# NETL Life Cycle Inventory Data
# Process Documentation File

**Process Name:** Coal/Biomass to Methanol to Gasoline

**Reference Flow:** 1 kg of FT Gasoline

**Brief Description:** The conversion of coal or coal and switchgrass to methanol and then to gasoline

## Section I: Meta Data

**Geographical Coverage:** United States **Region:** Midwest

**Year Data Best Represents:** N/A

**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:**

None.

**Tracked Input Flows:**

| | | |
|---|---|---|
| PRB coal | *[Technosphere]* | *PRB coal input* |
| Switchgrass (NETL) [Renewable primary products] | *[Technosphere]* | *Switchgrass input* |

| | |
|---|---|
| Natural gas burned in NGCC | *[Technosphere] Natural gas burned in NGCC* |
| Land use area, IL, no reversion [Land use] | *[Technosphere] Land use in Illinois from growing switchgrass* |

**Tracked Output Flows:**

| | |
|---|---|
| FT Gasoline [Valuable substance] | *Reference flow* |
| Carbon dioxide [Inorganic emissions to air] | *Emission to air* |
| Carbon dioxide [Inorganic intermediate products] | *Captured and compressed carbon dioxide, which will be injected into a saline formation* |
| FT LPG [Valuable substance] | *LPG is coproduced with gasoline* |
| Sulfur [Valuable substance] | *Sulfur is coproduced through recovery by the claus process* |

## Section II: Process Description

### Associated Documentation

This unit process is composed of this document and the data sheet (DS) *DS_Stage3_O_Coal_to_Methanol_to_Gasoline_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 the indirect liquefaction of PRB coal, or coal and switchgrass, by the C-MTG process. In this process the feedstocks are gasified, the syngas is reformed to produce methanol, and the methanol is converted to gasoline. The pure stream of carbon dioxide produced allows for carbon capture. The reference flow of this unit process is: 1 kg of FT Gasoline.

### Boundary and Description

**Figure 1** provides an overview of the boundary of this unit process and the inputs and outputs included in it. The feedstock fuels of PRB coal, or coal and switchgrass, are dried to remove excess moisture. They are then sent to a high-pressure, oxygen-blown Shell quench-type gasifier, which produces a stream of raw syngas. The high temperature entrained-bed gasifier uses a partial water quench and syngas cooler to cool the hot syngas stream and generate steam for the water gas shift reactors and power generation.

After passing through the water quench system, the syngas passes through a cyclone and a raw gas candle filter where a majority of the fine particles are removed and returned to the gasifier with the coal feedstock. Fines produced by the gasification system are recirculated to extinction. The dust removal efficiency of the cyclone is approximately 80 percent. Final dust removal is achieved in the wet scrubbing section, to lower the dust content of the syngas to <1 mg/Nm³, and to lower its halide content to <1 ppmv. The wet scrubbing system consists of a venturi scrubber followed by a packed bed wash column. A 3 percent by weight slurry bleed is fed to the primary wastewater treatment. Syngas is water saturated and leaves the wet scrubbing system at a temperature of 425 °F.

Syngas from the wet scrubber enters the sour shift and cooling section. In order to achieve a 2:1 ratio of $H_2$ to CO in the final syngas, approximately 55 to 60 percent of the syngas is shifted. The syngas to be shifted is heated in a feed/effluent exchanger to a temperature of 530 °F. This syngas passes through the 1$^{st}$ stage shift reactor where the shift reaction converts CO and $H_2O$ into $H_2$ and $CO_2$, and heats the outlet syngas to 895 °F. This syngas is then cooled to 505 °F for feeding the second stage

The syngas/steam mixture passes through the second stage shift reactor where the shift reaction converts additional CO and $H_2O$ into $H_2$ and $CO_2$, and heats the second-stage shift reactor outlet syngas to approximately 570 °F. After cooling, the shifted syngas from the second-stage shift reactor outlet mixes with the bypass syngas and is sent to low-temperature gas cooling then to the downstream Rectisol unit. A feature of this plant configuration is that $H_2S$ and $CO_2$ are removed within the same process, via the Rectisol unit.

$CO_2$-lean syngas with a $H_2$/CO ratio of 2:1 from the acid gas removal process is compressed from 490 psia to the synthesis loop operating pressure of 755 psia in the syngas compressor. The compressed synthesis gas will be mixed with the recycled make-up gas, heated to 400 ºF, and routed to the methanol reactor. The reactor is steam cooled and assumed to operate isothermally at 735 psia. In-line blowers, coolers, and knock-out drums are used within the synthesis loop to maintain pressure and remove crude methanol.

The basis for producing gasoline from synthesis gas via methanol is the Mobil methanol-to-gasoline (MTG) process. This proprietary process uses a zeolite catalyst to convert methanol to light liquid fuels, defined as less than C10 and some light gases (Meyers, 1984).

The MTG conversion is carried out in two steps. In the first step, crude methanol is vaporized and heated to reaction temperature by exchange with reactor effluent and then sent to the dimethyl ether (DME) reactor containing a dehydration catalyst (alumina) where approximately 75 percent of the methanol is dehydrated to an equilibrium mixture of methanol, DME, and water. The reaction is highly exothermic and the heat of reaction is 15-20 percent of the overall heat of reaction and is controlled by chemical equilibrium. In the second step, the equilibrium mixture is mixed with the recycle gas vapors separated from the three-phase product separator and passed into conversion reactors which contain a ZSM-5-based catalyst. The function of the recycle gas is to limit the temperature rise in the conversion reactor. In the conversion reactors the methanol and DME are essentially fully converted (99.99 percent) to gasoline-range hydrocarbons and water.

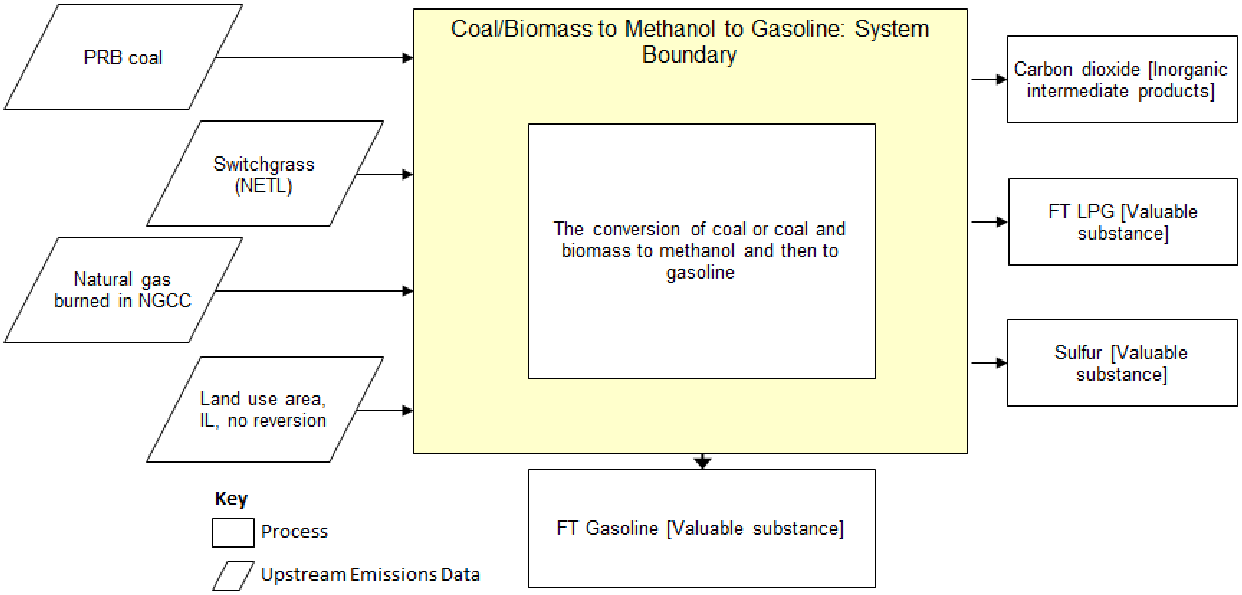
The heat from the product leaving the conversion reactors is retained to generate moderate- pressure steam in a boiler and to preheat the methanol feed to the DME reactor by heat exchange. The product is further cooled finally by air and water down to 100 ºF and then separated into three phases:

Gas Phase: Most (99.9 percent) of the gas phase is recycled to the MTG reactor inlet. The remaining gas is purged to the plant's fuel gas system.

Liquid Water Phase: The large volume of liquid water produced by the reactions contains about 0.1-0.2 wt% oxygenates (alcohols, ketones, and acids). The aqueous phase contains very little methanol and DME since essentially complete conversion of these compounds occurs over the catalyst.

Liquid Hydrocarbon Phase: The liquid hydrocarbon phase from the MTG reactor is called raw gasoline. The raw gasoline is processed in conventional fractionation columns to produce gasoline, LPG, and fuel gas. The produced gasoline contains 3-6 wt% durene (1, 2, 4, 5-tetramethyl benzene) while commercial gasoline specifications typically require less than 2.0 wt% durene. A heavy gasoline treatment (HGT) unit is provided to reduce the durene content to less than 2.0 percent by weight. The HGT unit fractionates raw gasoline into two parts. One part is a small volume, heavy fraction with a high durene concentration; the other part is a large volume, light fraction. The heavy fraction is heated and hydrotreated in a fixed-bed reactor (the HGT hydrotreator) to reduce its durene concentration. The hydrotreated heavy fraction is blended with the untreated light fraction to produce gasoline meeting the durene specification.

**Figure 1: Unit Process Scope and Boundary**




Three configurations are analyzed in this process. They are 100% coal with and without carbon dioxide capture, and 70% coal and 30% biomass with carbon dioxide capture. Key parameters for each of these configurations are provided in **Table 1**.

## Table 1: Parameters

| Parameter Name | Units | 100% Coal with Capture | 70% Coal with Capture | 100% Coal without Capture |
|---|---|---|---|---|
| PRB Coal | kg | 4.78 | 3.76 | 4.78 |
| Switchgrass | kg | 0.00 | 1.30 | 0.00 |
| Natural Gas | kg | 0.13 | 0.12 | 0.08 |
| LPG | kg | 0.15 | 0.14 | 0.15 |
| Sulfur | kg | 0.03 | 0.03 | 0.03 |
| $CO_2$ to Saline | kg | 4.56 | 4.55 | 0.00 |
| $CO_2$ to Air | kg | 0.88 | 0.91 | 5.30 |
| Land Use - Expected | $m^2$ | 0.00 | 0.88 | 0.00 |
| Land Use - Low | $m^2$ | 0.00 | 0.80 | 0.00 |
| Land Use - High | $m^2$ | 0.00 | 1.00 | 0.00 |

**Table 2: Unit Process Input and Output Flows**

| Flow Name | 100% Coal with Capture | 70% Coal with Capture | 100% Coal without Capture | Units (Per Reference Flow) |
|---|---|---|---|---|
| Inputs | | | | |
| PRB coal | 4.78 | 3.76 | 4.78 | kg |
| Switchgrass (NETL) [Renewable primary products] | 0 | 1.30 | 0 | kg |
| Natural gas burned in NGCC | 0.13 | 0.12 | 0.08 | kg |
| Land use area, IL, no reversion [Land use] | 0.00 | 0.88 | 0.00 | sqm |
| Outputs | | | | |
| FT Gasoline [Valuable substance] | 1.00 | 1.00 | 1.00 | kg |
| Carbon dioxide [Inorganic emissions to air] | 0.88 | 0.91 | 5.30 | kg |
| Carbon dioxide [Inorganic intermediate products] | 4.56 | 4.55 | 0 | kg |
| FT LPG [Valuable substance] | 0.15 | 0.14 | 0.15 | kg |
| Sulfur [Valuable substance] | 3.42E-02 | 2.63E-02 | 3.42E-02 | kg |

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

## Embedded Unit Processes

None.

## References


NETL 2013 — NETL. (2013). *Baseline Analysis of Subbituminous Coal and Biomass to Gasoline (Indirect Liquefaction by Methanol Synthesis)*.

Meyers 1984 — Robert A. Meyers, ed. in chief, *Handbook of Synfuels Technology,* ,TRW Chemical Technology Operations, Redondo Beach, California, 1984.

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 Retrived from http://www.netl.doe.gov/energy-analyses/refshelf/PubDetails.aspx?Action=View&PubId=409

## Section III: Document Control Information

**Date Created:** August 22, 2013

**Point of Contact:** Timothy Skone (NETL), Timothy.Skone@NETL.DOE.GOV

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Original/no revisions

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