NETL Life Cycle Inventory Data
Process Documentation File

Process Name:	Thermochemical Ethanol Plant Operation
Reference Flow:	1 kg of Ethanol (E95)
Brief Description:	Inputs and outputs for ethanol production by a thermochemical ethanol plant using cellulosic feedstocks. Includes addition of denaturant (gasoline) as 5 percent volume of final product.

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: Yes

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:

CASE_CS	*Allows the selection of corn stover feedstock (binary)*
CASE_SG	*Allows the selection of switchgrass feedstock (binary)*
FEED_CS_E100	*Feed rate of corn stover per unit production of pure ethanol (kg corn stover/kg ethanol)*

FEED_SG_E100	*Feed rate of switchgrass per unit production of pure ethanol (kg corn stover/kg ethanol)*

Tracked Input Flows:

Corn Stover	*Corn stover input to thermochemical ethanol plant*
Switchgrass	*Switchgrass input to thermochemical ethanol plant*
Gasoline (NETL) [Crude oil products]	*Gasoline input used as a denaturant in ethanol.*

Tracked Output Flows:

Ethanol (E95)	*1 kg of ethanol (E95) production (the reference flow of this unit process)*

Section II: Process Description

Associated Documentation

This unit process is composed of this document and the data sheet (DS) *DS_Stage3_O_EthanolThermochemical_2010.01.xls*, which provides additional details regarding calculations, data quality, and references as relevant.

Goal and Scope

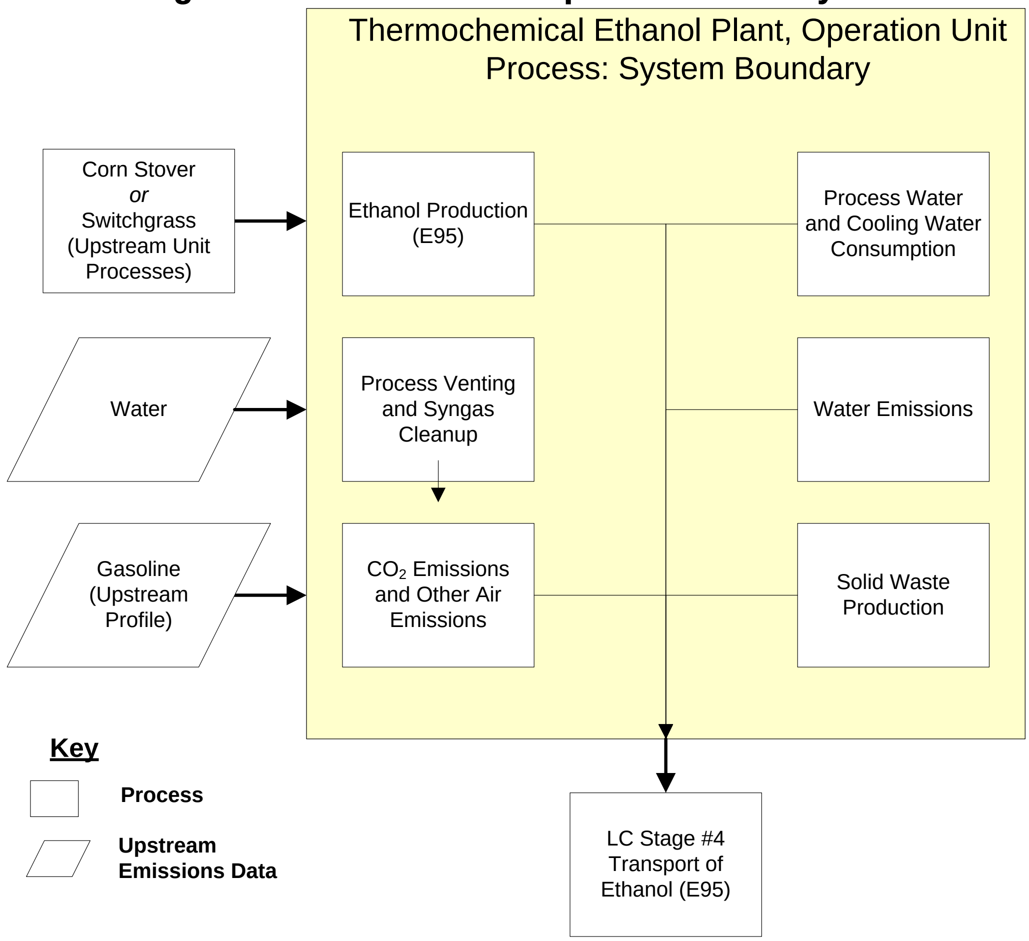
This unit process accounts for the operating activities for a thermochemical ethanol plant that uses cellulosic feedstock. All flows of this unit process are normalized to a reference flow for the production of 1 kg of ethanol that is denatured with gasoline at a concentration of 5 percent by volume (E95). The inputs to the process include water, corn stover or switchgrass, and gasoline. 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. Corn stover or switchgrass are two types of cellulosic feedstock that can be converted to ethanol via gasification followed by catalytic synthesis; the resource consumption and emissions associated with the upstream production and delivery of corn stover and switchgrass to the ethanol plant are not included in the boundaries of this unit process but are accounted for by upstream unit processes. Gasoline is used as a denaturant, making the product ethanol unfit for human consumption; the upstream resources and emissions associated with gasoline are not included in this unit process. The output of this unit process is E95 (a mixture that is 95 percent ethanol and 5 percent gasoline by volume), wastewater, and air emissions.

Boundary and Description

This unit process models the production of ethanol via a thermochemical ethanol plant that gasifies cellulosic feedstock and then catalytically converts the resulting synthesis gas to ethanol and other alcohols. The energy inputs and outputs of this process are provided in an NREL technoeconomic analysis of thermochemical ethanol production (Phillips 2007). This unit process describes activities that occur within Life Cycle (LC) Stage #3 of thermochemical ethanol production. The steps that precede this unit process include the production of corn stover or switchgrass in LC Stage #1, and the transport of corn stover or switchgrass in LC Stage #2. The step that immediately follows this unit process is the pipeline transport of ethanol 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 biomass 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.

This unit process has four adjustable parameters which allow the modeling of two types of cellulosic feedstocks used for thermochemical ethanol production. “CASE_CS” is an adjustable parameter that allows the selection of corn stover as the cellulosic feedstock to the thermochemical ethanol plant; the value of this parameter is “1” or “0”. “CASE_SG” is an adjustable parameter that allows the selection of switchgrass as the cellulosic feedstock to the thermochemical ethanol plant; the value of this parameter is “1” or “0”. Only one type of cellulosic feedstock can be modeled at a time, so “CASE_CS” and “CASE_SG” are mutually exclusive. “FEED_CS_E100” is an adjustable parameter that specifies the amount of corn stover per production of one kg of pure ethanol; the default value for this parameter is 3.12. “FEED_SG_E100” is an adjustable parameter that specifies the amount of switchgrass per production of one kg of pure ethanol; the default value for this parameter is 3.03.

Figure 1: Unit Process Scope and Boundary



The basis document for this unit process is a 2007 study conducted by NREL (National Renewable Energy Laboratory) that models the thermochemical conversion of biomass to ethanol. Hybrid poplar is the type of cellulosic feedstock used in the basis document (Phillips 2007); this unit process assumes that the operating characteristics of the thermochemical ethanol plant do not change significantly with changes in the type of cellulosic feedstock. The physical flows of the thermochemical ethanol plant are based on an ASPEN model that accounts for all process streams starting with the receipt of biomass feedstock and ending with production of ethanol. The properties of these streams were used to calculate the raw materials, utilities, and air emissions associated with the thermochemical production of ethanol.

The thermochemical ethanol plant of this unit process has an operating capacity of 61.8 MGY (million gallons per year). The first step at the thermochemical ethanol plant is feed handling and preparation, which dries the biomass feedstock. The next step is indirect gasification, which circulates synthetic olivine mineral between a gasifier and char combustor; the olivine supplies the heat that is necessary for the endothermic gasification reactions. Steam is injected into the gasifier to stabilize the flow of biomass and sand. The biomass converts to a mixture of syngas components (CO, H_2, CO_2, and

CH_4), tars, and a solid char that is composed of carbon residue. The gas that exits the gasifier is first cleaned with a scrubber, which removes particulates, ammonia, and tars. An additional gas-cleaning step uses an amine unit to recover carbon dioxide (CO_2) and hydrogen sulfide (H_2S) (the CO_2 is vented to the atmosphere and the H_2S is reduced to elemental sulfur and disposed as solid waste). It is necessary to remove these impurities in order to prevent contamination of the catalyst in the fixed bed reactor, the next step in the process, which converts the syngas to liquid alcohols. After alcohols are synthesized in the fixed bed reactor, they are routed to a flash separator, dehydrated using molecular sieves, and then fed to a distillation column that separates methanol and ethanol from the alcohols with higher molecular weights. A second distillation column separates the methanol and ethanol; the methanol is used to flush water from the molecular sieves and then recycle it to the entrances of the alcohol synthesis reactor. The design includes a conventional steam cycle that produces heat required for the gasifier and other operations, as well as electricity that can be used for internal operations or exported as a co-product. The integration of heat exchangers throughout the process allows the recovery of heat for the generation of steam.

The CO_2 emissions from the thermochemical ethanol plant include CO_2 from the vent stream of the synthesis gas cleanup process and the flue gas from the char combuster. Since the thermochemical ethanol plant of this unit process does not use fossil fuels, it is assumed that all CO_2 emissions from the unit process are biogenic. No data are available for the emission of methane, nitrous oxide, or other greenhouse gas emissions.

Other air emissions included in this unit process are hydrogen sulfide (H_2S) and ammonia (NH_3). Hydrogen sulfide is a byproduct of biomass gasification and must be removed from the process stream prior to the catalytic synthesis process. The syngas cleanup system removes the majority of the H_2S from the syngas stream and sends it to solid waste disposal. This unit process assumes that the composition of the flue gas from the syngas cleanup process is 10 ppm by volume (Philips et al 2007). The flow rate, temperature, pressure, and molar composition of bulk gases were used to calculate the mass of H_2S that is emitted by the syngas cleanup flue gas stream. Ammonia is emitted by the power generation processes at the thermochemical ethanol plant at a rate of 0.45 kg (1.0 lb) per hour (Phillips et al 2007). The flow rates of H_2S and ammonia emissions were converted to a basis of ethanol production by dividing them by the hourly flow rate of ethanol output.

Heavy metals such as lead and mercury are not present in the raw materials used by the thermochemical ethanol plant, and thus it is unlikely that significant levels of lead or mercury are released from this unit process.

The thermochemical ethanol plant uses water for steam generation and cooling towers. Water is lost through cooling tower evaporation and is also discharged as wastewater. The rates of water input are reported in the basis document as 1.94 kg of water per kg of ethanol production (Phillips et al 2007). The rates of wastewater discharge were estimated from output streams of the tar reforming/cleaning operations and the cooling system blowdown operations (Phillips et al 2007). When converted to a basis of ethanol production, the rate of wastewater discharge is 0.29 kg of wastewater per kg of ethanol production. The rate of wastewater discharge is less than the rate of water input because of water lost to evaporation.

The basis document (Phillips et al 2007) does not provide any data on the on the quality of wastewater from thermochemical ethanol plants. Furthermore, since thermochemical ethanol plants have not been commercialized, no primary data are available on the quality of wastewater discharges from such plants.

The properties of the thermochemical ethanol plant of this unit process 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 Thermochemical Ethanol Plant (Phillips 2007)

Property	Thermochemical Ethanol Plant
Raw Material Feedstock(s)	Corn Stover or Switchgrass
Ethanol output at 100% capacity, MGY (million L/yr)	61.8 (234)
Higher alcohol output at 100% capacity, MGY (million L/yr)	10.8 (40.9)
Geography	U.S. Midwest
Overall Plant Efficiency (% HHV)	47.4%

Table 2: Unit Process Input and Output Flows

Flow Name*	Thermo-chemical Ethanol Plant w/ Corn Stover Feedstock	Thermo-chemical Ethanol Plant w/ Switchgrass Feedstock	Units (Per Reference Flow)
Inputs			
Water (unspecified) [Water]	1.84	1.84	kg
Corn Stover	**2.98**	**0.00**	**kg**
Switchgrass	**0.00**	**2.89**	**kg**
Outputs			
Ethanol (E95)	1	1	kg
Carbon dioxide (biotic) [Inorganic emissions to air]	4.15	4.15	kg
Ammonia [Inorganic emissions to air]	1.54E-05	1.54E-05	kg
Hydrogen sulphide [Inorganic emissions to air]	3.06E-08	3.06E-08	kg
Water (returned to receiving body) [Water]	2.76E-01	2.76E-01	kg
Solid Waste (unspecified) [Solid Waste]	5.56E-04	5.56E-04	kg

* **Bold face** clarifies that the value shown *does not* include upstream environmental flows. Upstream environmental flows were added during the modeling process using GaBi modeling software, as shown in Figure 1.

Embedded Unit Processes

None.

References

Philips *et al*. 2007

Phillips, S., et al. 2007. *Thermochemical Ethanol via Indirect Gasification and Mixed Alcohol Sythesis of Lignocellulosic Biomass*. National Renewable Energy Laboratory, Golden, CO. NREL/TP-501-41168. http://www.nrel.gov/docs/fy07osti/41168.pdf (Accessed December 17, 2009).

Section III: Document Control Information

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Revision History:

Original/no revisions

How to Cite This Document: This document should be cited as:

NETL (2010). *NETL Life Cycle Inventory Data – Unit Process: Thermochemical Ethanol Plant Operation.* U.S. Department of Energy, National Energy Technology Laboratory. Last Updated: February 2010 (version 01). www.netl.doe.gov/energy-analyses (http://www.netl.doe.gov/energy-analyses)

Section IV: Disclaimer