Assessment of Well-to-Wheels Energy Use and Greenhouse Gas Emissions of Fischer-Tropsch Diesel

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Acronyms and Abbreviations

ATR	autothermal reforming
CD	conventional diesel
CH_4	methane
CI	compression ignition
CO	carbon monoxide
CO_2	carbon dioxide
DOE	Department of Energy
EPA	Environmental Protection Agency
EPACT	Energy Policy Act
FG	flared gas
FT	Fischer-Tropsch
FTD	Fischer-Tropsch diesel
GHG	greenhouse gas
GREET	Greenhouse gases, Regulated Emissions, and Energy use in Transportation
GWP	global warming potential
H_2	hydrogen
LHV	lower heating value
ULS	ultra-low sulfur
ULSD	ultra-low-sulfur diesel
MTBE	methyl tertiary butyl ether
N_2O	nitrous oxide
NG	natural gas
NNA	non-North American
NO_x	nitrogen oxides
OTT	Office of Transportation Technologies
P10	probability of 10%
P20	probability of 20%
P50	probability of 50%
P80	probability of 80%
P90	probability of 90%
PM_{10}	particulate matter with a diameter of 10 micrometers or less
POX	partial oxidation
PTW	pump to wheel
RFG	reformulated gasoline
S	sulfur
SA	standalone
SMR	steam methane reforming
SO_x	sulfur oxides
syngas	synthetic gas
VOC	volatile organic compound
WTP	well to pump
WTW	well to wheels

Units of Measure

^oC	degrees Celcius
Btu	British thermal unit(s)
g	gram(s)
gal	gallon(s)
kWh	kilowatt hour(s)
mmBtu	million Btu
ppm	part(s) per million
psi	pounds(s) per square inch

1. Introduction

The middle distillate fuel produced from natural gas (NG) via the Fischer-Tropsch (FT) process has been proposed as a motor fuel for compression-ignition (CI) engine vehicles. FT diesel could help reduce U.S. dependence on imported oil. The U.S. Department of Energy (DOE) is evaluating the designation of FT diesel as an alternative motor fuel under the 1992 Energy Policy Act (EPACT). As part of this evaluation, DOE has asked the Center for Transportation Research at Argonne National Laboratory to conduct an assessment of well-to-wheels (WTW) energy use and greenhouse gas (GHG) emissions of FT diesel compared with conventional motor fuels (i.e., petroleum diesel).

For this assessment, we applied Argonne's Greenhouse gases, Regulated Emissions, and Energy use in Transportation (GREET) model to conduct WTW analysis of FT diesel and petroleum diesel. This report documents Argonne's assessment. The results are presented in Section 2. Appendix A describes the methodologies and assumptions used in the assessment.

2. WTW Energy Use and GHG Emission Results of Fischer-Tropsch Diesel

2.1. Fuel Options and Key Assumptions

A WTW analysis includes the feedstock, fuel, and vehicle operation stages. The feedstock and fuel stages together are called "well-to-pump" (WTP) or "upstream" stages, and the vehicle operation stage is called the "pump-to-wheels" (PTW) or "downstream" stage. Argonne has developed the GREET model to estimate WTW energy use and emissions for combinations of various vehicle technologies and transportation fuels. The most recent GREET version is the beta version of GREET 1.6 (Wang 2001), which was used here to assess FT diesel energy and emission effects.

Because of potential technology improvements and economic and other factors that will affect the introduction of certain technologies, we encountered uncertainties in simulating future fuel production. To address the uncertainties, GREET 1.6 incorporates Monte Carlo simulations that we can use to conduct stochastic modeling of fuel production pathways. The Monte Carlo simulations require that we establish probability-based functions for key input parameters to generate energy and emission results with probability distributions. As part of this assessment, we conducted Monte Carlo simulations to estimate energy use and emissions of baseline petroleum gasoline and diesel.

Baseline Diesel Fuels. For comparison, our assessment included petroleum diesel as well as FT diesel. For petroleum diesel, we included a conventional diesel with a sulfur (S) content of 350 ppm and an ultra-low-sulfur (ULS) diesel with a sulfur content of 15 ppm. The U.S. Environmental Protection Agency (EPA) has adopted the ULS diesel requirement for implementation beginning in 2006.

Table 1 presents key assumptions for petroleum diesel that are used for GREET Monte Carlo simulations. In the table, P20 represents a probability of 20%, P50 a probability of 50%, and P80 a probability of 80%. A P20 value in the table means that there is a 20% chance that the actual

value may be below the presented value, a P50 value indicates a 50% chance that the actual value may be below the presented value, and a P80 value indicates an 80% chance that the actual value may be below the presented value. Statistically, the P50 value represents the average value for a given parameter, and P20 and P80 values represent the range for the given parameter. The probability distribution functions that are listed in Table 1 for energy efficiencies associated with petroleum recovery and petroleum refining to diesel fuels were developed for a previous Argonne study (see General Motors Corporation et al. 2001).

FT Diesel Production Options. Production of FT diesel consists of three steps: (1) production of synthetic gas (syngas), (2) synthesis of middle distillates, and (3) upgrading of products. The FT reaction is exothermic, and some excess steam is generated from the process. The generated steam can be exported to nearby facilities or used to generate electricity for export. We included three types of FT plant designs: with no steam or electricity co-generation (standalone [SA] plants), with steam co-generation, and with electricity co-generation.

Current economics and already proposed FT facilities strongly suggest that FT plants would be located outside of North America. Consequently, we evaluated FT diesel production outside of North America with non-North American (NNA) natural gas (NG). (Logistics for FTD production from Alaska North Slope gas fields, if any is produced there, are likely to be similar to those for NNA gas.) We also included flared gas (FG) from NNA sources as a technically feasible pathway. We realize that the amount of FG available worldwide for FT diesel production will be limited. Furthermore, in almost all instances that "associated gas" would be used to produce FTD or other products, that gas would be flared up until the time when it is captured for production of FTD or other products, but this does not establish that the gas would otherwise be flared over the long term. Our inclusion of FG-based FT diesel production is solely for the purpose of completeness in our technical analysis; it by no means implies that we believe that a significant amount of FT diesel will be produced from FG.

Our assumptions for FT diesel production are presented in Table 1. They are based on data published in the literature, input from oil companies during preparation of Argonne's portion of the General Motors study (General Motors Corporation et al. 2001), and data provided by the three FT companies that submitted FT diesel petitions to DOE (Mossgas, Rentech, and Syntroleum). The carbon efficiency for FT facilities, as presented in Table 1, is defined as carbon in products generated by FT facilities divided by carbon in NG feedstock to FT facilities. The carbon efficiency is used to calculate carbon dioxide (CO_2) emissions from FT facilities. Note that throughout this report, energy efficiencies and energy use results are based on lower heating values of fuels.

Table 1. Probability Distribution Functions for Key Parameters in Production of Petroleum and FT Diesel[a]

Parameter	Parametric Assumptions		
	P20[b]	P50[b]	P80[b]
Petroleum diesel			
Petroleum recovery efficiency (%)[c]	96.0	98.0	99.0
Petroleum refining efficiency (%): 350-ppm S diesel	88.0	89.0	90.0
Petroleum refining efficiency (%): 15-ppm S diesel	85.0	87.0	89.0
FT diesel production: standalone design			
Recovery efficiency (%): NNA NG and FG	96.0	97.5	99.0
Processing efficiency (%): NNA NG and FG	96.0	97.5	99.0
FT diesel production efficiency (%)[d]	54.0	61.0	68.0
FT diesel production: electricity co-generation			
FT diesel production efficiency (%)[c, e]	49.0	53.0	57.0
Electricity co-generation (kWh/mmBtu of FT diesel)[d]	16.6	23.6	30.5
FT diesel production: steam co-generation			
FT diesel production efficiency (%)[c, e]	49.0	53.0	57.0
Steam co-generation (Btu/mmBtu of FT diesel)[d]	189,000	268,000	347,000
FT facility carbon conversion efficiency (%)[d]	62.5	71.3	80.0

[a] A normal distribution function is assumed for each parameter, except as noted.
[b] Values are for probabilities of 20%, 50%, and 80%, respectively, except as noted.
[c] A triangle distribution function was assumed for petroleum recovery efficiency.
[d] Values are for probabilities of 10%, 50%, and 90%, respectively.
[e] FT facility energy efficiencies here are based on energy contents in produced energy products except for co-generated steam and electricity, which are taken into account via a displacement approach inside of the GREET model. For details of this methodology, see Wang and Huang (1999).

In their petitions to DOE to designate FT diesel as an alternative fuel, Mossgas, Rentech, and Syntroleum each provided information on the energy and carbon conversion efficiency of their FT processes and facilities. We applied company-specific efficiency data in the GREET model and calculated energy use and GHG emissions for the FT facilities and processes specified by the three companies. Table 2 presents key parameters for the FT facilities and processes described by the three companies. Input parameters other than those specified in Table 2 were GREET default assumptions (which is also true for simulations of generalized FT diesel production processes presented in Table 1).

Table 2. Characteristics of Company-Specific FT Facilities and FT Diesel[a]

Parameter	Mossgas[b]	Rentech[c]	Syntroleum[d]
Standalone facility energy efficiency: %	62.0[e]	54.0	49.0
FT facilities with electricity co-generation			
Energy efficiency: %[f]	NP[g]	49.6	Excluded[h]
Electricity generation: kWh/mmBtu of FT diesel	NP	21.9	Excluded
FT facilities with steam co-generation			
Energy efficiency: %[f]	NP	NP	49.0
Steam production: Btu/mmBtu of FT diesel	NP	NP	347,000[i]
FT facility carbon efficiency: %	78.3	68.4	72.0
FT facility FT diesel yield: Btu % or vol.% of all fuel products	40	71[j]	70
FT diesel fuel characteristics[k]			
Density: grams/gallon	3,057	2,932	2,915
Carbon content: wt. %	85.25	NP	85.0
Lower heating value: Btu/gallon	125,718	126,190	121,600

[a] From data provided by Mossgas, Rentech, and Syntroleum to DOE. Among the three companies, Syntroleum provided energy efficiency and carbon efficiency for FG-based FT facilities. However, our recent investigation indicated that the energy efficiency value provided by Syntroleum was originally from a previous Argonne study. Thus, it was determined here that the energy efficiency value was not Syntroleum-specific efficiency. Consequently, we decided not to include in this report the FG-based standalone case provided by Syntroleum.

[b] From Knottenbelt and Murdoch (2001) and Knottenbelt (1999). Mossgas submitted data only for standalone FT facilities (facilities that do not produce electricity or steam for export).

[c] From Sheppard (2001) and Rentech, Inc. (1999). Rentech submitted data for standalone facilities and facilities that co-produce FT fuels and electricity. We used the information presented in Rentech's ATR flow sheet dated October 15, 2001.

[d] From Woodward (2001) and Syntroleum (2000). Syntroleum submitted data for three cases – standalone facilities, facilities that co-produce FT fuels and electricity, and facilities that co-produce FT fuels and steam. Syntroleum's case for co-generating FT fuels and electricity is not included in this report; see Footnote h for details. Syntroleum submitted data for standalone FT facilities based on flared gas as well as natural gas. Syntroleum's flared gas case is not included in this report; see Footnote a for details.

[e] A small amount of electricity is inputted to Mossgas facilities. The energy efficiency here is based on the energy content of 3,413 Btu per kWh of electricity. Energy loss of electricity generation (about 65%) is taken into account inside of the GREET model during GREET simulations.

[f] FT facility energy efficiencies here are based on energy contents in produced energy products except for co-generated steam and electricity, which are taken into account via a displacement approach inside of the GREET model. For details of this methodology, see Wang and Huang (1999).

[g] NP = Not provided.

[h] Syntroleum provided information for a case under which both steam and electricity are co-generated with FT fuels (the power and steam case). Syntroleum's information indicated that more steam (in Btu) is generated under this case than under the case of steam co-generation only. While the Syntroleum-presented power and steam case may be possible, the generated steam under this case could be very low-quality steam whose usefulness is not clear. In the earlier version of our report, we assumed that the steam would be used to generate electricity at a low generation efficiency (i.e., 20% efficiency). However, with that assumption, the case analyzed in the earlier version was not a

Syntroleum case any more. Absent a Syntroleum facility-specific electric generation efficiency value, and a steam pressure value (see Footnote i), we decided not to include Syntroleum's power and steam case in this revision.
[i] Syntroleum specified that the produced steam is with 700 psi pressure.
[j] This is volumetric based share.
[k] The information is used to calculate energy use and carbon emissions during the pump-to-wheels stage.

Table 2 shows data for FT facilities or processes as reported by the three petitioning companies. Admittedly, each company's technology, facility design, energy feedstock inputs, and product slate can be distinctly different. In particular, the Mossgas design produces gasoline, diesel fuel, LPG blending components (propane, butylenes, and butane), and other energy products such as light alcohol, fuel oil, etc. The Mossgas facility product slate is 47% gasoline, 40% diesel fuel, 5% LPG blending components, and 8% of other energy products (based on energy contents of products) (Knottenbelt and Murdoch, 2001). Of the total energy feedstock inputs to Mossgas facilities, 82% is natural gas, 15% is condensates, and 3% is electricity (based on energy content of these input items).

The Syntroleum design uses natural gas as the only energy feedstock input and produces diesel fuel and naphtha (Woodward, 2001). On the energy basis, the Syntroleum design may produce 70% diesel fuel and 30% naphtha (by energy content) (see Wang and Huang 1999).

The Rentech design uses natural gas as the only energy feedstock input and produces diesel fuel and naphtha (Sheppard, 2001). On the volumetric basis, the Rentech design was presented to produce 71% diesel and 29% naphtha.

The above information on feedstock inputs and product outputs shows that the Mossgas design is distinctly different from the designs by Rentech and Syntroleum. The Mossgas design seems to be intended for production of both gasoline and diesel, while the designs by Rentech and Syntroleum are intended for FT diesel production. In evaluating WTW energy and GHG emission impacts of FT diesel in this study, we face the issue of allocating energy use and GHG emissions among multiple products from FT facilities. In our analysis, we allocated energy and emissions among fuel products based on energy shares of produced products. Other approaches are available to address co-product issues (see General Motors Corporation et al., 2001). However, these other approaches require detailed information on individual processes within a FT facilities. Because of the proprietary nature of FT process designs at this time, such information is not available to us.

2.2. Calculations of PTW Energy Use and GHG Emissions

GREET calculates PTW energy use and GHG emissions for each mile driven on the basis of vehicle fuel economy and per-mile emission rates. For this assessment, per-mile energy and emission results are converted into results per mmBtu of fuel used by vehicles by dividing per-mile results by per-mile energy use by vehicles. This conversion cancels out the effect of vehicle fuel economy on per-mmBtu results.

To calculate the PTW GHG emissions associated with fuel combustion, we need to determine the fuel density, carbon content, and Btu content of vehicular fuels. We applied data from Argonne's previous work and from the three FT companies — listed in Table 3 — to GREET to conduct PTW calculations. We did not have enough data to establish probability distribution

functions for the fuel characteristics of petroleum diesel, so we used point estimates. For FT diesel, we established probability distribution functions on the basis of data provided by the three FT companies. These probability distribution functions were used for simulations of generalized FT diesel production processes. For simulations of company-specific FT diesel production processes, we used the company-specific fuel characteristics presented in Table 2.

Table 3. Parametric Values of Fuel Characteristics for GREET Simulations[a]

Fuel Characteristic	Parametric Value		
	P20[b]	P50[b]	P80[b]
Conventional diesel			
Energy content (Btu/gal): lower heating value (LHV)		128,500	
Density (g/gal)		3,240	
Carbon content (% by weight)		87.0	
Ultra-low-sulfur diesel			
Energy content (Btu/gal): LHV		128,000	
Density (g/gal)		3,240	
Carbon content (% by weight)		87.0	
FT diesel			
Energy content (Btu/gal): LHV[c]	121,600	123,895	126,190
Density (g/gal)[c]	2,915	2,986	3,057
Carbon content (% by weight)[c]	85.0	85.1	85.25

[a] Fuel characteristics for conventional diesel and ultra-low-sulfur diesel are from GREET 1.6 default assumptions. Fuel characteristics for FT diesel are from data provided by the three FT companies (see Table 2).
[b] Values are for probabilities of 20%, 50%, and 80%, respectively. We did not have probability distribution functions for the characteristics of conventional diesel and ultra-low-sulfur diesel, so we used point estimates (under P50) for their fuel characteristics.
[c] A normal distribution function is assumed for each parameter.

2.3. WTW Energy Use and GHG Emission Results

Table 4 presents energy use and GHG emission results for the FT diesel assessment. The table is divided into three groups. The first group includes two baseline fuels: conventional diesel and ultra-low-sulfur diesel. The second group includes four FT diesel options with generalized FT production processes. The third group includes five FT diesel production options specified in the petitions to DOE by the three FT diesel companies.

For the first two groups, GREET simulations were conducted with probability distribution functions, so the results for the two baseline petroleum diesel fuels and four FT diesel general

production options are presented with probability distributions of 10%, 50%, and 90%. The values at 10% probability (P10) mean that 10% of FT diesel plants may have results below these values, the values at 50% probability (P50) mean that 50% of FT diesel plants may have results below these values, and the values at 90% probability (P90) mean that 90% of FT diesel plants may have results below these values. Statistically, P50 values represent average values, and P10 and P90 values represent the potential ranges of results.

For the third group, point estimates — rather than probability-based estimates — were generated from GREET simulations because the information provided by the three FT diesel companies is not adequate for probability-based estimates for specific FT process designs. For the same FT facility design (e.g., standalone facility design), the results from company-specific designs generally fall within the P10 to P90 ranges of the same FT design evaluated in the second group. Thus, the results for general FT production options may be used in EPACT rulemaking to determine the energy and GHG emission effects of FT diesel.

This assessment presents estimates of total energy use, fossil energy use, petroleum use, and emissions of the three GHGs (CO_2, CH_4, and N_2O). Total energy use here includes all energy sources (non-renewable and renewable). Fossil energy includes three non-renewable fossil energy sources: petroleum, NG, and coal. The separation of energy use into the three groups helps identify whether a new fuel/vehicle system can achieve overall energy benefits (based on total energy use), reduce fossil energy use, and displace petroleum use. Emissions of the three GHGs are combined together with their GWPs (1 for CO_2, 21 for CH_4, and 310 for N_2O) to derive CO_2-equivalent GHG emissions.

Figures 1–4 graphically present the WTW total energy use, fossil energy use, petroleum use, and GHG emissions results for the two baseline fuels and four general FT diesel options. In the four figures, the bars represent average values, while the lines superposed the bars represent ranges. Figure 1 shows that the three FT diesel production options (with NG as the feedstock) increase total energy use by roughly 500,000 Btu per mmBtu of FT diesel, relative to the two baseline petroleum diesels. Note that co-generation of electricity in FT plants actually results in increased total energy use, relative to FT plants without electricity export, because (1) FT plant designs with electricity export are subject to an energy efficiency penalty (see Table 1), and (2) we assumed that the electricity from FT plants would displace electricity generation from NG-fired combined-cycle turbines, which have an electricity generation efficiency of greater than 50%. Displacement of efficient electricity generation (from the combined-cycle turbines) by FT plant electricity results in fewer energy and GHG emission benefits from the co-generated electricity.

Figure 1 also reveals that if steam is co-generated from FT plants, total energy use for FT diesel is reduced, relative to standalone FT plants. Furthermore, if FG is used as the feedstock in FT plants, total energy use for FT diesel is minimal, because FG is otherwise wasted.

Figure 2 shows fossil energy use for the six options. The patterns of fossil energy use are similar to those for total energy use. That is, use of NG-based FT diesel increases fossil energy use significantly, while FG-based FT diesel reduces fossil energy use significantly.

Figure 3 shows petroleum use for production and use of FT diesel and petroleum diesel fuels. Because FT diesel is produced from NG rather than petroleum, use of FT diesel results in huge reductions in petroleum use, relative to the two baseline petroleum diesels.

Figure 4 shows GHG emissions for the six fuel options. Overall, FT plants with standalone and electricity co-generation designs result in higher GHG emissions than the two baseline petroleum diesels. However, if FT plants are designed with steam export, production and use of FT diesel may actually result in reductions in GHG emissions, although GHG emissions associated with FT diesel production are subject to great uncertainties (wide range of results). If FG is the feedstock for FT diesel production, use of FT diesel results in huge GHG emission reduction benefits because of the elimination of gas flaring during FT diesel production.

The energy use and GHG emissions results presented here are based on mmBtu of fuel delivered and used. Use of petroleum diesel and FT diesel in internal combustion engines may result in different engine efficiencies. A complete comparison among these fuels — including an examination of engine efficiency (or vehicle fuel economy), as well as fuel characteristics — should be conducted. As part of such a study, the per-mmBtu results presented here need to be adjusted to per-mile results. However, use of petroleum diesel and FT diesel in diesel engines results in small differences in Btu-based vehicle fuel economy. Parallel conclusions regarding per-mile changes between petroleum and FT diesel could be drawn from the conclusions regarding per-mmBtu changes provided in Table 4 and in Figures 1–4.

Table 4. Well-to-Wheels Results: Conventional Diesel, Ultra-Low-Sulfur Diesel, and FT Diesel (Energy in Btu and Emissions in g/mmBtu of Fuel Delivered and Used)

	Well-to-Pump					Pump-to-Wheels					Well-to-Wheels				
	Total Energy	Fossil Energy	Petroleum	CO_2	GHGs	Total Energy	Fossil Energy	Petroleum	CO_2	GHGs	Total Energy	Fossil Energy	Petroleum	CO_2	GHGs
Conventional Diesel, 350 ppm S Content															
10%	161,644	158,600	74,566	12,785	14,967	1,000,000	1,000,000	1,000,000	80,425	81,738	1,161,644	1,158,600	1,074,566	93,210	96,704
50%	186,060	182,551	85,322	14,510	16,737	1,000,000	1,000,000	1,000,000	80,424	81,925	1,186,060	1,182,551	1,085,322	94,934	98,662
90%	211,110	207,158	96,011	16,273	18,529	1,000,000	1,000,000	1,000,000	80,422	82,185	1,211,110	1,207,158	1,096,011	96,695	100,713
Ultra-Low-Sulfur Diesel, 15 ppm S Content															
10%	169,227	165,886	77,446	13,318	15,507	1,000,000	1,000,000	1,000,000	80,739	82,053	1,169,227	1,165,886	1,077,446	94,057	97,560
50%	214,029	210,184	99,033	16,518	18,797	1,000,000	1,000,000	1,000,000	80,738	82,240	1,214,029	1,210,184	1,099,033	97,256	101,037
90%	261,894	257,240	121,531	19,897	22,258	1,000,000	1,000,000	1,000,000	80,737	82,491	1,261,894	1,257,240	1,121,531	100,634	104,750
FT Diesel: Standalone Plants															
10%	562,879	562,480	14,737	24,974	27,215	1,000,000	1,000,000	0	74,736	76,501	1,562,879	1,562,480	14,737	99,710	103,716
50%	748,273	747,471	20,594	34,263	36,503	1,000,000	1,000,000	0	75,175	76,676	1,748,273	1,747,471	20,594	109,437	113,178
90%	988,533	987,938	27,123	44,088	46,338	1,000,000	1,000,000	0	75,685	76,998	1,988,533	1,987,938	27,123	119,773	123,336
FT Diesel: Plants with Electricity Export															
10%	694,481	693,944	15,015	18,744	20,677	1,000,000	1,000,000	0	74,736	76,501	1,694,481	1,693,944	15,015	93,480	97,178
50%	857,089	856,232	21,028	29,032	31,014	1,000,000	1,000,000	0	75,175	76,676	1,857,089	1,856,232	21,028	104,207	107,690
90%	1,044,105	1,043,450	27,857	39,958	41,942	1,000,000	1,000,000	0	75,685	76,998	2,044,105	2,043,450	27,857	115,643	118,940
FT Diesel: Plants with Steam Export															
10%	471,148	470,593	14,855	4,645	5,913	1,000,000	1,000,000	0	74,736	76,501	1,471,148	1,470,593	14,855	79,381	82,415
50%	657,483	656,779	20,387	16,805	18,143	1,000,000	1,000,000	0	75,175	76,676	1,657,483	1,656,779	20,387	91,979	94,818
90%	870,053	868,887	26,490	29,363	30,870	1,000,000	1,000,000	0	75,685	76,998	1,870,053	1,868,887	26,490	105,049	107,868
FT Diesel: Standalone Plants with Flared Gas															
10%	-949,203	-949,548	16,358	-76,546	-76,789	1,000,000	1,000,000	0	74,736	76,501	50,797	50,452	16,358	-1,810	-288
50%	-887,594	-888,343	22,364	-63,720	-63,697	1,000,000	1,000,000	0	75,175	76,676	112,406	111,657	22,364	11,455	12,979
90%	-819,302	-820,607	29,004	-52,395	-52,236	1,000,000	1,000,000	0	75,685	76,998	180,698	179,393	29,004	23,290	24,762

Results for FT Facilities Specified by Three Individual Companies

Mossgas SA	748,995	741,948	21,604	31,780	34,157	1,000,000	1,000,000	0	76,000	77,523	1,748,995	1,741,948	21,604	107,780	111,680
Rentech SA	972,742	971,956	20,773	40,884	43,126	1,000,000	1,000,000	0	72,406	73,929	1,972,742	1,971,956	20,773	113,290	117,056
Syntroleum SA	1,173,026	1,172,171	21,905	41,019	43,262	1,000,000	1,000,000	0	74,704	76,227	2,173,026	2,172,171	21,905	115,723	119,489
Rentech Electricity	1,001,934	1,001,147	20,875	31,760	33,750	1,000,000	1,000,000	0	72,406	73,929	2,001,934	2,001,147	20,875	104,166	107,679
Syntroleum Steam	714,586	713,879	20,329	13,057	14,188	1,000,000	1,000,000	0	74,704	76,227	1,714,586	1,713,879	20,329	87,761	90,415

Notes: SA = standalone; FG = flared gas; electricity = plant design with electricity export; steam = plant design with steam export.

Figure 1. WTW Total Energy Use (in Btu/mmBtu of Fuel Delivered and Used)

Figure 2. WTW Fossil Energy Use (in Btu/mmBtu of Fuel Delivered and Used)
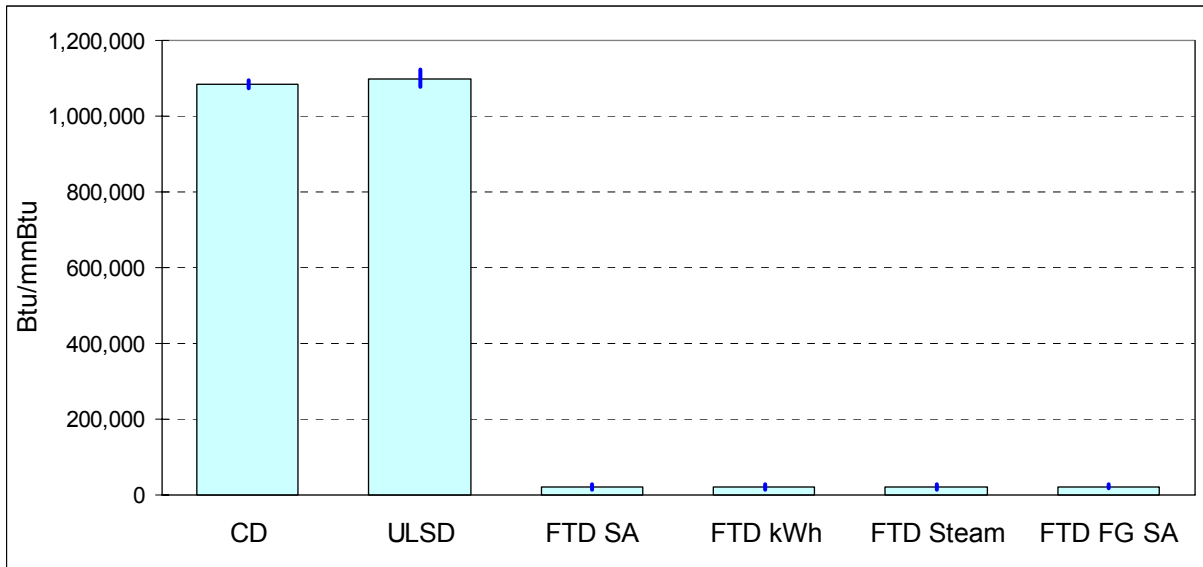
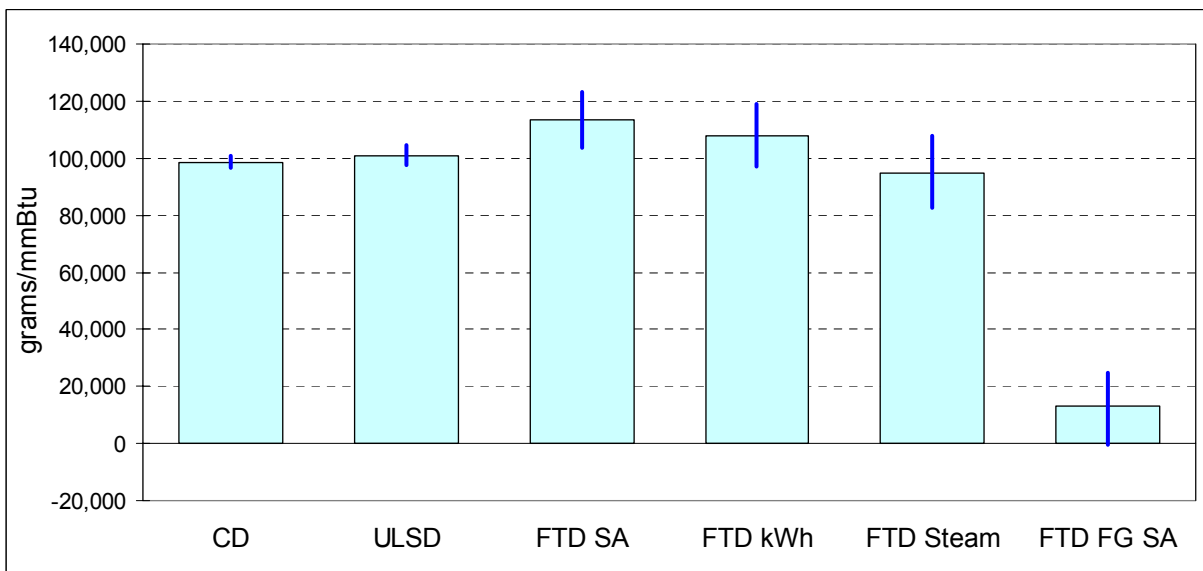Figure 3. WTW Petroleum Use (in Btu/mmBtu of Fuel Delivered and Used)

Figure 4. WTW GHG Emissions (in g/mmBtu of Fuel Delivered and Used)

3. Acknowledgments

4. References

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Appendix A

A.1 Analytical Approach

A WTW analysis of a vehicle/fuel system covers all stages of the fuel cycle — from energy feedstock recovery (wells) to energy delivered at vehicle wheels (wheels). Since 1995, with funding from DOE's Office of Transportation Technologies (OTT), Argonne has been developing the GREET model as an analytical tool for use by researchers and practitioners to estimate WTW energy use and emissions associated with transportation fuels and advanced vehicle technologies. Argonne released the first version of the GREET model — GREET 1.0 — in June 1996 (Wang 1996). Since then, Argonne has released a series of GREET versions with revisions, updates, and upgrades. The most recent version is the beta version of GREET 1.6 (Wang 2001). This version was used for the FT diesel assessment described here. The model and associated documents are posted at Argonne's GREET website at http://greet.anl.gov.

Figure A1 presents the stages and activities covered in GREET WTW simulations of vehicle/fuel systems. A WTW analysis includes the feedstock, fuel, and vehicle operation stages. The feedstock and fuel stages together are called "well-to-pump" or "upstream" stages, and the vehicle operation stage is called the "pump-to-wheels" or "downstream" stage. In GREET, WTW energy and emission results are presented separately for each of the three stages shown in Figure A1.
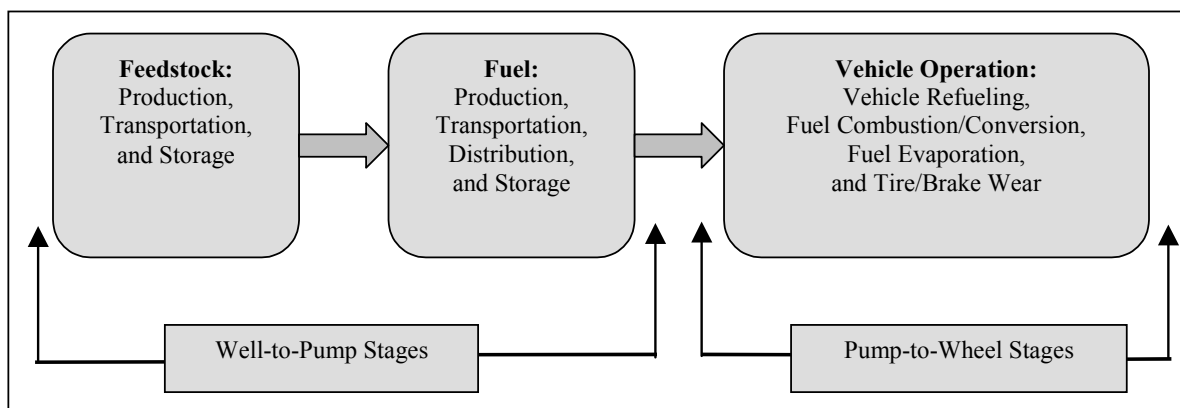

Figure A1. WTW Stages of Vehicle/Fuel Systems Covered in the GREET Model

For a given transportation fuel/vehicle technology combination, the GREET model separately calculates:

1. Fuel-cycle energy consumption for
   a) Total energy (all energy sources),
   b) Fossil fuels (petroleum, NG, and coal), and
   c) Petroleum;
2. Fuel-cycle emissions of GHGs
   a) Carbon dioxide (CO_2) (with a global warming potential [GWP] of 1),

b) Methane (CH_4) (with a GWP of 21), and

c) Nitrous oxide (N_2O) (with a GWP of 310); and

3. Fuel-cycle emissions of five criteria pollutants (separated into total and urban emissions)

a) Volatile organic compounds (VOCs),

b) Carbon monoxide (CO),

c) Nitrogen oxides (NO_x),

d) Particulate matter with a diameter of 10 micrometers or less (PM_{10}), and

e) Sulfur oxides (SO_x).

This assessment presents estimates of total energy use, fossil energy use, petroleum use, and emissions of the three GHGs (CO_2, CH_4, and N_2O). Total energy use here includes all energy sources (non-renewable and renewable). Fossil energy includes three non-renewable fossil energy sources: petroleum, NG, and coal. The separation of energy use into the three groups helps identify whether a new fuel/vehicle system can achieve overall energy benefits (based on total energy use), reduce fossil energy use, and displace petroleum use. Emissions of the three GHGs are combined together with their GWPs (1 for CO_2, 21 for CH_4, and 310 for N_2O) to derive CO_2-equivalent GHG emissions.

In this assessment, WTW results are separated into WTP and PTW stages. WTP stages comprise two groups of activities: production- and transportation-related activities. Production-related activities include petroleum refining, FT diesel production, etc. Transportation-related activities include petroleum transportation, diesel transportation and distribution, and FT diesel transportation and distribution. Details regarding the methods used to calculate energy use and emissions for the WTP stages are presented in Wang (1999), Wang and Huang (1999), He and Wang (2000), and General Motors Corporation et al. (2001).

Figure A2 shows GREET calculation logic for energy use and emissions of fuel production-related activities. For a given production activity, GREET calculates energy use and emissions by means of input assumptions regarding energy conversion efficiency, process fuel shares, combustion technology shares, emission factors associated with combustion technologies powered by different fuel types, and facility locations. Of these input parameters, the energy conversion efficiency for a given activity is the key parameter in determining both energy use and emissions associated with the activity.
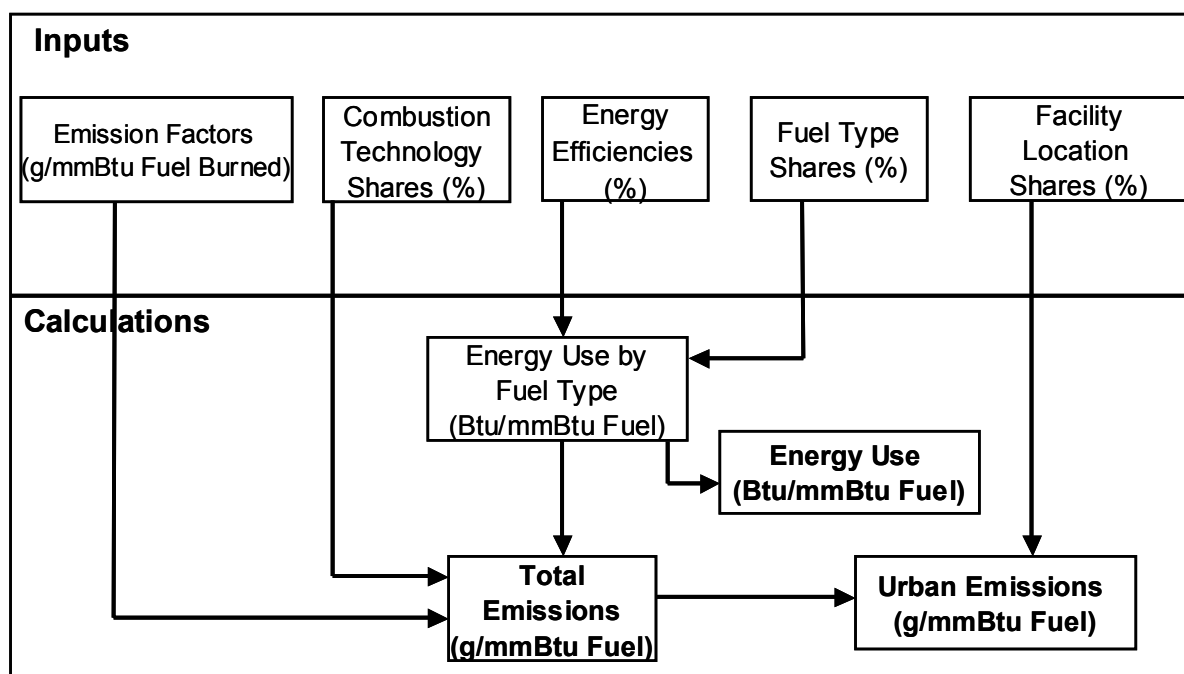
Figure A2. GREET Energy and Emission Calculation Logic for Production-Related Activities

Figure A3 presents GREET calculation logic for energy use and emissions of transportation-related activities. To calculate energy use and emissions for transportation of a given fuel or energy feedstock, GREET takes input parameters such as transportation distance, transportation mode shares, energy intensity and emission factors of transportation modes, and share of process fuels for transportation modes. Usually, energy use and emissions from transportation-related activities are far less than those from production-related activities.

For PTW (vehicle operation) stages, GREET calculates per-mile energy use and emissions by means of input parameters of vehicle fuel economy and tailpipe and evaporative emissions. In this assessment, DOE requested that PTW results, as well as WTP results, be presented per unit of energy delivered and used. For WTP stages, GREET directly calculates energy use and emissions per mmBtu of fuel delivered at the fuel pump. In this analysis, PTW per-mile energy use and emission results from GREET simulations are converted to per-mmBtu energy use and emissions by applying the vehicular fuel use in Btu per mile that is calculated in GREET to per mile PTW results.
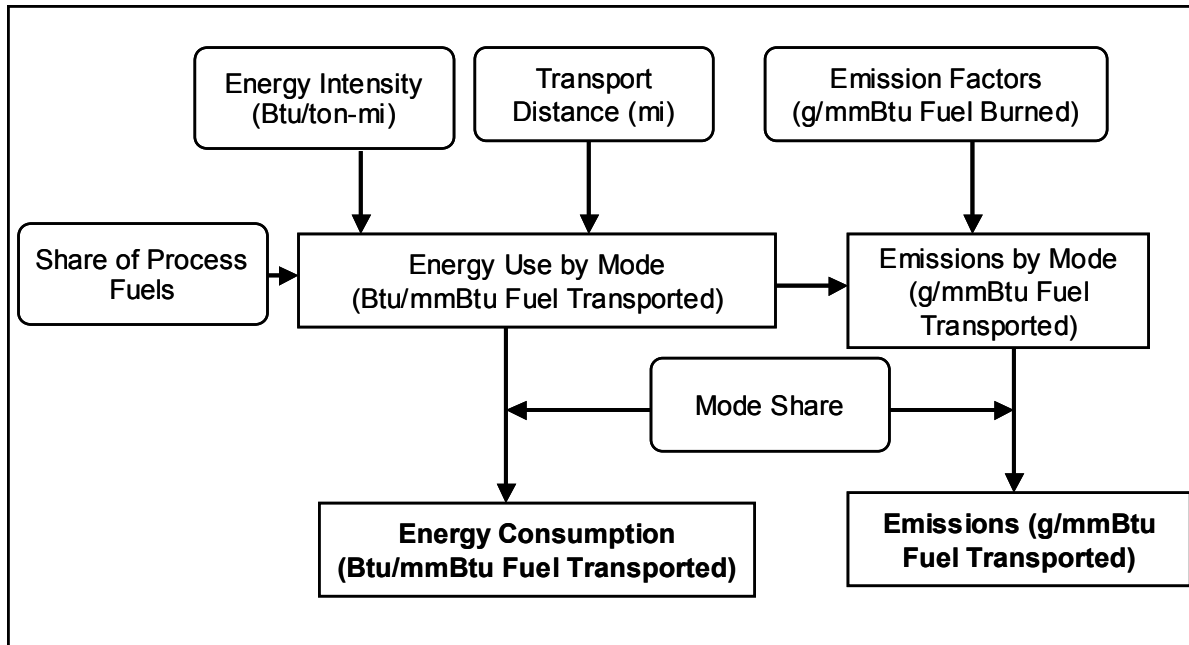
Figure A3.   GREET Energy and Emission Calculation Logic for Transportation-Related Activities

A.2 Pathway Specifications for This Assessment

Baseline Petroleum Diesel Fuels.   Since 1996, Argonne has been evaluating the energy and emission impacts of baseline gasoline and diesel fuels. For FT diesel comparisons, petroleum diesel is the baseline fuel because both petroleum diesel and FT diesel can be used in CI engines. For baseline diesel fuel, we included a conventional diesel with a sulfur content of 350 ppm and an ULS diesel with a sulfur content of 15 ppm. EPA has proposed the ULS diesel requirement for implementation beginning in 2006.

Figure A4 is a flowchart of the WTP stages included in GREET for petroleum diesel. The two key stages are petroleum recovery and petroleum refining. Probability distribution functions for the energy efficiencies of these two stages were developed for a previous Argonne study (see General Motors Corporation et al. 2001) and are presented in Table 1 (Section 2) of this report.

Figures A5–A6 show transportation logistics for petroleum and diesel. Detailed descriptions of other parametric assumptions regarding the transportation-related activities shown in Figure A3 are presented in He and Wang (2000).
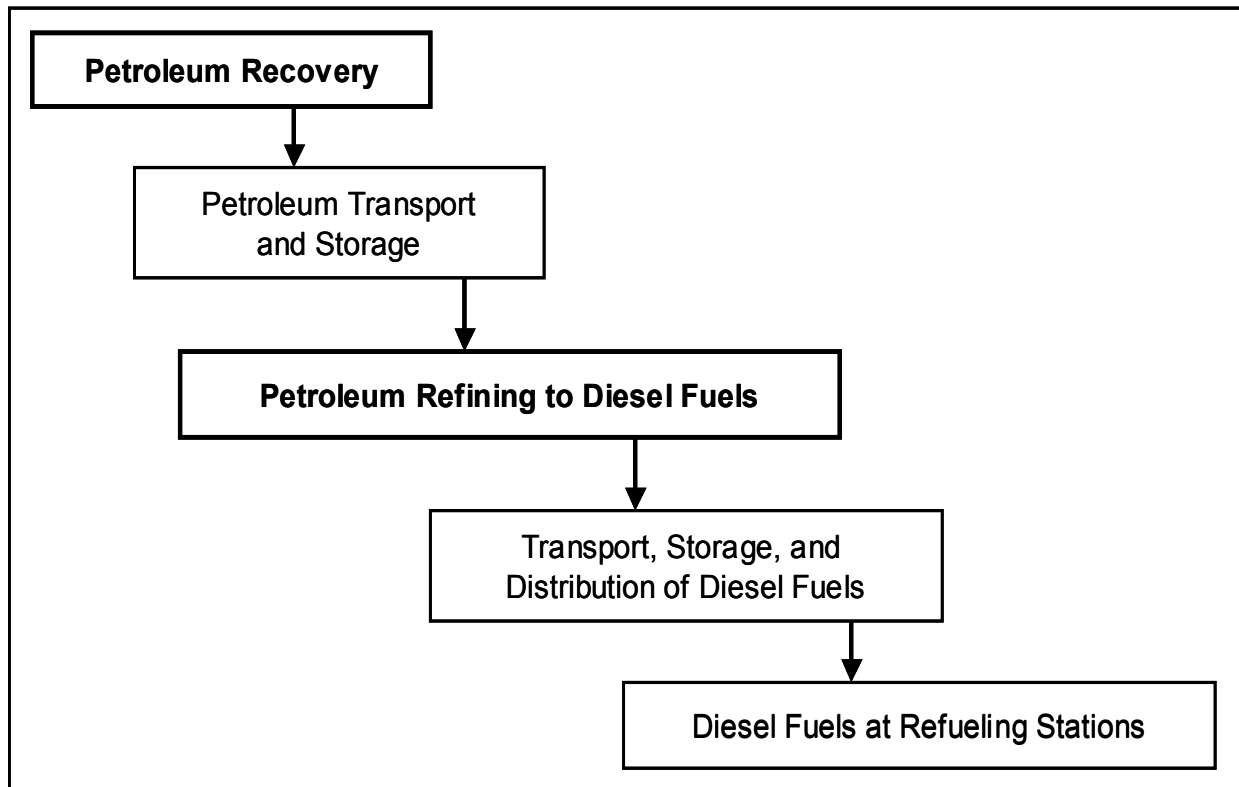
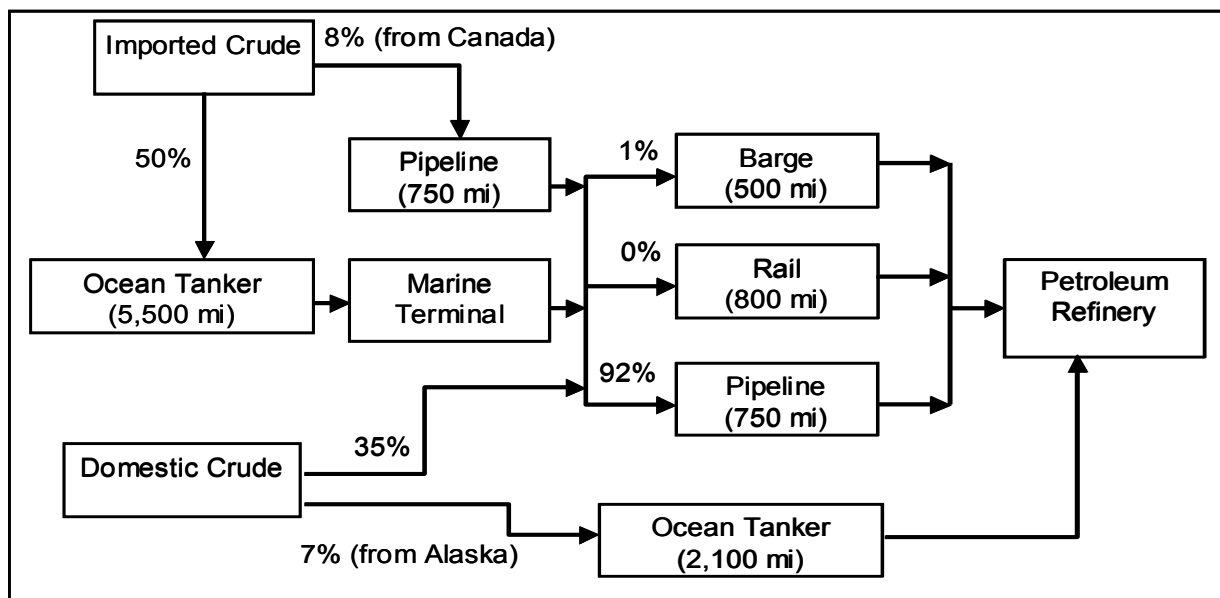Figure A4. WTP Stages of Baseline Petroleum Diesel

Figure A5. Transportation Logistics of Petroleum from Oil Fields to Petroleum Refineries for U.S. Petroleum Fuel Production
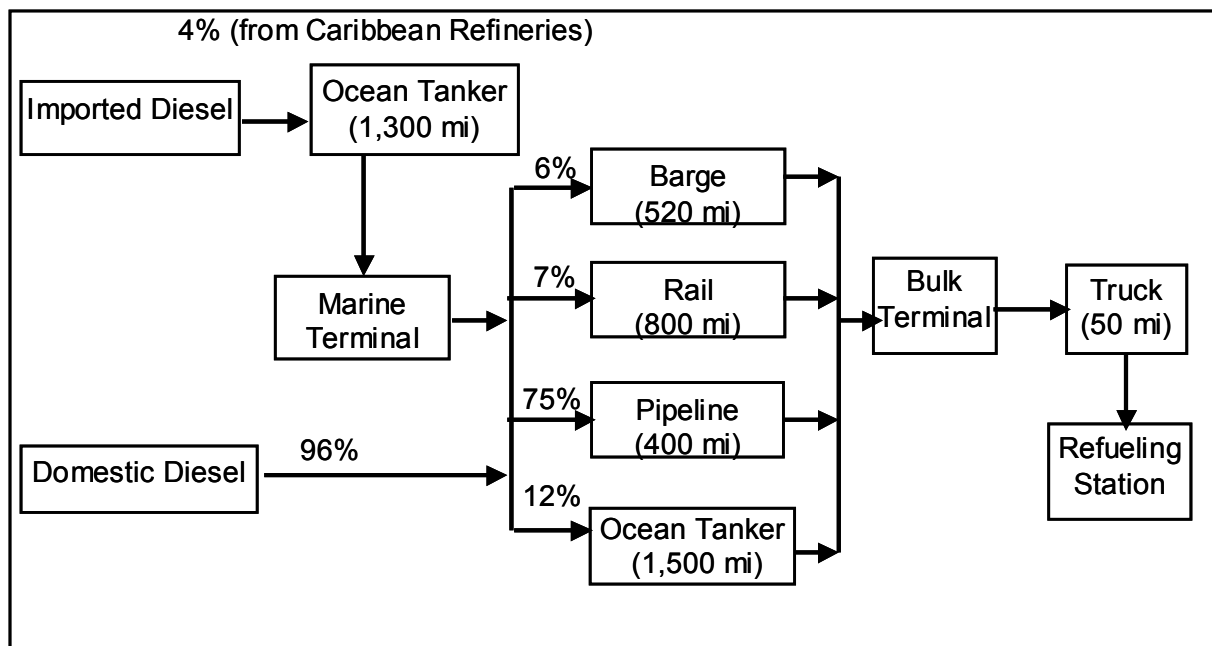
Figure A6. Transportation Logistics of U.S. Diesel from Petroleum Refineries to Refueling Stations

Generalized FT Diesel Production Processes. Production of FT diesel consists of three steps: (1) production of synthetic gas (syngas), (2) synthesis of middle distillates, and (3) upgrading of products. At the syngas production stage, NG feed is converted into syngas (a mixture of CO and hydrogen [H_2]). Steam methane reforming (SMR), partial oxidation (POX), or autothermal reforming (ATR) technologies can be used to generate syngas.

The next stage in FT diesel plants is FT synthesis. With the help of catalysts, the reaction produces a variety of hydrocarbon liquids including middle distillates and naphtha. The product mix from the process depends on the catalyst used and the operating temperature of the reactor. For example, an operating temperature of 180–250°C helps produce predominately middle distillates and wax; an operating temperature of 330–350°C helps produce gasoline and olefins. The FT reaction is exothermic, and some excess steam is generated from the process. The generated steam can be exported to nearby facilities or used to generate electricity for export. We included three types of FT plant designs: with no steam or electricity co-generation (SA plants), with steam co-generation, and with electricity co-generation.

Figure A7 presents the WTP stages of FT diesel production pathways. Current economics and already proposed FT facilities strongly suggest that FT plants would be located outside of North America. Consequently, we evaluated FT diesel production outside of North America with non-North American (NNA) natural gas (NG). (Logistics for FTD production from Alaska North Slope gas fields, if any is produced there, is likely to be similar to that for NNA gas.) We also included flared gas (FG) from NNA sources as a technically feasible pathway. We realize that the amount of FG available worldwide for FT diesel production will be limited. Furthermore, in almost all instances that "associated gas" would be used to produce FTD or other products, that gas would be flared up until the time when it is captured for production of FTD or other

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products, but this does not establish that the gas would otherwise be flared over the long term. Our inclusion of FG-based FT diesel production is solely for the purpose of completeness in our technical analysis; it by no means implies that we believe that a significant amount of FT diesel will be produced from FG.

The key WTP stages (in bold in Figure A7) for FT diesel production are gas recovery, gas processing, and FT diesel production. The largest efficiency losses for FT pathways occur during the FT diesel production stage. Table A1 summarizes data regarding FT diesel production. The data were provided by the three companies (Mossgas, Rentech, and Syntroleum) that are petitioning DOE to designate FT diesel as an alternative fuel. On the basis of data published in the literature, input from oil companies during preparation of Argonne's portion of the General Motors study (General Motors Corporation et al. 2001), and data provided by the three FT companies, we made parametric assumptions for this assessment; these assumptions are provided in Table 1 (Section 2) of this report. Carbon efficiency for FT diesel production in Table A1 is defined as the amount of carbon in products of FT plants divided by the amount of carbon in NG feedstock to FT plants. The carbon efficiency is used to calculate CO_2 emissions from FT plants.
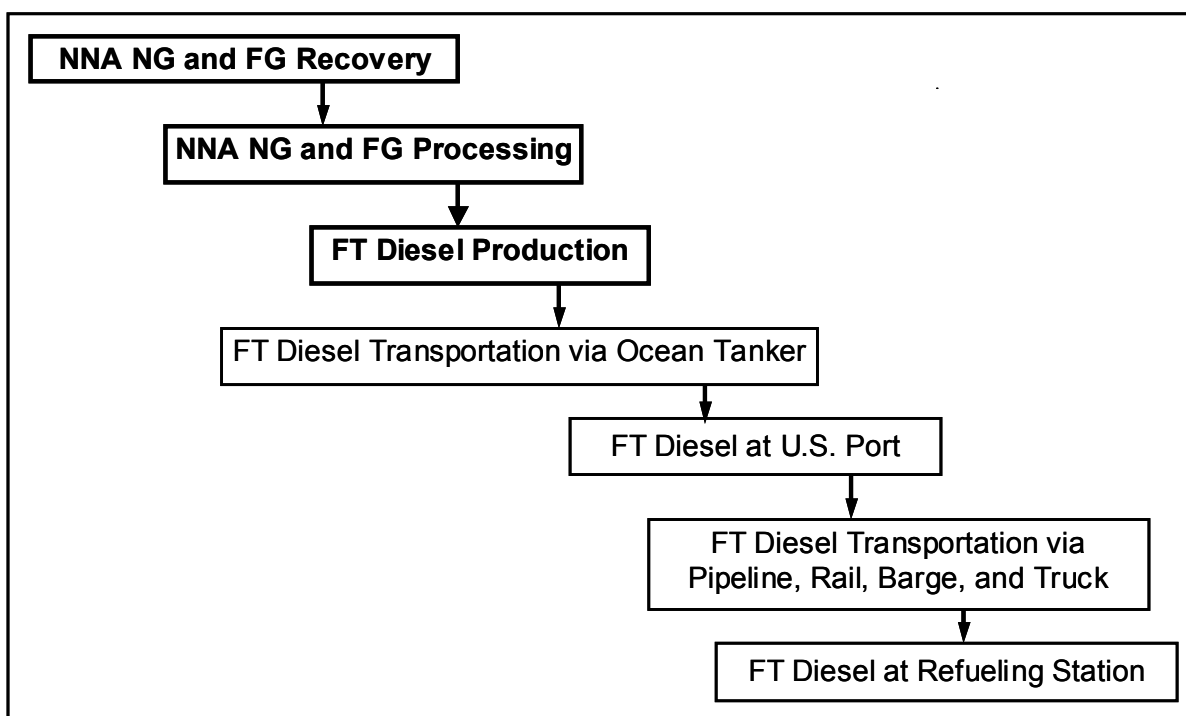

Figure A7. WTP Stages of FT Diesel Pathways

Figure A8 presents transportation logistics for FT diesel from NNA production sites to U.S. refueling stations. As the figure implies, we assumed that FT diesel would be primarily produced in the Middle East and North Africa, where inexpensive NG is available. Some FT projects have been proposed in Asia, Australia, sub-Saharan Africa, and South America. The transportation distance for FT diesel from these locations to the United States will be shorter than the distance from the Middle East and North Africa. But, overall, FT diesel transportation distance has a very small effect on FT diesel's energy use and GHG emissions.
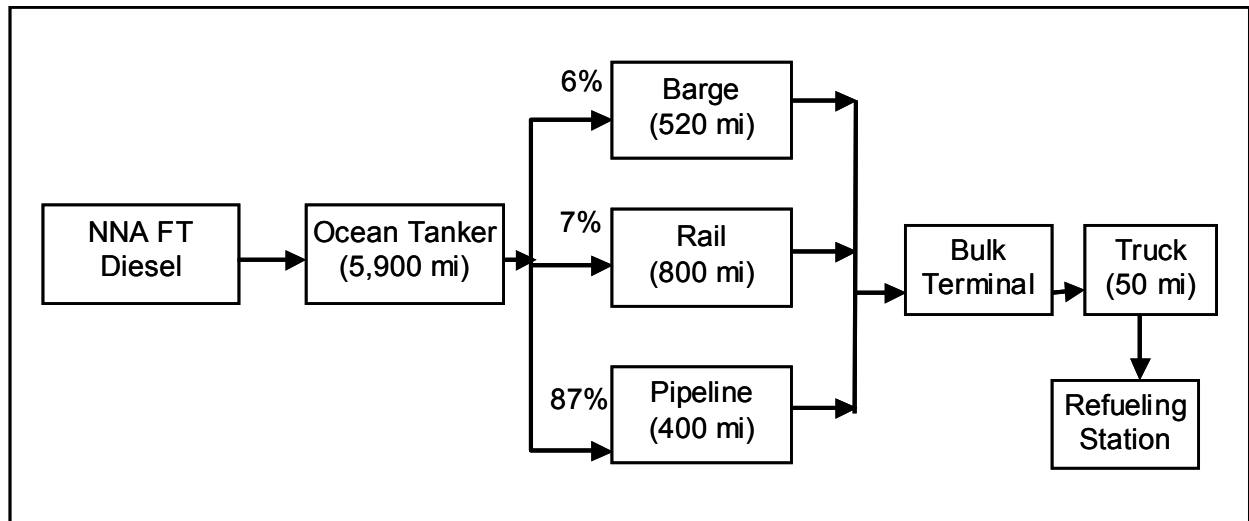

Figure A8. Transportation Logistics of Non-North American FT Diesel to U.S. Refueling Stations