NETL Life Cycle Inventory Data
Process Documentation File

Process Name:	Petroleum Refinery: Gasoline, Diesel, Kerosene-Based Jet Fuel Products
Reference Flow:	1 kg of Refinery Product
Brief Description:	Operations of an industry average U.S. domestic petroleum refinery, adjustable to produce one of three refinery products under one of 14 fuel production scenarios. Purchased energy, water, emissions to air and water, and water use are inventoried.

Section I: Meta Data

Geographical Coverage:	US	**Region:**	US
Year Data Best Represents:	2005; 2030		
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:

FENERGY	*Fraction of refinery energy attributable to a chosen refinery product (dimensionless)*
FH2	*Fraction of hydrogen consumption attributable to a chosen refinery product (dimensionless)*

DELTA_GHGA	*Adjusts refinery CO_2 (carbon dioxide) emissions according to a change in crude oil source (dimensionless)*
APIGRAVITY	*Density of crude oil feedstock, in units of API degrees (API degrees)*
SULFURCONTENT	*Sulfur content of crude oil feedstock (percent)*
RHO_BBL	*Density of refinery product (kg/bbl)*

Tracked Input Flows:

Crude Oil NETL [Crude oil products]	*Crude oil feedstock*
Hard coal free customer USA [Hard coal products]	*Coal purchased for energy generation at the refinery*
Natural gas USA [Natural gas products]	*Natural gas purchased for energy generation at the refinery*
Power [Electric power]	*Electricity purchased for utility requirements at the refinery*
Steam mix (kg) [Thermal energy]	*Steam purchased for utility requirements at the refinery*

Tracked Output Flows:

Refinery product [Crude oil products]	*1 kg of petroleum refinery product (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_Petroleum_Refinery_2010.02.xls*, which provides additional details regarding calculations, data quality, and references as relevant.

Goal and Scope

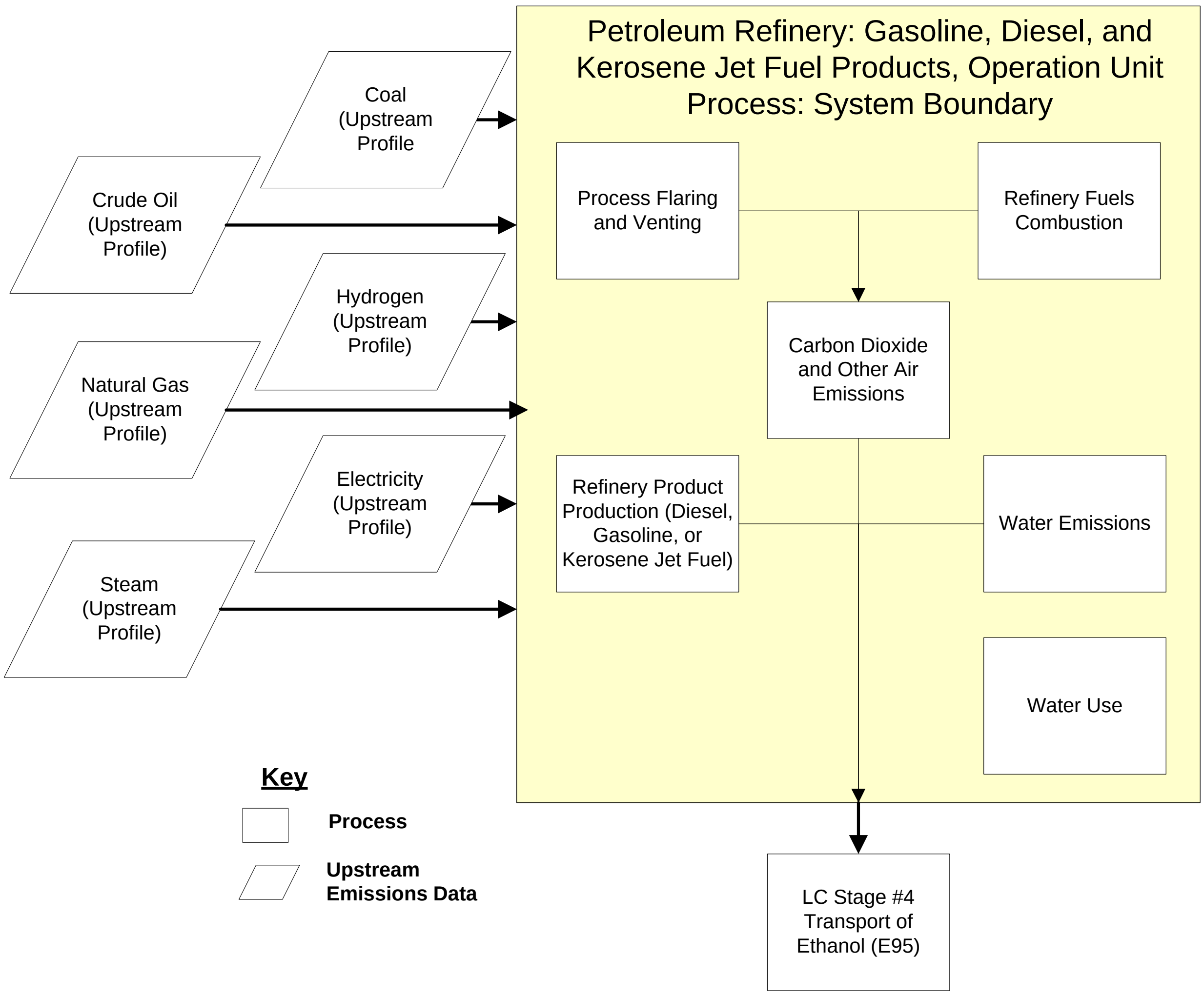
This unit process accounts for the operating activities of an industry average petroleum refinery operating in the United States during a single year (2005 or 2030). The process is based on the reference flow of 1 kg of refinery product, and includes parameters that allow the modeling of gasoline, diesel, and jet fuel production. Adjustable parameters also enable the modeling of 14 different fuel production scenarios, each using different crude oil sources and/or temporal boundaries (2005; 2030). The tracked inputs to the process include crude oil, coal, natural gas, steam, and electricity. 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. Crude oil is transformed into a variety of products via physical separation and chemical transformation processes; the resource consumption and emissions associated with the upstream production and delivery of crude oil from various country mixes are not included in the boundaries of this unit process but are accounted for by upstream unit processes. The outputs of this unit process are refinery product (gasoline, diesel, or jet fuel, depending on the chosen parameters) water, air emissions, and water emissions.

Boundary and Description

This unit process models the production of refinery products (gasoline, diesel, or jet fuel) by a conventional petroleum refinery. The energy inputs and outputs for this process were provided in the NETL Petroleum Baseline Report (NETL 2008). This unit process describes activities that occur within Life Cycle (LC) Stage #3 of a petroleum refinery. The baseline data used for the development of this unit process are representative of 2005 refinery operations using the U.S. national average crude oil supply, but by incorporating parameters that adjust greenhouse gas emissions and some other air pollutants (SO_2, PM10, NOx, and NH_3) according to crude oil quality, this unit process can be used to model a wide range of scenarios of crude oil quality. The steps that precede this unit process include the extraction of crude oil in LC Stage #1 and mixed-mode transport of crude oil in LC Stage #2. The step that immediately follows this unit process is the pipeline transport of refinery product diesel 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 crude oil, coal, natural gas, steam, and electricity 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 6 adjustable parameters, which allow the modeling of three refinery products (gasoline, diesel, and jet fuel) and crude oil with varying density and sulfur characteristics. “FENERGY” is an adjustable parameter that allocates the energy use of the refinery among refinery co-products and is based on the relative volumetric throughput of each co-product for refinery sub-process (e.g., atmospheric distillation, vacuum distillation, hydrotreating, isomerization, etc.) and the energy consumption of each refinery sub-process. “FH2” is an adjustable parameter that allocates the hydrogen use of the refinery among refinery co-products and is based on the relative hydrogen demands of each refinery co-product. More details on the development of “FENERGY” and “FH2” are provided in the NETL baseline study on petroleum refining (NETL 2008). “DELTA_GHGA” is an adjustable parameter that adjusts the GHG (greenhouse gas) emissions from the refinery based on changes in crude oil quality (sulfur content and density). “APIGRAVITY” is an adjustable parameter that specifies the density of crude oil input; the values of “APIGRAVITY” used by this unit process are from NETL’s source-specific petroleum refining model (NETL 2009) and range from 22.6 (Venezuela heavy crude) to 44.8 (Algeria crude). The units for “APIGRAVITY” are API degrees, where low values represent heavy crude oil and high values represent light crude oil. "SULFURCONTENT" is an adjustable parameter that specifies the sulfur content (in percent by weight) in crude oil; the values of "SULFURCONTENT" used by this unit process are from NETL's source-specific petroleum refining model (NETL 2009) and range from 0.1 (Algeria crude) to 3.0 (Mexico crude). "RHO_BBL" is an adjustable parameter that specifies the density of refinery products and allows the translation of volumetric flows to the basis of mass of production; the value of "RHO_BBL" is 117.3 kg/barrel for gasoline, 134.6 kg/barrel for diesel, and 128.1 kg/barrel for jet fuel. All of the adjustable parameters are located on the Scenarios tab of the DS and utilized in background calculations in other tabs of the DS to support the results on the Data Summary tab. While these parameters are adjustable, the UP has been preloaded with values for 14 difference crude oil source mixes and the three refinery products of interest (gasoline, diesel, and jet fuel).

The crude type and product are selected on the Scenarios tab of the DS. This selection retrieves the adjustable parameter values, which are then used in other supporting calculations on background tabs in the DS to determine the GHG emissions for the refinery. However, by using additional energy and hydrogen allocation factors as specified in the NETL petroleum baseline study (NETL 2008) and additional greenhouse gas emission factors as specified in the NETL source-specific refinery model, the refinery operations for other refinery products (including residual fuel oil, coke, light ends, and heavy ends) could also be modeled by this unit process with some adjustments to the background calculations and allocation factors.

Data for GHG emissions and purchased energy use are taken exclusively from the NETL petroleum baseline study, and details on the development of energy and greenhouse gas data are provided in the documentation of the NETL petroleum baseline study (NETL 2008). NETL expanded upon the Petroleum Baseline study by developing heuristics that adjust the GHG emissions from refinery operations based on changes in crude oil quality (NETL 2009). The heuristics were developed by performing linear regression on the relationships between crude quality and the known throughput of key refinery operations. For a more detailed explanation of these heuristics, see "An Evaluation of the Extraction, Transport and Refining of Imported Crude Oils and the Impact on Life Cycle Greenhouse Gas Emissions" (NETL 2009). The development of other environmental metrics, including criteria air pollutants and other air emissions, water use, and water quality are discussed below.

An attempt was made to develop these heuristics based on refinery-specific data for each of the 148 operating petroleum refineries in the United States using data extracted from EPA's 2005 National Emissions Inventory (EPA 2009a). Due to a lack of data for crude oil quality as received by individual refineries, no significant trends between crude oil quality and emissions were identified for refinery-specific data. Since strong correlations could not be determined based on refinery-specific data, data for the entire U.S. petroleum sector was used to develop correlations between crude oil quality and non-GHG emissions. Annual data from 1990 through 2008 (EPA 2009b) was plotted versus the average crude oil quality, refinery fuel consumption, and refinery output for each year from 1990 through 2008 (EIA 2009). Since the data for crude oil quality was at the same level of detail as the sector-wide emissions, the emissions reported by the entire U.S. petroleum sector demonstrate relatively strong trends between crude quality and four non-greenhouse gas emissions: sulfur dioxide (SO_2), ammonia (NH_3), nitrogen oxides (NO_X), and particulate matter < 10 microns (PM_{10}). The sector trends (EPA 2009b) for these four emissions were applied to the refinery-specific data (EPA 2009a) in order to adjust non-greenhouse gas refinery emissions according to crude oil quality. The emissions of other air pollutants (volatile organic compounds, carbon monoxide, lead, and mercury) did not exhibit strong relationships between crude quality and sector-wide emissions, and thus no adjustments are made to these emissions. The 2005 refinery emissions of volatile organic compounds, carbon monoxide, lead, and mercury are used to represent all scenarios of this unit process.

Detailed water use data, including water consumption data, were not found to be publicly available. Note that water use and consumption are not tracked under the National Pollutant Discharge Elimination System (NPDES) data reporting program. Several references for refinery water use were identified; however, review of those documents revealed that each relied on a single document from which refinery water use values were derived (Gleick 1994). Water consumption data for traditional refining, as well as refining that incorporates reforming and hydrogenation, are included in that report, and were scaled according to the proportion of US refineries using traditional (7 percent) versus reforming and hydrogenation pathways (93 percent) in 2007, according to ANL (2008).

In order to estimate the emissions of water quality constituents from the refinery, water quality emissions data from National Pollutant Discharge Elimination System (NPDES) permitting reports were reviewed for a total of 49 presently operational US refineries for which NPDES reporting data are readily available (EPA 2009c). Of those 49 refineries, 34 were found to have NPDES water quality data that were useful for this analysis.

As needed, reported water quality emissions data were converted to a concentration basis (e.g., mg of constituent per L of water). Correlative analysis was completed on the resulting data to evaluate trends among the concentration of the various indicated wastewater constituents and wastewater volume, refinery capacity, refinery complexity, API gravity, and sulfur percent, as defined for the analysis of refinery air quality constituents. However, no significant or discernable trends were indicated. Therefore, average water quality emissions values were calculated for each constituent, according to the emissions values indicated in the NPDES permit reports (EPA 2009c).

The properties of the 2005 baseline petroleum refinery of this analysis are shown in **Table 1**. Parameter values for 42 unique pathways, including those shown in Table 1, are provided in the DS sheet for this unit process. **Table 2** provides a summary of modeled input and output flows for the 2005 baseline petroleum refinery. Additional details regarding input and output flows, including calculation methods, are contained in the associated DS sheet.

Table 1: Properties of 2005 U.S. National Average Petroleum Refinery

	2005 National Average, Gasoline	2005 National Average, Diesel	2005 National Average, Jet Fuel
Crude oil average API Gravity (API degrees)	30.4	30.4	30.4
Crude oil average sulfur content (%w)	1.42%	1.42%	1.42%
Share of refinery energy to co-products (proportion)	0.474	0.249	0.0612
Share of refinery hydrogen use to co-products (proportion)	0.430	0.377	0.0902
Product density (kg/barrel)	117	135	128

Table 2: Unit Process Input and Output Flows

Flow Name*	2005 National Average, Gasoline	2005 National Average, Diesel	2005 National Average, Jet Fuel	Units (Per Reference Flow)
Inputs				
Crude Oil NETL [Crude oil products]	1.00	1.00	1.00	kg
Hard coal free customer USA [Hard coal products]	5.25E-05	4.76E-05	3.01E-05	kg
Hydrogen [Inorganic intermediate products]	1.45E-03	2.20E-03	1.36E-03	kg
Natural gas USA [Natural gas products]	2.58E-02	2.79E-02	1.75E-02	kg
Power [Electric power]	5.18E-05	4.70E-05	2.97E-05	MWh
Steam mix [Thermal energy]	1.14E-01	1.03E-01	6.54E-02	MJ
Water [Water]	1.68	1.47	1.54	kg
Outputs				
Refinery product [Crude oil products]	1	1	1	kg
Aluminum [Heavy metals to fresh water]	5.37E-07	4.68E-07	4.92E-07	kg
Ammonia [Inorganic emissions to air]	3.68E-06	3.34E-06	2.11E-06	kg
Ammonia [Inorganic emissions to fresh water]	5.81E-06	5.07E-06	5.32E-06	kg
Antimony [Heavy metals to fresh water]	4.76E-09	4.15E-09	4.36E-09	kg
Arsenic (+V) [Heavy metals to fresh water]	1.52E-08	1.33E-08	1.39E-08	kg
Cadmium (+II) [Heavy metals to fresh water]	1.46E-09	1.27E-09	1.34E-09	kg
Carbon dioxide [Inorganic emissions to air]	3.22E-01	3.06E-01	1.93E-01	kg
Carbon monoxide [Inorganic emissions to air]	1.27E-04	1.15E-04	7.26E-05	kg
Chromium (unspecified) [Heavy metals to fresh water]	2.63E-08	2.29E-08	2.41E-08	kg
Copper (+II) [Heavy metals to fresh water]	2.20E-08	1.92E-08	2.02E-08	kg
Cyanide [Inorganic emissions to fresh water]	4.32E-08	3.76E-08	3.96E-08	kg
Iron [Heavy metals to fresh water]	1.12E-06	9.76E-07	1.03E-06	kg
Lead (+II) [Heavy metals to fresh water]	5.15E-08	4.49E-08	4.71E-08	kg
Lead (+II) [Heavy metals to air]	1.43E-09	1.29E-09	8.18E-10	kg
Mercury (+II) [Heavy metals to fresh water]	2.58E-10	2.25E-10	2.36E-10	kg
Mercury (+II) [Heavy metals to air]	2.16E-10	1.96E-10	1.24E-10	kg
Methane [Organic emissions to air (group VOC)]	2.82E-04	2.56E-04	1.62E-04	kg
Nickel (+II) [Heavy metals to fresh water]	4.08E-07	3.56E-07	3.74E-07	kg
Nitrogen dioxide [Inorganic emissions to air]	2.05E-04	1.86E-04	1.17E-04	kg
Nitrous oxide (laughing gas) [Inorganic emissions to air]	5.48E-06	4.97E-06	3.14E-06	kg
NMVOC (unspecified) [Group NMVOC to air]	1.54E-04	1.40E-04	8.83E-05	kg
Particulate Matter, unspecified [Other emissions to air]	3.58E-05	3.25E-05	2.06E-05	kg

Phosphorus [Inorganic emissions to fresh water]	5.13E-07	4.47E-07	4.70E-07	kg
Silver [Heavy metals to fresh water]	4.64E-09	4.05E-09	4.25E-09	kg
Sulphur dioxide [Inorganic emissions to air]	2.70E-04	2.45E-04	1.55E-04	kg
Zinc (+II) [Heavy metals to fresh water]	7.08E-07	6.17E-07	6.49E-07	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

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Section III: Document Control Information

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