NETL Life Cycle Inventory Data
Process Documentation File

Process Name:	CBTL Zero Sulfur Diesel
Reference Flow:	1 kg of Diesel
Brief Description:	Coal-and-Biomass-to-liquids (CBTL) via Fischer-Tropsch synthesis using Illinois No. 6 or PRB as the coal and switchgrass as the biomass feedstock where applicable.

Section I: Meta Data

Geographical Coverage: United States   **Region:** Midwest or Mountain West

Year Data Best Represents: 2013

Process Type: Energy Conversion (EC)

Process Scope: Gate-to-Gate Process (GG)

Allocation Applied: No

Completeness: All Relevant Flows Captured

Flows Aggregated in Data Set:

☑ Process   ☑ Energy Use   ☐ Energy P&D   ☐ Material P&D

Relevant Output Flows Included in Data Set:

Releases to Air:	☑ Greenhouse Gases	☐ Criteria Air	☐ Other
Releases to Water:	☐ Inorganic	☐ Organic Emissions	☐ Other
Water Usage:	☐ Water Consumption	☐ Water Demand (throughput)	
Releases to Soil:	☐ Inorganic Releases	☐ Organic Releases	☐ Other

Adjustable Process Parameters:

CO2_air	*[kg/kg] kg CO_2 emission to air per kg diesel*
CO2_saline	*[kg/kg] kg CO_2 captured per kg diesel*
Diesel	*[kg/kg] kg diesel produced*
Elec	*[MWh/kg] MWh power exported per kg diesel*

Naphtha	*[kg/kg] kg naphtha produced per kg diesel*
I6	*[kg/kg] kg Illinois No. 6 coal per kg diesel*
PRB	*[kg/kg] kg PRB coal per kg diesel*
Switchgrass	*[kg/kg] kg switchgrass per kg diesel*
LU_IL	*[sqm/kg] square meter per kg diesel*
LU_MT	*[sqm/kg] square meter per kg diesel*

Tracked Input Flows:

Hard Coal (Illinois No 6) [Intermediate]	*[Technosphere] Illinois No. 6 coal feedstock to CBTL plant*
Rosebud Coal (NETL) [Hard coal products]	*[Technosphere] PRB coal feedstock to CBTL plant*
Switchgrass (NETL) [Renewable primary products]	*[Technosphere] Switchgrass feedstock to CBTL plant*
Land use area, IL, no reversion [Land use]	*[Resource] Land use area, Illinois*
Land use area, MT, no reversion [Land use]	*[Resource] Land use area, Montana*

Tracked Output Flows:

FT Diesel [Valuable substances]	*Reference flow*
Carbon dioxide [Inorganic emissions to air]	*Emission to air*
FT Naphtha [Valuable substances]	*Coproduct*
Electricity [Electric power]	*Coproduct*
Carbon dioxide [Inorganic intermediate products]	*Sent to sequestration*

Section II: Process Description

Associated Documentation

This unit process is composed of this document and the data sheet (DS) *DS_Stage3_O_CBTL_Zero_Sulfur_Diesel_2013.01.xlsx*, which provides additional details regarding relevant calculations, data quality, and references.

Goal and Scope

This unit process provides a summary of relevant input and output flows associated with coal-and-biomass-to-liquids (CBTL) via Fischer-Tropsch (FT) synthesis using Illinois No. 6 or PRB as the feedstock and switchgrass as the biomass feedstock where applicable. The reference flow of this unit process is: 1 kg of Diesel

Boundary and Description

This unit process provides a summary of relevant input and output flows associated with coal-and-biomass-to-liquids (CBTL) via Fischer-Tropsch (FT) synthesis using Illinois No. 6 or Powder River Basin (PRB) coal, and switchgrass. The Rosebud mine in Montana is used as the source for PRB coal.

Two broad design approaches were considered: (1) a facility that is designed to primarily produce liquid fuels, and (2) a poly-generation plant that is designed to co-produce electric power for sale into the grid. In the fuels-focused production facility, a portion of the unconverted syngas is recycled back to the FT reactors, resulting in a greater percentage of the original carbon in the feedstock being converted into liquid fuels.

Both the fuels-focused facility (i.e. the "recycle" configuration) and the once-through configuration are designed to produce 50,000 barrels per day (bpd) of FT liquids, comprised of 34,000 bpd of FT diesel (or 69 percent of the product) with the balance consisting of FT naphtha. The FT diesel is completely fungible in today's fueling infrastructure and can be used as a drop-in fuel, while the FT naphtha is assumed to be sold for use as an ethylene cracker feedstock.

All configurations use Siemens entrained flow gasification with full water quench to produce the raw synthesis gas from the coal feed. Raw synthesis gas (syngas) conditioning is accomplished using conventional cold gas cleaning for sulfur removal and recovery and for bulk carbon dioxide (CO_2) removal. Synthesis is accomplished using low temperature Fischer-Tropsch (FT) slurry phase reactor technology using iron based FT catalysts.

For plants cases designated "Once-Through", the clean syngas is passed through the FT reactors one time only. After product recovery and CO_2 removal, the unconverted syngas and light hydrocarbons are sent to gas turbines for power generation. These configurations produce liquid fuels and a large quantity of power as a co-product. Plant cases designated "Recycle" use the recycle configuration where most of the unconverted syngas and light hydrocarbons are recycled back to the FT reactors (after CO_2 removal) to increase the liquid production. The balance of the unconverted syngas and light hydrocarbons are diverted to the gas turbines for power generation.

The inputs to this unit process are Illinois No. 6 coal or Powder River Basin (PRB) coal, and switchgrass, in the applicable cases. The CBTL process produces diesel, naphtha, electricity, and CO_2 that can be sent to a saline aquifer sequestration site. The reference flow of this unit process is 1 kg of diesel. All input and output

DF_Stage3_O_CBTL_Zero_Sulfur_Diesel_2013.1.docx

flows are expressed on the basis of this reference flow. The boundaries of this unit process are shown in **Figure 1**.

Figure 1: Unit Process Scope and Boundary
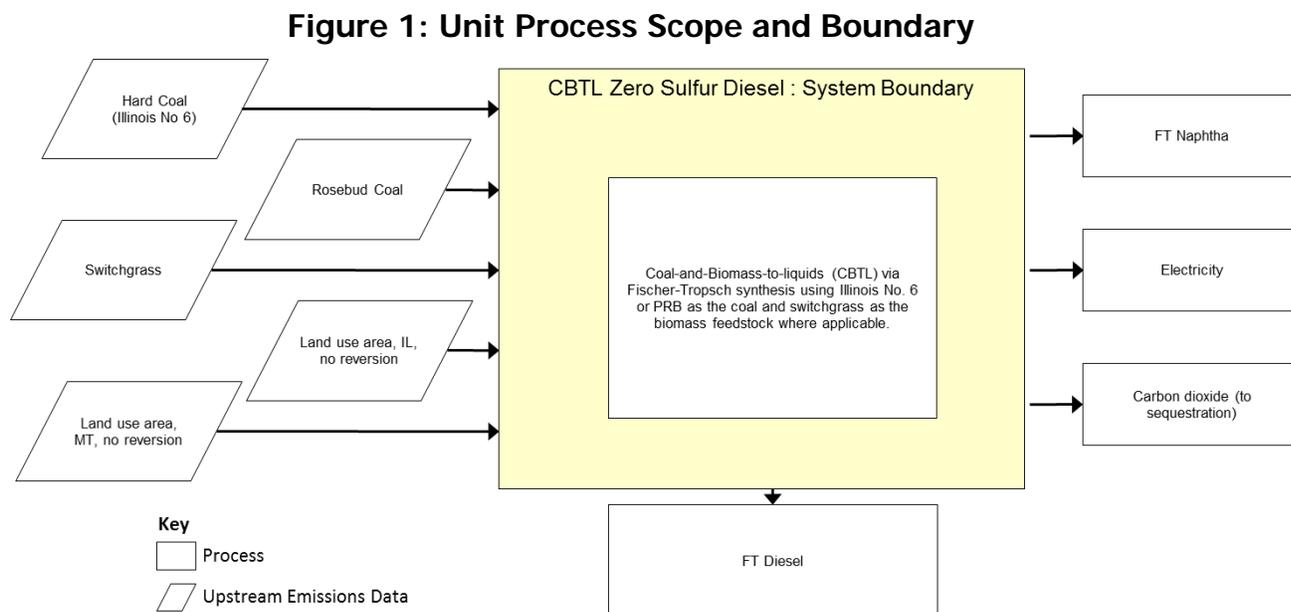
There are sixteen capture configurations analyzed in this report and four venting configurations. The Case Identifier is a five character code based on the specific case configuration. The first character denotes the coal type with "B" denoting bituminous and "S" denoting subbituminous. The second character denotes the recycle configuration. "R" denotes simple recycle and "O" denotes once-through. The third character denotes the cooling configuration. "W" refers to the system where mechanical draft, water-cooled cooling towers are used for the plant cooling duties. "A" denotes configurations with maximum air cooling and "H" denotes the hybrid cooling scheme. The fourth and fifth characters designate the mass fraction of biomass on an as-received basis. For the venting configurations the letter "V" is added to the five character code.

For example, Case "BRW00" is shorthand for bituminous coal, recycle mode, water cooling, and no biomass and BRW00V designates the CO_2 venting configuration. In a similar manner, "BOW15" is bituminous coal, once-through mode, water cooling, with 15 percent biomass. For the subbituminous coal cases, "SRA00" means subbituminous coal, recycle, air cooling, and no biomass. Similarly, "SOH15" is subbituminous coal, once-through mode, hybrid cooling, with 15 percent biomass. **Table 1** summarizes the sixteen cases.

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Table 1: CBTL Case Descriptions

Case Name	Coal Type	Recycle Configuration	Cooling Configuration	Biomass Percentage	CO₂ Venting
BRW00	I6	Recycle	Water	None	Sequestered
BRW00V	I6	Recycle	Water	None	Vented
BOW00	I6	Once-through	Water	None	Sequestered
BOW00V	I6	Once-through	Water	None	Vented
BRW15	I6	Recycle	Water	15%	Sequestered
BOW15	I6	Once-through	Water	15%	Sequestered
SRW00	PRB	Recycle	Water	None	Sequestered
SRW00V	PRB	Recycle	Water	None	Vented
SRA00	PRB	Recycle	Air	None	Sequestered
SRH00	PRB	Recycle	Hybrid	None	Sequestered
SOW00	PRB	Once-through	Water	None	Sequestered
SOW00V	PRB	Once-through	Water	None	Vented
SOA00	PRB	Once-through	Air	None	Sequestered
SOH00	PRB	Once-through	Hybrid	None	Sequestered
SRW15	PRB	Recycle	Water	15%	Sequestered
SRA15	PRB	Recycle	Air	15%	Sequestered
SRH15	PRB	Recycle	Hybrid	15%	Sequestered
SOW15	PRB	Once-through	Water	15%	Sequestered
SOA15	PRB	Once-through	Air	15%	Sequestered
SOH15	PRB	Once-through	Hybrid	15%	Sequestered

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Table 2: Unit Process Input and Output Flows

Flow Name	Plant Configuration					
	BRW00	BRW00V	BOW00	BOW00V	BRW15	BOW15
Inputs						
Hard Coal (Illinois No 6) [kg]	4.86	4.89	5.48	5.56	4.40	4.98
Switchgrass [kg]	0.00	0.00	0.00	0.00	0.78	0.88
Direct Land Use, IL [sqm]	0.00	0.00	0.00	0.00	0.52	0.59
Outputs						
F-T Diesel [kg]	1.00	1.00	1.00	1.00	1.00	1.00
F-T Naphtha [kg]	0.42	0.42	0.42	0.42	0.42	0.42
Electricity [MWh]	5.98E-04	1.19E-03	2.27E-03	3.10E-03	2.80E-04	1.83E-03
Carbon dioxide to Saline Aquifer (captured) [kg]	6.17	0.00	6.89	0.00	6.25	7.01
Carbon dioxide (air emission) [kg]	0.88	6.92	1.60	8.68	0.86	1.61

Flow Name	Plant Configuration							
	SRW00	SRW00V	SRA00	SRH00	SOW00	SOW00V	SOA00	SOH00
Inputs								
Rosebud Coal **[kg]**	6.26	6.25	6.47	6.36	7.02	7.17	7.01	7.01
Outputs								
F-T Diesel [kg]	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00
F-T Naphtha [kg]	0.42	0.42	0.42	0.42	0.42	0.42	0.42	0.42
Electricity [MWh]	0.00E+00	5.26E-04	0.00E+00	0.00E+00	1.30E-03	2.45E-03	1.09E-03	1.22E-03
Carbon dioxide to Saline Aquifer (captured) [kg]	6.43	0.00	6.62	6.51	7.14	0.00	7.14	7.14
Carbon dioxide (air emission) [kg]	0.76	7.17	0.94	0.84	1.42	8.84	1.42	1.42

Flow Name	Plant Configuration					
	SRW15	SRA15	SRH15	SOW15	SOA15	SOH15
Inputs						
Rosebud Coal **[kg]**	5.81	6.03	5.88	6.29	6.29	6.29
Switchgrass [kg]	1.03	1.06	1.04	1.11	1.11	1.11
Direct Land Use, MT [sqm]	2.06	2.14	2.08	2.23	2.23	2.23
Outputs						
F-T Diesel [kg]	1.00	1.00	1.00	1.00	1.00	1.00
F-T Naphtha [kg]	0.42	0.42	0.42	0.42	0.42	0.42
Electricity [MWh]	0.00E+00	0.00E+00	0.00E+00	1.09E-03	8.61E-04	1.01E-03
Carbon dioxide to Saline Aquifer (captured) [kg]	6.82	7.06	6.89	7.19	7.34	7.34
Carbon dioxide (air emission) [kg]	1.04	1.26	1.10	1.52	1.51	1.51

* **Bold face** clarifies that the value shown *does not* include upstream environmental flows.

DF_Stage3_O_CBTL_Zero_Sulfur_Diesel_2013.1.docx

Embedded Unit Processes

None.

References

NETL, 2013   NETL. (2013).Production of Zero Sulfur Diesel Fuel from Domestic Coal: Configurational Options to Reduce Environmental Impact. DOE/NETL-2012/1542.

NETL, 2011   NETL. (2011). Calculating Uncertainty in Biomass Emissions Model, Version 2.0 (CUBE 2.0): Model and Documentation. (DOE/NETL-2012/1538). Pittsburgh, PA: National Energy Technology Laboratory Retrieved from http://www.netl.doe.gov/energy-analyses/refshelf/PubDetails.aspx?Action=View&PubId=409.

Section III: Document Control Information

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