NETL Life Cycle Inventory Data
Process Documentation File

Process Name: CTL Plant Operation with Bituminous Coal Feed

Reference Flow: 1 kg of Fischer-Tropsch diesel (FTD)

Brief Description: Inputs and outputs for Fischer-Tropsch diesel production by a 50,000 barrel per day CTL plant using Illinois No. 6 bituminous coal feed. Includes scenarios for CCS and ATR (autothermal reforming). Naphtha is a co-product of all CTL cases.

Section I: Meta Data

Geographical Coverage: US **Region:** Midwest

Year Data Best Represents: 2009

Process Type: Energy Conversion (EC)

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

Allocation Applied: No

Completeness: All Relevant Flows Recorded

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 Pollutants	☐ Other
Releases to Water:	☒ Inorganic Emissions	☐ Organic Emissions	☐ Other
Water Usage:	☒ Water Consumption	☒ Water Demand (throughput)	
Releases to Soil:	☐ Inorganic Releases	☐ Organic Releases	☐ Other

Adjustable Process Parameters:

COALFEED	*Feedrate of coal to CTL plant (ton/day)*
DIESELFLOW	*Production rate of FT (Fischer-Tropsch) diesel (barrels/day)*
CAP_FAC	*Capacity factor of CTL plant (dimensionless)*
HHVI6COAL	*Higher heating value of Illinois No. 6 bituminous coal feedstock (MMBtu/ton)*

NAPFLOW	*Production rate of naphtha, a co-product (barrels/day)*
ELCFLOW	*Excess electricity generated by CTL plant (MWh/day)*
CO2SEQFLOW	*Mass capture rate of CO_2 from CTL plant (ton/day)*
CO2FLOW	*CO_2 released to atmosphere from CTL plant (ton/day)*
STACK_OUT	*Volumetric flow rate of stack gas from CTL plant (ft^3/hr)*
PROD_OUT	*Volumetric flow rate product gas from CTL plant (ft^3/hr)*
SOLIDFLOW	*Mass flow rate of solid waste from CTL plant (lb/hr)*
H2O_CCS	*Rate at which water use increases with addition of a CCS or CCS+ATR system (dimensionless)*
H2OFLOW_IN	*Water input to CTL plant (L/MMBtu)*
H2OFLOW_OUT	*Water output from CTL plant (L/MMBtu)*
HG_RECOVERY	*[dimensionless] Fraction of mercury that is not removed from flue gas and is released to air; based on 90% recovery.*

Tracked Input Flows:

Hard Coal (Illinois No. 6) [Intermediate]	*Bituminous coal input to CTL plant*

Tracked Output Flows:

FTD diesel	*1 kg of Fischer-Tropsch diesel production (reference flow)*
Naphtha (NETL)	*Mass of naphtha is co-produced per kg of Fischer-Tropsch diesel production*

Power [Electric Power]	*Excess electricity generated by CTL plant and sold to the grid*
CO_2 sent to sequestration	*Mass of CO_2 that is captured for sequestration per kg of FTD production*

Section II: Process Description

Associated Documentation

This unit process is composed of this document and the data sheet (DS) *DS_Stage3_O_CTL_2010.01.xls*, which provides additional details regarding calculations, data quality, and references as relevant.

Goal and Scope

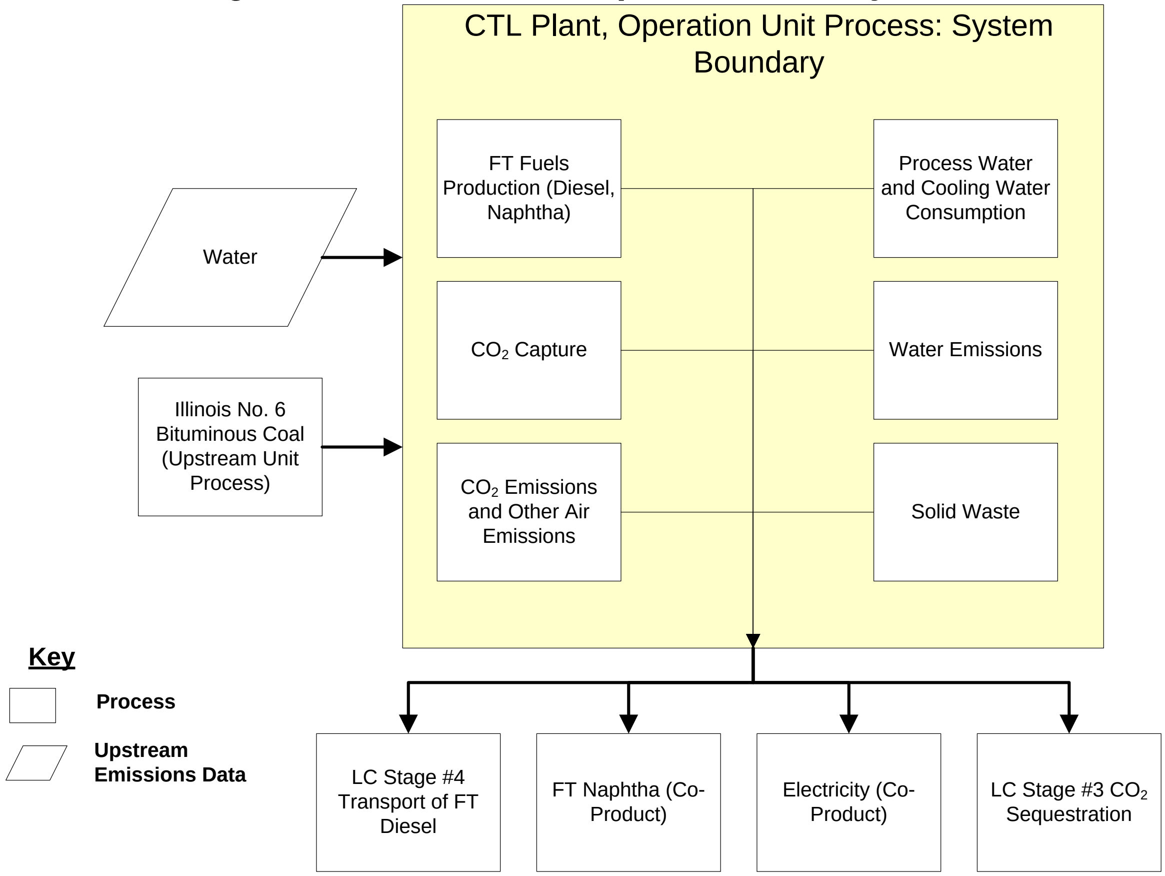
This unit process accounts for the operating activities for a CTL (coal to liquids) plant that uses Illinois No. 6 bituminous coal as a feedstock. The unit process is based on the reference flow of 1 kg of FT (Fischer-Tropsch) diesel production. The inputs to the process include water and bituminous coal. Water is used for cooling and other process-related utilities; water is assumed to enter the boundaries of this unit process having no upstream resource consumption or environmental emissions.

Illinois No. 6 bituminous coal is a fossil feedstock that is converted to diesel via gasification, followed by catalyzed synthesis; the resource consumption and emissions associated with the upstream production and delivery of Illinois No. 6 bituminous coal to the CTL plant are not included in the boundaries of this unit process, but are accounted for in separate unit processes. The outputs of this unit process are FTD (the reference flow of this unit process), naphtha (a co-product of this unit process), electricity, water, air emissions, and water emissions.

Boundary and Description

This unit process models the production of diesel fuel via coal gasification and FT synthesis. The energy inputs and outputs for this process were provided in the NETL CBTL Baseline Report (NETL 2009). This unit process describes activities that occur within Life Cycle (LC) Stage #3 of FTD production. The steps that precede this unit process include the extraction and processing of Illinois No. 6 bituminous coal in LC Stage #1, and the rail transport of Illinois No. 6 coal in LC Stage #2. The step that immediately follows this unit process is the pipeline transport of FTD in LC Stage #4. **Figure 1** provides an overview of the boundary of this unit process. Rectangular boxes represent relevant sub-processes, while trapezoidal boxes indicate upstream data that are outside of the boundary of this unit process. As shown, upstream resources and emissions associated with the production and delivery of coal are accounted for outside of the boundary of this unit process, while water is assumed to enter the boundary of the unit process with no upstream resources or emissions. The methods for calculating these operating activities are described below.

Figure 1: Unit Process Scope and Boundary



This unit process has 15 adjustable parameters, which enhance the versatility of this unit process, and allow the modeling of several scenarios. Unless noted otherwise, these adjustable parameters are based on data from the NETL baseline report on CBTL plants (NETL 2009). “COALFEED” is an adjustable parameter that is based on NETL data for CBTL plants and describes the rate at which the CTL plant consumes fossil feedstocks. “DIESELFLOW” is an adjustable parameter for the production rate of FTD. “CAP_FAC” is an adjustable parameter that describes the operating time of the CTL plant, and allows an accurate translation between instantaneous and annual flows of the CTL plant; the default value for “CAP_FAC” is 0.85 (i.e., 85 percent), which is specified in the baseline document for this unit process (NETL 2009) and accounts for plant downtime due to maintenance or interruptions in feedstock supply.

“HHVI6COAL” is an adjustable parameter that describes the higher heating value of Illinois No. 6 coal (NETL 2007) feedstock and is a necessary factor for the normalization of water use rates and stack flow rates, which are expressed on the basis of volume per MMBtu of feedstock input, to the production of one kg of FTD. “NAPFLOW” is an adjustable parameter that represents the mass of naphtha that is co-produced per kg of

FTD production. “ELCFLOW” is the excess electricity produced by the CTL plant. “CO2SEQFLOW” and “CO2FLOW” are adjustable parameters that represent the mass of CO_2 (carbon dioxide) that is captured for sequestration, and the mass of CO_2 that is released to the atmosphere, respectively. “STACK_OUT” is an adjustable parameter that represents the volumetric flow rate of the stack gas, and allows the calculation of SO_x (sulfur oxides) and NO_x (nitrogen oxides) emissions to air.

“PROD_OUT” is an adjustable parameter that represents the volumetric flow rate (in ft^3/hr) of the gas stream that exits the gasifier, and is used to calculate H_2S (hydrogen sulfide) emissions from the CTL plant. “SOLIDFLOW” is an adjustable parameter that represents the mass of ash and other solid wastes from the CTL plant. “H2O_CCS” is an adjustable parameter that represents the change in water input to the CTL plant when a CCS system is added; this change in water input is based on the NETL data for an IGCC power facility (NETL 2007). “H2OFLOW_IN” and “H2OFLOW_OUT” are adjustable parameters that are also based on NETL data for an IGCC (Integrated Gasification Combined Cycle) power facility (NETL 2007), and represent the water consumption of the CTL plant. Finally, “HG_RECOVERY” is the fraction of mercury in the stack gas that is not captured by environmental controls and is released to the atmosphere.

Naphtha is a co-product of FTD. This unit process does not use co-product allocation to apportion environmental burdens between FTD and naphtha. Rather, the mass of naphtha per production of one kg of FTD is shown as an output, and the recommended approach for co-product management is system expansion wherein naphtha that is co-produced by CTL plants which displaces naphtha that is produced by conventional routes. No life cycle data are available for the production of naphtha by conventional routes in the United States. Thus, for the life cycle of CTL fuels, NETL uses life cycle data for jet fuel to represent the conventional naphtha routes that are displaced by FT naphtha. That is, for every kg of FT naphtha that is produced by a CTL plant, one kg of jet fuel is displaced from the energy supply system. Alternatively, one could use the available GaBi profile for naphtha produced in the European Union. The displacement of conventional routes to naphtha production are outside the scope of this unit process; only the mass of naphtha that is co-produced per unit of FTD production is shown in this unit process.

Electricity is a co-product of FTD only for the CTL case in which no CCS or CCS+ATR technologies are used. The CTL plant of this unit process generates excess electricity at a rate of 35 MWh per day. To model the co-production of electricity from the CTL plant, NETL recommends system expansion with the displacement of grid electricity. Only the flow of co-product electricity is shown in this unit process; the reduction in environmental burdens (resource consumption and environmental emissions) due to the displacement of electricity is modeled outside of this unit process. For electricity displacement, NETL recommends a fuel profile as shown in the EPA eGRID database (EPA 2009).

The NETL CBTL baseline (NETL 2009) provides data for CO_2 emissions, H_2S emissions, and slag (solid waste) output. The inventories for other environmental emissions were determined from other sources. NO_x and PM emissions from CTL plants are based on data in the NETL baseline report on fossil energy plants (NETL 2007), which include data for an IGCC plant with bituminous coal as a feedstock. The mercury content in Illinois No. 6 bituminous coal is based on a study of mercury control technologies (Lee et al. 2006) and on the assumption that 90 percent of mercury is captured by environmental controls. Similarly, based on the composition of the Illinois No. 6 coal, the extent to which the gas streams of a CTL plant are cleaned, and baseline data provided by NETL studies on power generation (NETL 2007), NH_3 and Pb emissions were assumed to be negligible. Because no combustion processes are considered (e.g., no auxiliary boilers or other units are used for onsite energy generation) no other combustion-related emissions (such as carbon monoxide and hydrogen chloride) are calculated.

Water use was not given in the NETL CBTL Baseline report. An EIS on a smaller CTL plant was used as a data source for water input, consumption, and discharge (DOE 2007). Water increases due to CCS addition were based on the percent increase reported in the NETL baseline report on fossil energy plants (NETL 2007). This is noted at a data limitation as no distinction was made between water use increases with CCS and CCS + ATR. Emissions to water were determined based on the calculated water output and effluent water quality data from an IGCC plant (NETL 2002). Water emissions that were calculated as 0.1 ppm (parts per million) or greater were included in the water quality data for this unit process. This includes the waterborne emission of NH_3, cyanide (CN^-), nickel (Ni), selenium (Se), and zinc as significant waterborne outputs. Both the water quantity and quality data are considered data limitations for this unit process.

Solid waste is dominated by ash created during gasification, which is given in the NETL CBTL baseline report. Additionally, the FT process uses an iron catalyst that would contribute to solid waste as it degrades and is replaced. Data on FT catalyst productivity and loss (degradation) rate were taken from an NREL report of FT production of mixed alcohols from biomass (Phillips *et al.* 2007). When calculated, the loss of catalyst was less than 0.01 percent compared to slag output, and was therefore considered insignificant.

Properties of CTL plants that use Illinois No. 6 coal as a feedstock are shown in **Table 1**. **Table 2** provides a summary of modeled input and output flows. Additional details regarding input and output flows, including calculation methods, are contained in the associated DS sheet.

Table 1: Properties of Illinois No. 6 Bituminous Coal CTL Plants (NETL 2009)

Property	50,000 BPD CTL	50,000 BPD CTL w/ CCS	50,000 BPD CTL w/ CCS +ATR
Diesel Output (tonne/day)	4,633	4,635	4,639
Naphtha Output (tonne/day)	1,576	1,574	1,572
Coal Input (tonne/day)	19,703	19,245	20,897
CO2 Capture (tonne CO2e/day)	0	24,173	29,346
CO2 Emissions (tonne/day)	26,401	1,967	917
Solid Waste Flow (tonne/day)	2,036	1,989	2,160
Electricity output (MJ/day)	3,041,280	0	0

Table 2: Unit Process Input and Output Flows

Flow Name*	5,000 BPD BTL, switchgrass	5,000 BPD BTL w/ CCS, switchgrass	5,000 BPD BTL w/ CCS + ATR, switchgrass	Units (Per Reference Flow)
Inputs				
Water (unspecified) [Water]	33.4	35.0	37.9	L
Hard Coal (Illinois No. 6) [Intermediate]	**4.25**	**4.15**	**4.50**	**kg**
Outputs				
Fischer-Tropsch diesel (FTD)	1	1	1	kg
Naphtha (NETL) [Organic intermediate products]	0.340	0.340	0.339	kg
Power [Electric power]	0.656	0.000	0.000	MJ
Carbon dioxide [Inorganic intermediate products]	0.00	5.21	6.33	kg
Water (returned to receiving body) [Water]	13.96	14.62	15.86	kg
Carbon dioxide [Inorganic emissions to air]	4.844	0.361	0.168	kg
Nitrogen dioxide [Inorganic emissions to air]	6.57E-05	6.68E-05	7.26E-05	kg
Sulphur dioxide [Inorganic emissions to air]	7.15E-04	6.98E-04	7.57E-04	kg
Particulate Matter, unspecified [Other emissions to air]	3.96E-04	3.87E-04	4.20E-04	kg
Mercury (+II) [Heavy metals to air]	3.83E-08	3.74E-08	4.05E-08	kg
Hydrogen Sulfide [Other emissions to air]	1.71E-07	1.69E-07	1.59E-07	kg
Ammonium / ammonia [Inorganic emissions to fresh water]	1.23E-04	1.29E-04	1.40E-04	kg
Cyanide [Inorganic emissions to fresh water]	2.01E-06	2.10E-06	2.28E-06	kg
Nickel (+II) [Heavy metals to fresh water]	1.59E-06	1.67E-06	1.81E-06	kg
Selenium [Heavy metals to fresh water]	1.93E-06	2.02E-06	2.19E-06	kg
Zinc (+II) [Heavy metals to fresh water]	1.90E-06	1.99E-06	2.16E-06	kg
Solid Waste (unspecified) [Solid Waste]	3.74E-01	3.65E-01	3.96E-01	kg

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

Embedded Unit Processes

None.

References

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Section III: Document Control Information

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