cultivation inputs for each feedstock; however, not all oils are chemically equal and this analysis does not reflect the physical properties of any single oil type.

¹⁹ Richards (2000) and Mortimer and Elsayed (2006) estimated one-way transport distances of 90 km and 130 km, respectively.

Table S17 presents the actual distributions of fatty acid carbon chain lengths for rapeseed oils.²⁰ An example of a shortcoming of the assumption used in this analysis is the treatment of oils containing unsaturated carbon chains. The presence of double bonds within a carbon chain would lead to additional hydrogen consumption during the deoxygenation process in order to saturate the molecule, however, such effects are ignored herein.

Table S17: Component fatty acid profiles for renewable oils considered in this work

Fatty Acid Components (weight %)	Caprylic (8:0)	Capric (10:0)	Lauric (12:0)	Myristic (14:0)	Palmitic (16:0)	Palmitoleic (16:1)	Stearic (18:0)	Oleic (18:1)	Linoleic (18:2)	Linolenic (18:3)	Arachidic (20:0)	Gadoleic (20:1)	Behenic (22:0)	Eruic (22:1)
Rapeseed (B. campestris)	—	—	—	—	4	—	2	33	18	9	—	12	—	22
Rapeseed (B. napus)	—	—	—	—	3	—	1	17	14	9	—	11	—	45
Notes:														
1. Information from: DeMan et al. (1999)														

Equation 7 can be re-written in a mass balance form for easier comparison to experimental data.



The feedstock, key products and process energy needed per pound of HRD are summarized in Table S18.

Table S18: Experimental and theoretical requirements for the creation of renewable diesel

Feedstock (lb)	Experimental			Theoretical
	Low	Baseline	High	
Oil	100	100	100	100
H ₂ (51586 Btu/lb)	1.5	2.72	3.8	3.4
Key Products (lb)				
HRD (18908 Btu/lb)	83.0	84.19	86	86.2
Propane Mix Gas (18568 Btu/lb)	2.0	4.75	5	5.0
Process Energy (Btu)				
Electricity	5785	6942	8099	--
Natural Gas	8950	8950	8950	--

Notes:

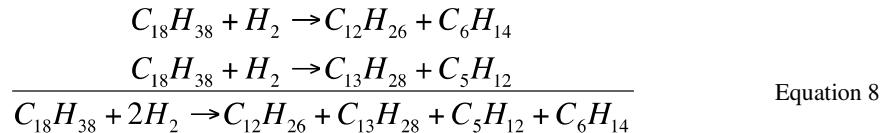
1. Steam is assumed to be produced from natural gas at 80% efficiency
2. Energy contents are taken from GREET (2008)
3. Experimental data taken from Appendix 2 of Huo et al. (2008) with modifications per recommendations from UOP (Kalnes, 2009)

Further refinement of HRD is required for the creation of HRJ. The strategy to estimate the process requirements of HRJ was to use the experimental data for the creation of HRD and subsequently estimate the additional requirements to convert the HRD into HRJ. For this analysis, HRD and HRJ are assumed to be symmetrical distributions of straight chains hydrocarbons centered on C₁₂ and C₁₈ respectively. The mechanism by which hydrocarbon chains crack is through smaller molecules, (e.g., pentane (C₅H₁₂) and hexane (C₆H₁₄)) breaking off the end. The dominant effect that takes place is the reduction of C₁₈ to C₁₃ by cracking pentane and C₁₂ by cracking hexane (Kalnes, 2009). Other reactions are also occurring where molecules from the distribution about C₁₈ crack to those from the distribution about C₁₂. To account fully for this effect would entail including the statistical nature by which chemical reactions are more likely to

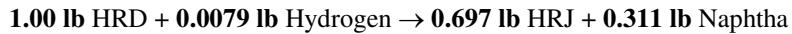
²⁰ The notation for denoting carbon chain length and number of double bonds is (chain length):(number of double bonds). For example, a chain length of 18 with 2 double bonds is expressed as 18:2.

take place. In keeping with the level of detail required of this analysis, the aforementioned effects were assumed to cancel out if the two distributions have the same shape about their mean.

Making use of these arguments simplifies the analysis to two chemical reactions converting diesel fuel to jet fuel:



Written in mass balance form and normalized for one lb of HRD, the overall equation governing the formation of HRJ from renewable oil can be expressed as:



Although variations in carbon chain length are not captured in this analysis, fatty acids with carbon chain length distributions around 12 are better suited for use as feedstock for jet fuel because higher blending percentages can be used without the need for hydrocracking. Furthermore, carbon chain lengths closer to 12 would result in a higher yield of jet fuel per unit mass of oil input.

Naphtha in this case is a combination of 46% C₅H₁₂ and 54% C₆H₁₄ by mass. Using these ratios of HRD to HRJ, the process energies from Table S18 were modified to reflect the energy requirements to create HRJ as shown in Table S19. Based on discussions with experts at UOP (Kalnes, 2009), it is assumed that total process energies (natural gas and electricity) will increase by 10% to 30% per pound of renewable feedstock when including the hydrocracking required for the formation of HRJ. The total hydrogen consumption is the sum of that needed to first make HRD and then to crack it to HRJ. In all cases where renewable oils are processed into finished fuel products, energy and emissions were allocated based on energy content.

Table S19: Energy requirements for the creation of HRJ

Feedstock (lb)	Emissions Scenarios		
	Low	Baseline	High
Oil	100	100	100
H ₂ (51586 Btu/lb)	2.15	3.38	4.48
Key Products (lb)			
HRJ (18950 Btu/lb)	57.8	58.7	59.9
Naphtha (19215 Btu/lb)	25.8	26.2	26.8
Propane Mix Gas (18568 Btu/lb)	2.0	4.8	5.0
Process Energy (Btu)			
Electricity	6364	8330	10529
Natural Gas	9845	10740	11635

The hydropyrolysis step of converting renewable oil into HRD has a mass yield of 84% and results in 8.7 gCO₂/MJ. After making the aforementioned changes, hydropyrolysis renewable oil into HRJ has a mass yield below 60% and results in 10.3 gCO₂/MJ. The emissions associated with hydrogen production in this work are representative of steam reforming of natural gas and are consistent with default GREET assumptions. While these results provide a first approximation of mass and energy inputs, they do not reflect the impact of oil composition on process inputs or differences in real world production scenarios.

4.1.6 Results

The life cycle GHG emissions from the production and use of HRJ fuel from rapeseed oil are given in Table S20. The life cycle GHG emissions range from 0.45 to 0.87 times those of conventional jet fuel; however, nitrous oxide emissions represent between 39% and 44% of the total. Edwards et al. (2007) found

nitrous oxide emissions from rapeseed production to be of similar magnitude using an independent, well-validated soil chemistry model (DNDC, version 82N). The variation in the biomass credit is due to minor changes in the allocation scheme through the pathway. The transportation of oil across the Atlantic is responsible for only 0.6 g CO₂e/MJ; these emissions would not have been incurred had the fuel been processed and used within Europe.

Nitrous oxide emissions represent more than approximately 40% of the total life cycle GHG emissions from the rapeseed to HRJ pathway. As such, the consequences of the uncertainty associated with IPCC correlations are more important for this pathway.

Table S20: Summary of results from renewable jet fuel production and use from rapeseed

	Low	Baseline	High
Key Assumptions			
Total Biomass Yield (Mg/ha/yr)	2.79	3.35	3.89
Seed Oil Fraction	45%	44%	41%
Life Cycle CO₂ Emissions by Stage			
Biomass Credit (gCO ₂ /MJ)	-73.7	-70.5	-68.9
Recovery of feedstock (gCO ₂ /MJ)	13.6	17.2	26.4
Transportation of feedstock (gCO ₂ /MJ)	3.2	3.1	3.1
Processing of feedstock to fuel (gCO ₂ /MJ)	7.1	10.3	13.2
Transportation of jet fuel (gCO ₂ /MJ)	0.6	0.6	0.6
Combustion CO ₂ (gCO ₂ /MJ)	70.4	70.4	70.4
WTT GHG Emissions by Species			
WTT CO ₂ emissions (gCO ₂ /MJ)	-49.2	-39.2	-25.7
WTT CH ₄ emissions (gCO ₂ e/MJ)	1.0	1.3	1.7
WTT N ₂ O emissions (gCO ₂ e/MJ)	17.6	22.4	29.5
Total WTW GHG Emissions (gCO₂e/MJ)	39.8	54.9	75.9
Life Cycle GHG Emissions Relative to Baseline Conventional Jet Fuel	0.45	0.63	0.87

5 Summary of Life Cycle GHG Emissions

Table S21 summarizes the results of the life cycle GHG emissions for the baseline scenario of jet fuel from conventional crude oil, coal and switchgrass via F-T processing without CCS and rapeseed oil via hydroprocessing. The ‘biomass credits’ given to biofuels from the CO₂ absorbed during biomass growth are explicitly broken out in these results; these credits are largely the reason why these fuels offer the potential for reduced GHG emissions. The ‘biomass credit’ for BTL is larger because biomass is used to power the entire fuel production process.

Table S21: Baseline life cycle GHG emissions for all fuel pathways studied.

	Biomass Credit	Recovery	Feedstock Transport	Processing	Fuel Transport	Combustion	WTT N ₂ O	WTT CH ₄	Land Use Change	Total
Crude to conventional jet fuel	0.0	4.2	1.5	5.5	0.8	73.2	0.1	2.3	0.0	87.5
Coal to F-T fuel (no carbon capture)	0.0	0.8	0.1	117.2	0.6	70.4	0.0	5.7	0.0	194.8
Switchgrass to F-T fuel	-222.7	6.4	0.6	152.1	0.5	70.4	10.3	0.2	0.0	17.7
Rapeseed oil to HRJ	-70.5	17.2	3.1	10.3	0.6	70.4	22.4	1.3	0.0	54.9

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