Petroleum Refinery Life Cycle Inventory Model (PRELIM)

PRELIM v1.0

User guide and technical documentation

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1.3 Acknowledgement

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1.4 Acronyms and abbreviations

%wt +°C: Percentage on weight basis e.g., 1gram per kilogram equals 0.1 %wt Temperature over specific value in Celsius
AGO: Atmospheric gas oil
AR: Atmospheric residue
CCQMP: Canadian Crude Quality Monitoring Program
CVRSMD: Coefficient of variation of the root-mean-square deviation
FCC: Fluid catalytic cracker
GHG: Greenhouse gas
GO-HC: Gas oil hydrocracker
H: Hydrogen
HHV: High-heating value
HTSD: High Temperature Simulated Distillation
HVGO: Heavy vacuum gas oil
iC5: Isopentane
KW: Watson characterization factor
LCA: Life cycle assessment
LHV: Low-heating value
LPG: Liquefied petroleum gas
LSR: Light straight run
LVGO: Light vacuum gas oil
MCF: Million cubic feet
MCR: Micro carbon residue
NG: Natural gas
PFD: Process flow diagram
PRELIM: Petroleum Refinery Life Cycle Inventory Model
RFG: Refinery fuel gas
S: Sulphur
SD: Standard Deviation
SMR: Steam methane reforming
SR: Straight run
t: (metric) tonne
TBP: Temperature boiling point
ULSD: Ultra-low sulphur diesel
Vol: Volume
VR: Vacuum residue

1.5 Changes and updates from previous versions of PRELIM

A previous version of PRELIM was published in 2012 in Environmental Science & Technology (Abella et al., 2012). This version of PRELIM (version 1.0) was released in March 6, 2015.

1.6 Working with PRELIM: a quick reference guide

This section provides a summary of the documentation to give the user a quick overview of PRELIM's main features to start using the model within minutes.

1.6.1 Technical requirements

PRELIM is constructed using Microsoft Excel and has successfully been tested with Microsoft Excel 2007 and more recent versions for both Windows and Macintosh computers.

PRELIM is a complex Excel spreadsheet that can be resource-intensive for some computers and results in Excel instability. If this happens, one easy fix is to restart your computer prior to launching the PRELIM model.

1.6.2 Running a crude oil assay from the assay library

The `Main Input & Output` worksheet contains all the main options to run the model for one or all crude assays available in the model.

The user can run a crude assay in PRELIM by selecting an assay in the dropdown menu of the `Basic input` section. The properties of the active assay are available below in the PRELIM format (see section 2.3.5 to learn about the format), and main results in terms of energy use and GHG emissions are displayed in real time to the right of the input cells in the `Main results` box.

Detailed results are available on the `Results Single Assay` worksheet. Even more detailed results for each of the two refinery configurations are displayed on the `CokingRefinery Detailed Results` and the `HydroRefinery Detailed Results` worksheets.

The user can also run the model for all crude assays available in the assay inventory by clicking the `All assays in inventory` button available in the `Additional inputs and options` section.

A set of dropdown menus and checkboxes listed in the `Additional inputs and options` section of the `Main Input & Output` worksheet allows the user to override the default refinery configuration and specify enabled process units, the source of the natural gas consumed in the refinery, the electricity source, the allocation method, allocated products, the heating value, and the global warming potential of GHG emissions used in the model.

1.6.3 Advanced options

The `Expert Inputs` worksheet provides the user with two additional tools:

- A blank assay to input a custom assay in the PRELIM format; and
- A crude blender tool to create a custom assay from existing crude assays.

The resulting custom assays are then made available in the top dropdown menu of the `Main Input & Output` worksheet.

2 Introduction

The Petroleum Refinery Life Cycle Inventory Model (PRELIM) is a mass and energy based process unit-level tool for the estimation of energy use and greenhouse gas (GHG) emissions associated with processing a variety of crude oils within a range of configurations in a refinery. PRELIM aims to inform policy analysis by providing a transparent model including data, assumptions and detailed results.

This user guide and technical documentation introduces PRELIM and details the calculations and data sources used in the model. First, PRELIM's motivation and the model construction are described. Then, the user guide introduces the PRELIM interface and outlines how the user can interact with each of the worksheets. Next, the technical documentation explains the calculations involved in each of the calculation worksheets and details the methods and assumptions used to estimate the energy use and associated GHG emissions for each process unit and at a total refinery level.

The PRELIM model was built using Microsoft Excel to ensure transparency and maximum accessibility. PRELIM is freely available for download from the Life Cycle Assessment of Oil Sands Technologies research group website (University of Calgary): http://ucalgary.ca/lcaost/prelim.

2.1 Model motivation

PRELIM was developed to offer a free, flexible, transparent, and open-source tool that captures the impact of crude oil quality and refinery configuration on energy use and GHG emissions, combining a life cycle approach with linear programming modeling methods to overcome existing life cycle model limitations. Further documentation and examples can be found in Abella et al. (2012).

As both US and Canadian refineries have shifted to accommodate increased use of different crudes (e.g., oil sands derive products, Bakken light crudes). It is possible to estimate the energy and GHG emissions from any crude oil produced globally. The potential use of PRELIM includes running scenarios for policy analysis purposes to explore the implications of processing crudes of different qualities and in different refinery configurations as an example. The target audience includes researchers and decision-makers from government, academia, and industry.

2.2 PRELIM model goals

The release of the PRELIM model as an open source tool had the following objectives:

1. Build a rigorous, engineering-based model of energy use and GHG emissions from oil processing in a refinery, using a life cycle approach;
2. Work with refinery experts to validate assumptions and data;
3. Use detailed data (public wherever possible) to provide maximum accuracy and flexibility;
4. Document sources of all equations, parameters, and input assumptions;
5. Provide a model that is free to access, use, and modify by any interested party; and
6. Provide a data framework that can be integrated as a module in a Well-To-Wheel (i.e., life cycle) model.

As stated, one of the goals of PRELIM is the generation of comprehensive documentation to allow effective use and modification of the tool by the user. Data input and features that can be overridden are documented in each worksheet. This document explains PRELIM's calculations and assumptions and provides information on model data sources.

2.3 PRELIM model construction

2.3.1 Software

PRELIM is a stand-alone, spreadsheet-based model that operates in Microsoft Excel. It has successfully been tested with Microsoft Excel 2007, 2010, and 2013 for PC and Macintosh.

PRELIM is a complex Excel spreadsheet that can be resource-intensive for some computers and results in Excel instability. If this happens, one easy fix is to restart your computer prior to launching the PRELIM model.

2.3.2 Color-coding

The PRELIM model uses a color-coding system to allow the user to easily navigate the model: inputs and results worksheet tabs have are red, calculations worksheet tabs are blue, and data and constant worksheet tabs are green.

In addition, the following color-coding is used in the spreadsheets:

- **A cell with a red background** indicates that this value is a constant and can be overridden by expert users in the `Constants` worksheet;
- **A value with a white background** typically indicates a calculated value; and
- the `Process Correlations` worksheet uses a specific color-coding that is indicated at the top of the spreadsheet.

Some color-shading is also used in this document to help navigate the documentation:

- `This format` refers to a worksheet in the PRELIM model; and
- `This format` refers to a header or an option in the PRELIM model.

System boundary

The system boundary of PRELIM includes all major process units used in a refinery to process oil. Twenty-four process units can be enabled using one of the ten available configurations. The system boundary also includes the upstream energy use and GHG emissions associated with input energy sources (i.e., electricity, natural gas).

Upstream (e.g., extraction, processing, transport) and downstream (e.g., transport, use of transportation fuel in a vehicle) energy and GHG emissions are not included in PRELIM.

The model focuses on combustion emissions. Fugitive GHG emissions are not considered in the current version of PRELIM.

2.3.3 Modeling approach

PRELIM is built using a systems level approach by employing refinery linear modelling methods to represent a range of possible configurations reflecting currently operating refineries in North America. The systems level approach frames the level of detail for modelling in order to obtain a tool of wide applicability in the assessment of refinery energy use and GHG emissions for crudes of different quality, and allows for the easy incorporation of model results in Well-To-Wheel analyses. The refinery linear modelling methods allow for process unit and overall refinery mass balances to overcome the lack of crude specificity of previous life cycle models and to explore the use of alternative life cycle inventory allocation methods at the refinery sub-process level. Since the model structure allows for the integration of key life cycle assessment concepts (i.e., goal and scope definition, functional unit, and allocation) as recommended by the International Standard ISO 14041, the model is titled the Petroleum Refinery Life-cycle Inventory Model.

The two main inputs required to run PRELIM are the refinery configuration and the crude quality information (described below in sections 2.3.5 and 2.3.6).

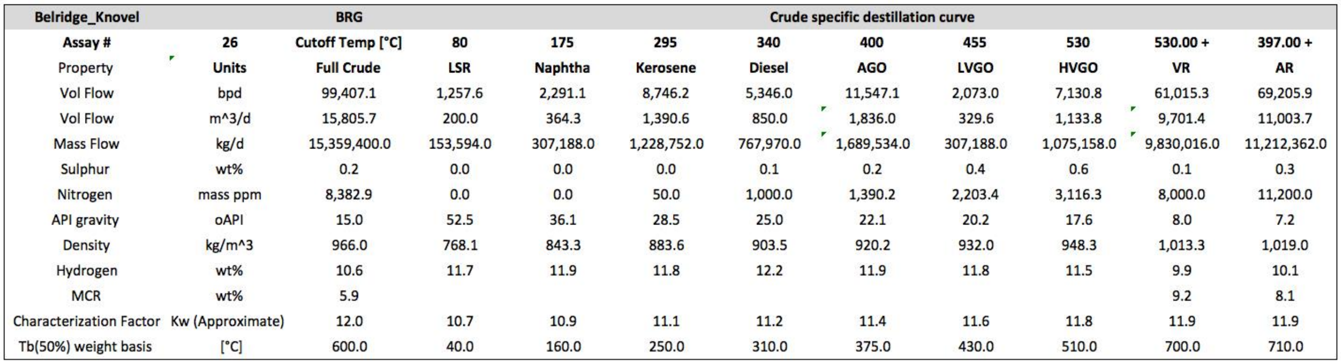
2.3.4 Model structure – refinery configuration

PRELIM can simulate up to ten specific refinery configurations. All configurations include crude distillation, hydrotreating, and naphtha and catalytic reforming processes. Additional process units can be enabled including gas oil hydrocracking, fluid catalytic cracking, coking, and residual hydrocracking. There are two major refinery configurations: coking refinery and hydrocracking refinery (also called hydro refinery). The first four configurations (0, 1, 2, and 3) will generate identical results for both major refinery types as these configurations use the same hydroskimming and medium conversion process units (see section 3.1.1.2.3 for more details). Configurations 4, 5, and 6 are specific to the coking refinery and configurations 7, 8, and 9 are specific to the hydro refinery. PRELIM also includes supporting process units such as steam methane reforming, and pollution control units such as flue gas treatment and sulphur recovery.

Figure 3 and Figure 4 in section 4.2.2 display a process flow diagram (PFD) for each of the major refinery configurations (note that supporting process units are not displayed on the PFDs).

2.3.5 The PRELIM crude assays

PRELIM uses crude oil quality information as the starting point for model calculations. This information is supplied as a crude oil "assay" and must to be entered in a specific format. The PRELIM format uses five parameters to characterize the quality of the whole crude: crude distillation curve, sulphur content, API gravity, carbon residue content, and hydrogen content. The crude is also separated into nine fractions associated with a specific cut-temperature. The five quality parameters are also specified for each of the nine fractions in addition to the whole crude. A total of 62 parameters are input to the model for each crude. Figure 1 provides an example of a crude oil assay.



Belridge_Knovel		BRG				Crude specific destillation curve					
Assay #	**26**	**Cutoff Temp [°C]**	**80**	**175**	**295**	**340**	**400**	**455**	**530**	**530.00 +**	**397.00 +**
Property	**Units**	**Full Crude**	**LSR**	**Naphtha**	**Kerosene**	**Diesel**	**AGO**	**LVGO**	**HVGO**	**VR**	**AR**
Vol Flow	bpd	99,407.1	1,257.6	2,291.1	8,746.2	5,346.0	11,547.1	2,073.0	7,130.8	61,015.3	69,205.9
Vol Flow	m^3/d	15,805.7	200.0	364.3	1,390.6	850.0	1,836.0	329.6	1,133.8	9,701.4	11,003.7
Mass Flow	kg/d	15,359,400.0	153,594.0	307,188.0	1,228,752.0	767,970.0	1,689,534.0	307,188.0	1,075,158.0	9,830,016.0	11,212,362.0
Sulphur	wt%	0.2	0.0	0.0	0.0	0.1	0.2	0.4	0.6	0.1	0.3
Nitrogen	mass ppm	8,382.9	0.0	0.0	50.0	1,000.0	1,390.2	2,203.4	3,116.3	8,000.0	11,200.0
API gravity	oAPI	15.0	52.5	36.1	28.5	25.0	22.1	20.2	17.6	8.0	7.2
Density	kg/m^3	966.0	768.1	843.3	883.6	903.5	920.2	932.0	948.3	1,013.3	1,019.0
Hydrogen	wt%	10.6	11.7	11.9	11.8	12.2	11.9	11.8	11.5	9.9	10.1
MCR	wt%	5.9								9.2	8.1
Characterization Factor	Kw (Approximate)	12.0	10.7	10.9	11.1	11.2	11.4	11.6	11.8	11.9	11.9
Tb(50%) weight basis	[°C]	600.0	40.0	160.0	250.0	310.0	375.0	430.0	510.0	700.0	710.0

Figure 1: An example of crude oil assay in the PRELIM format

The model includes a crude assay inventory that includes crude oils that have been characterized and organized into the PRELIM format. As of November 2014, there are 51 crudes in the inventory. However, crude oils are added to the inventory regularly. Crude oil assays available publicly often are not presented in the PRELIM format. For example, the cut temperatures used in the format of the Chevron, Exxon, BP and Statoil assays are presented in Table 1. Several new assays from these companies' websites as well as from the Knovel crude oil database have been transformed into PRELIM format. Permission was granted from these sources to use these data. The original crude assays from these sources were transformed before being added to the crude oil assay inventory of the current version of the model.

Table 1: Cut temperatures in Chevron, Exxon, BP and Statoil Assays

	C5s	**Naphtha**	**Kerosene**	**Diesel**	**AGO**	**LVGO**	**HVGO**	**VR**	**AR**				
Cutoff Temp (End) in Model [°C]	80	180	290	343	399	454	525	525	399				
BP[1]	C_5-95	Naphtha	Naphtha	Kerosene	Atm Gas Oil	Vac. Gas Oil	Vac. Gas Oil	Heavy Vac. Gas Oil	Residue				
	95	149	175	232	342	369	509	550	585				
Chevron[2]	Light Naphtha	Medium Naphtha	Heavy Naphtha	Kerosene	Atm Gas Oil	Light VGO	Heavy VGO	Vacuum Residue	Atm Residue				
	80	150	200	260	340	450	570	End	End				
Exxon[3]	Butane and Lighter	Light Naphtha C5	Heavy Naphtha	Kerosene	Diesel	Vacuum Gas Oil	Vacuum Residue						
	15	74	165	250	343	537	815						
Stat Oil[4]					**Atmospheric Cuts**						**Vacuum Cuts**		
	65	100	150	200	250	300	350	370	FBP	450	500	550	FBP

[1] Source: http://www.bp.com/en/global/bp-crudes/assays.html (last accessed on September 1st, 2014)
[2] Source: http://crudemarketing.chevron.com (last accessed on September 1st, 2014)
[3] Source: http://www.exxonmobil.com/crudeoil (last accessed on September 1st, 2014)
[4] Source: http://www.statoil.com/en/OurOperations/TradingProducts/CrudeOil/Crudeoilassays/Pages/default.aspx (last accessed on September 1st, 2014)

Knovel assay format is not mentioned in this table because Knovel assay format can slightly vary from one assay to another. You can learn more about the Knovel assay formats at this URL: http://app.knovel.com

The method used to convert an assay into the PRELIM format is explained in section 4.3.1 as well as in Abella et al. (2012). This method has been evaluated as described in the section 5.3.

2.4 Spreadsheet organization

PRELIM is divided into three types of worksheets: (i) inputs and results worksheets, (ii) calculation worksheets, and (iii) data and constants worksheets. Inputs and results worksheets tabs have a red background, calculations worksheets tabs are blue, and data and constant worksheets tabs are green.

The `Overview` worksheet includes the model's authors and version, provides a brief description of each of the worksheets as well as the copyright statement.

3 A guide to the user interface

The `Input and Output` worksheets comprise the main interface for the user and allow selection of basic and advanced options. They can be used to run a case for one or all crude oil assays in the assay inventory. Key results are also presented in this worksheet. Output worksheets allow the user to explore aggregated and the detailed results of the model. All input and output worksheets have red-coloured tabs.

These worksheets do not contain any calculations since their purpose is mainly to provide input to the model and display results. This section presents the interface, how the user can interact with the model as well as how the worksheets are linked.

3.1 Main Input & Output

The `Main Input & Output` worksheet's purpose is two-fold: on the left side, the `Main inputs` box groups all basic options to run the model for one or all crude oil assays; on the right side, the `Main results` box displays live updates to the main results for the selected assay.

All input parameters are prepopulated with default values and options. Any change will trigger the model to recalculate the results.

3.1.1 Main inputs box

The main user interface includes:

- **Buttons that contain hyperlinks** to allow the user to access other worksheets of the model relevant to a particular activity;
- **Buttons that activate macros** to run specific features of PRELIM such as running all assays in the assay inventory; and
- **Dropdown menus and checkboxes** that are built Excel form controls. These form controls are not linked to macros but are typically linked to cells located on the calculations worksheets.

Each time the model starts, PRELIM loads in each of the dropdown menus and checkboxes the same values as the ones active when the model was last saved. When a user selects a new crude assay, the model automatically updates the active refinery configuration for both of the refinery types using the method described in section 4.2.2.1. However, there is one exception to this: the active configuration is *not* updated if the user has overridden it by forcing the use of a specific configuration in the `Process unit configuration` option in the `Main input & Output` worksheet. Selecting `Default value` in the dropdown menu will allow PRELIM to use again the default calculated value.

3.1.1.1 Basic input

The first section in this worksheet, under the header `Basic input`, provides a crude oil assay dropdown menu. The selected crude assay's properties are copied from the `Assay Inventory` worksheet and displayed in the table below the dropdown menu in the PRELIM format. The user can select a new assay from the inventory. Note that selecting another crude oil assay automatically triggers the model to recalculate the energy and GHG emissions using the new crude assay data. The `Main results` box to the right of the inputs is automatically updated.

3.1.1.2 Other inputs and options

The second section, called `Additional inputs and options`, offers additional options for the user to modify. This section includes three subsections.

3.1.1.2.1 More options

The `More options` subsection includes three buttons:

- `View assay inventory` links to the `Assay Inventory` worksheet and displays all the crude oil assays available in the model in the PRELIM format. Any changes to an assay can only be made in the assay inventory worksheet;
- `Input custom assay` links to a blank table in the `Expert Inputs` worksheet where the user can add a custom crude oil assay in the PRELIM format. Once added to the table, the user must select `Use Custom Assay` in the `Basic input` dropdown menu to run the new assay in the model; and
- `Create crude blend` links to the `Crude blender` tool in the `Expert Inputs` worksheet that allows the user to blend crude assays from the assay inventory. Once completed, the user must select `Use Custom Blend` in the `Basic input` dropdown menu to run the created blend in the model (see 3.2.2 for more details).

3.1.1.2.2 Display detailed results

The `Display detailed results` subsection has two buttons allowing further exploration of the results:

- `Current assay` displays detailed results for the current assay available on `Results Single Assay` worksheet. These results are more detailed than the `Main results` box on the `Main Input & Output` worksheet.

> Even more detailed results are available for each of the refineries: `CokingRefinery Detailed Results` and `HydroRefinery Detailed Results` display the breakdown of energy inputs and outputs as well as the GHG emissions per process unit.

- `All assays in inventory` runs a macro (`Float all assays`) that successively runs the model for each of the crude oil assays available in the `Assay Inventory` worksheet, including the `Custom Assay` and the `Custom Blend` that are set in the `Expert Inputs` worksheet.

> Note: Running the `All assays in inventory` macro can take up to 2 minutes on some computers. These include Macintosh computers due the fact Microsoft Excel software differs quite significantly from PC's version. It is recommended that the user does not do anything while the macro is running. The macro will automatically redirect the user to the `Results All Assays` worksheet once the process is completed.

3.1.1.2.3 Additional input and options

The `Additional inputs and options` subsection allows the user to define additional inputs and options such as the refinery configuration, the allocation method, the products that emissions should be allocated to, and the heating value used in the model calculations (i.e., HHV vs. LHV).

3.1.1.2.3.1 Refinery configuration

This set of options allows the user to enable or disable processes in the coking refinery and hydrocracking refinery. These options include:

- `Process unit configuration`: each crude oil assay is associated with a default configuration for both refinery types (see section 4.2.2 for details on how the default configuration is obtained). Each refinery type has a dropdown menu that allows for selecting the `Default value` (first option) or forcing the use of a specific refinery configuration. Processes included in each of the configurations are listed in the table to the right of the override options. Also, Table 2 below details the process units that are enabled in each of the configurations. Section 4.2.1 presents flow diagrams of all configurations and how the process units are connected.
- `Naphtha catalytic reformer options`: the dropdown menu allows the user to override the reformer configuration, which by default uses straight run naphtha (`SR Naphtha`) as input, and combines it with the stream coming from the coking/hydrocracking naphtha hydrotreater (`Heavy Naphtha)` unit as input to the catalytic naphtha reformer. Note: this option only applies if a deep conversion configuration is active.
- `Electricity source`: the dropdown menu allows the user to pick the electricity source and currently offers two options: electricity generated from a coal-fired power plant (`Coal-Fired power Plant 100%`); or electricity generated from a natural gas-fired power plant (`NG-fired Power Plant`).

Table 2: Process units enabled in each configuration

		Coking and hydrocracking refineries				Coking refinery			Hydrocracking refinery		
	Process units	**Config. 0**	**Config. 1**	**Config. 2**	**Config. 3**	**Config. 4**	**Config. 5**	**Config. 6**	**Config. 7**	**Config. 8**	**Config. 9**
Hydroskimming process units	Desalter	x	x	x	x	x	x	x	x	x	x
	Atmospheric tower furnace	x	x	x	x	x	x	x	x	x	x
	Atmospheric tower	x	x	x	x	x	x	x	x	x	x
	Naphtha hydrotreater	x	x	x	x	x	x	x	x	x	x
	Isomerisation unit	x	x	x	x	x	x	x	x	x	x
	Catalytic naphtha reformer	x	x	x	x	x	x	x	x	x	x
	Kerosene hydrotreater	x	x	x	x	x	x	x	x	x	x
	Merox unit	x	x	x	x	x	x	x	x	x	x
	Diesel hydrotreater	x	x	x	x	x	x	x	x	x	x
Medium conversion process units	Vacuum tower furnace		x	x	x	x	x	x	x	x	x
	Vacuum tower		x	x	x	x	x	x	x	x	x
	Gas oil hydrocracker			x	x		x	x		x	x
	Gas oil hydrocracker fractionator			x	x		x	x		x	x
	Fluid catalytic cracker feed hydrotreater		x		x	x		x	x		x
	Fluid catalytic cracker		x		x	x		x	x		x
	Fluid catalytic cracker main fractionator		x		x	x		x	x		x
	Alkylation unit		x		x	x		x	x		x
Coking units	Coking furnace					x	x	x			
	Coking					x	x	x			
	Coking fractionator					x	x	x			
	Coking naphtha hydrotreater					x	x	x			
Hydrocracking process units	Residue hydrocracker furnace								x	x	x
	Residue hydrocracker								x	x	x
	Residue hydrocracker fractionator								x	x	x
	Residue hydrocracker naphtha hydrotreater								x	x	x

A high-level process flow diagram shows how all process units are connected in section 4.2.1. A process flow diagram for each refinery configuration is also available in section 4.3.

3.1.1.2.3.2 Allocation method

The model can present results for two different functional units – per bbl of input crude or per MJ of final product (e.g., gasoline). This means that the energy and GHG emissions can be estimated for the entire refinery or for an individual final product. In order to present the results per final product, allocation of energy and emissions is required. The `Allocation method` option allows the user to select the allocation method used to process crude oil assays. Allocation is made on a process unit level and results in cumulative energy and emissions estimates for each refinery final product. Four methods are available:

- `Mass Basis`: calculations are made based on the mass of the streams going into and out of each process unit;
- `Energy Basis`: calculations are made based on the energy of the streams going into and out of each process unit;
- `Market Value Basis`: calculations are made based on the market value of the streams going into and out of each process unit (see note below); and
- `Hydrogen Content Basis`: calculations are made based on the hydrogen content of the streams going into and out of each process unit.

> Note regarding the `Market Value Basis`: prices used to calculate the value are located at the bottom of the `Constants` worksheet. Product prices were obtained from historical North American data from Platts (http://www.platts.com/product-list/all/all/market-data) and CMAI (www.cmaiglobal.com). These numbers can be overridden to reflect the current market.

3.1.1.2.3.3 Allocated products

The `Allocation products` option allows the user to pick the products that have energy use and emissions assigned to them. PRELIM is focused on exploring impacts of refining transportation fuels. Therefore, three products are included in all configurations and are not available in this menu: `Blended Gasoline`, `Jet-A/AVTUR`, and `ULSD` (Ultra Low-Sulphur Diesel). Five products are optional and can be enabled or disabled: `Fuel Oil`, `Bunker C`, `Surplus NCR Hydrogen`, `Coke/HC residue`, (depending on the refinery type), and `Sulphur`.

3.1.1.2.3.4 Heating value

This dropdown menu offers a choice in the heating value used in the model: `Lower Heating Values (LHV)` or `Higher Heating Values (HHV)`. The heating value of a product corresponds to the amount of heat released during the combustion of that product.

3.1.1.2.3.5 Global warming potential values

This dropdown menu allows the user to pick the global warming potential (GWP) and the lifetime to be used in PRELIM. Available values include values from IPCC Fourth Assessment Report (AR4) and IPCC Fifth Assessment Report (AR5) for 20 and 100 years.

3.1.2 Main results box

The `Main results` box displays aggregated results for the selected crude assay in terms of energy use (top left), associated GHG emissions (top right), as well as the product slate (bottom). These numbers are generated and regenerated every time a change is made to the input parameters on this worksheet.

3.1.2.1 Energy use

The `Energy use` section presents all energy commodities (electricity, heat, steam, hydrogen, and refinery fuel gas) used in each of the two refinery types for the same crude oil assay. The unit is MJ of energy consumed/bbl of crude. A figure below the energy use table offers a visual comparison of the results for the coking and the hydrocracking refineries.

> Note: a negative hydrogen value indicates a surplus of hydrogen.

3.1.2.2 Greenhouse gas emissions

The `Greenhouse gas emissions` section presents the GHG emissions associated with each of the energy commodities used in each of the two refineries for the same crude oil assay. The unit is kg of CO_2e/bbl of crude. The figure below the GHG emissions table allows a visual comparison of the results for the coking and the hydrocracking refineries.

The `See more results` button links to the `Results Single Assay` worksheet and displays more detailed results for the selected assay.

3.1.2.3 Product slate

The `Product slate` section presents the share of final products in bbl of product per day (table on the left) as well as a percentage (table on the right).

3.1.2.4 Energy consumption and GHG emissions by unit of final product

The `Energy consumption and GHG emissions by unit of final product` section at the bottom presents the energy allocated to refinery products in MJ/MJ of final product. Note that a zero value may indicate that the product has not been allocated any emissions in the `Additional inputs and options` (option `Pick allocation products`). The GHG emissions allocated to refinery products in g CO2e/MJ of final product is also presented for all products to which emissions have been allocated.

3.2 Expert inputs

In the current version, the `Expert Inputs` worksheet allows the user to access two features: input a custom assay, and blend crude oil assays from the assay inventory. Other features will be released in future versions of PRELIM.

3.2.1 Input Custom Assay

In the `Input Custom Assay` section, the user can fill in the blue-shaded fields in the blank assay template with the assay's properties. These properties need to be in the PRELIM assay format (see section 2.3.5 for details on the PRELIM format). Volume flow and API gravity will be automatically calculated from the input fields.

This custom assay is automatically copied into the `Assay Inventory` worksheet and can be used in the model by selecting `Use Custom Assay` in the `Main Input & Output` worksheet's dropdown menu.

> Note: you can customize the name of the custom assay by modifying cell `F6` on the `Expert Inputs` worksheet.

3.2.2 Crude Blender

The `Crude Blender` section displays a table where the user can select between 2 and 10 crude oil assays from the assay inventory and specify the amount of each crude in the blend using a mass ratio. Note that each cell in the `Crude Assays` column contains a dropdown menu that contains all available assays.

Clicking the `Create Blend` button then runs a macro (`Blending WeightAverageMethod`) that automatically calculates the properties of the resulting blend on a mass basis. After the user specifies the desired crude oil assays and the desired mass fractions of those crude oils in the final blended assay, the corresponding fractions of the individual crude oil assays selected to be blended are assumed to be mixed and thermodynamic mixing rules are used to calculate the mixture properties and to generate the blended assay. These properties are displayed below as well as in the `Assay Inventory` worksheet in the PRELIM format.

The blended crude assay can be used in the model by selecting `Use Custom Blend` in the `Main Inputs` worksheet's dropdown menu.

3.2.3 Advanced features in development

This section contains some features currently in development. It is not recommended to use these features as this may result in inaccurate results or the model becoming unstable.

3.3 Results for a single assay

The `Results Single Assay` worksheet displays results that are updated every time a change is made to an input parameter for the selected crude oil assay based on selected options in the `Main Input & Output` worksheet. Results are displayed in terms of energy use and GHG emissions, first for the coking refinery (blue headings) then for the hydrocracking refinery (red headings).

Two buttons on the right side of the table link to more detailed results for the coking refinery and hydrocracking refinery respectively.

3.4 Results for all assays

The `Results All Assay` worksheet displays results for all crude assays available in the `Assay Inventory` worksheet using the appropriate configuration that is chosen based on the criteria described in section 4.2.2.1 (or selected configuration if it is overridden). This worksheet is updated when the (`Float all assays`) macro is run by clicking the `All assays in inventory` button located in the `Display detailed results` subsection in the `Main Input & Output` worksheet. The macro iteratively calculates, copies, and pastes the results from each assay in this worksheet. When completed, the worksheet displays results for all assays available in the inventory, using the same format as the `Results Single Assay` worksheet.

An `Erase results` button in the top left corner of the worksheet allows the user to delete all current results on this worksheet.

> Note: running the macro and displaying this worksheet can take up to 20 seconds depending on your computer's specifications.

3.5 Coking refinery detailed results

The `CokingRefinery Detailed Results` worksheet displays detailed results for the selected crude oil assay using the coking refinery. This worksheet contains three main types of information:

- The `Process Energy Inputs and Outputs` table displays the input and output energy for each of the enabled process units;
- The `Process Life Cycle GHG Emissions` table displays the greenhouse gas emissions associated with the energy use of each of the enabled process units; and
- The `Contributors to the coking refinery's GHG emissions` figure presents the distribution of the contribution to greenhouse emissions per energy source on a process unit basis.

This worksheet is a display-only worksheet and does not offer any interactivity to the user.

3.6 Hydrocracking refinery detailed results

The `HydroRefinery Detailed Results` worksheet displays detailed results for the selected crude oil assay using the hydrocracking refinery. Detailed results contains three main types of information:

- The `Process Energy Inputs and Outputs` table displays the input and output energy for each of the enabled process units;
- The `Process Life Cycle GHG Emissions` table displays the greenhouse gas emissions associated with the energy use of each of the enabled process units; and
- The `Contributors to the hydrocracking refinery's GHG emissions` figure presents the distribution of the contribution to greenhouse emissions per energy source on a process unit basis.

This worksheet is a display-only worksheet and does not offer any interactivity to the user.

4 Technical documentation: calculation, data, and constants worksheets

This section provides technical documentation for the calculation, data and constants worksheets to explain how PRELIM works at a detailed level. More specifically, it details the relationship between the worksheets and how PRELIM models the refinery's process units in terms of assumptions, constants, and calculations.

4.1 Sources

Unless specified in the model or the documentation, PRELIM uses the following sources for default values, calculations, and equations:

- Gary, J.; Handwerk, G.; Kaiser, M., Petroleum Refining Technology and Economics Fifth ed.; CRC Press: New York, 2007.
- Parkash, S. Refining Processes Handbook, Burlington: Elsevier, 2003.

A complete list of references used to build, document, and validate the PRELIM model is available in section 4.4.3.2.

The data available in PRELIM for process unit energy requirements are presented as a default as well as with a range of plausible values for each parameter derived from the literature. The data were compared with confidential information and evaluated in consultation with industry experts to verify the values and their ranges are appropriate. Having said this, process energy requirements can vary greatly from refinery to refinery. Therefore, the user is able to override the data in these cells to reflect a specific refinery or scenario.

Some cells in the calculation worksheets have comments to explain calculations or provide the user with a source. Cells that are commented typically display a red triangle in their top right corner.

> Note: you may need to activate the comment display option in Microsoft Excel to be able to display comments.

4.2 General modeling methods

4.2.1 Model overview

Figure 2 presents a simplified process flow diagram (PFD) of the overall refinery model structure and how the process units are connected. A total of 10 refinery configurations are available in the model, through two refinery types: a coking and a hydrocracking refinery. These two structures include only "major" refinery processes (defined either by installed capacity in North America or by its potential for widespread adoption within the next 20 years) that are related to the production of transportation fuels. A detailed process flow diagram for each refinery configuration is available in sections 4.4.3, 0, and 4.4.5. Each refinery configuration is modelled at a process unit level, an improvement over current public Well-To-Wheel models (e.g., GREET [Argonne National Laboratory, The Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) Model. http://greet.es.anl.gov], and GHGenius [Natural Resources Canada, GHGenius A model for life cycle assessment of transportation fuels. http://www.ghgenius.ca]). Due to this, more detailed modelling is possible and is discussed throughout this section. A material balance connects the different process units along with flow splitters that together simulate different refinery configurations.

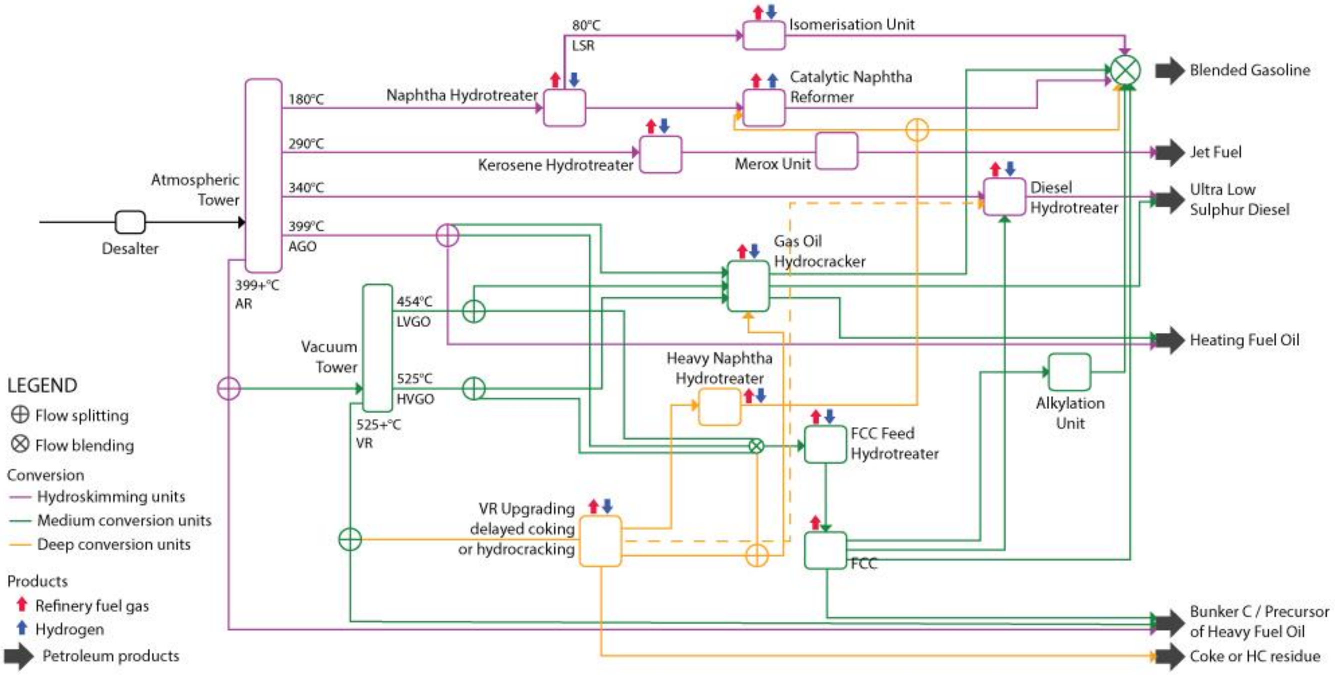


Figure 2: PRELIM simplified process flow diagram

> Flow splitters allow for different configurations based on three major refinery categories. The Atmospheric Residue (AR) flow splitter sends the AR to the Heavy Fuel Oil pool for a Hydroskimming Refinery. Otherwise, it is sent to Vacuum Distillation to simulate other refinery categories (Medium and Deep Conversion Refineries). The Vacuum Residue (VR) flow splitter sends VR to the Fuel Oil pool for a Medium Conversion Refinery or to VR Upgrading for a Deep Conversion Refinery. Atmospheric Gas Oil (AGO), Light Vacuum Gas Oil (LVGO), Heavy Vacuum Gas Oil (HVGO), and Coking or Gas Oil Residue Hydrocracking (GO-Resid HC) split swing cuts send the gas oils either to Gas Oil Hydrocracking or Fluid Catalytic Cracking or to both processes to simulate different types of Medium and Deep Conversion Refineries. Hydrotreated Heavy Naphtha can be sent either to the Naphtha Catalytic Reformer to increase hydrogen production or to the Gasoline pool. Brown dashed lines represent Hydrocracked Diesel intermediate product that is only produced if the VR upgrading uses Residue Hydrocracking, and optional blending of heavy naphtha in the gasoline pool. Abbreviations: Treatment (T) of Refinery Fuel Gas and sulphur recovery processes, Steam Methane Reforming (SMR) process to produce hydrogen if naphtha catalytic reformer supply is not sufficient, FCC Coke-Burned (C-B). Note that no process associated with recovery of Liquefied Petroleum Gas is included. The scheme shows distillation cut temperatures (°C) used in this study.

All configurations include atmospheric crude distillation, hydrotreating, and naphtha catalytic reforming process units. The configurations are differentiated by whether or not a vacuum crude distillation process unit and the following conversion technologies are present: gas oil hydrocracking and/or fluid catalytic cracking (referred to hereafter as FCC); delayed coking or residue hydrocracking. The thermal cracking technologies (e.g. FCC and delayed coking) increase the hydrogen to carbon ratio through carbon rejection while the hydrocracking technologies (gas oil and residue hydrocracking) modify the hydrogen to carbon ratio by adding hydrogen produced through a separate process unit (steam methane reforming referred to hereafter as SMR).

Each configuration requires a different amount of energy to process a crude and produces a different slate (i.e., volume and type) of refinery final products including transportation fuels (i.e., gasoline, kerosene, and diesel) as well as heavy fuel oil, hydrogen from the naphtha catalytic reforming process, refinery fuel gas (i.e., gas produced as a by-product in process units within the refinery), and the possible production of coke or hydrocracking residue. Liquefied Petroleum Gas (LPG) is an alternative final product in refineries and is treated in a simplified way in the current version of PRELIM (section 4.2.6).

For each process unit, the model calculates the energy that it requires and predicts the quantity and destination of products exiting the process unit using the following data: process unit energy requirements, process unit intermediate product yields, intermediate product characteristics (API, sulphur, and hydrogen content), and crude assay information. PRELIM also calculates the upstream energy use and GHG emissions associated with the energy sources (i.e., electricity and natural gas)(Baumann et al., 2004). Fugitive GHG emissions from the refinery tend to be an order of magnitude lower than combustion emissions (EPA, 2009) and are not considered in the current version of PRELIM.

PRELIM can calculate overall refinery energy and GHG emissions on a per barrel of crude or per megajoule (MJ) of crude basis as well as for a particular final product on a per MJ basis of product (e.g. per MJ of gasoline). For the latter type of functional unit, an allocation process of the energy use (amount and type) occurs at the refinery process unit level. That is, at each process unit, the amount and type of energy used is allocated to the process unit throughputs. In the next process unit, the sum of the energy embedded in the process feed (calculated by the allocation in preceding processes) and energy used in that process unit is similarly allocated to the process unit throughputs. Energy use and type of energy are traced through the entire refinery to the final products (Wang et al., 2004). PRELIM allows the flexibility to choose which products are assigned emissions (e.g., to transportation fuels only, transportation fuels plus coke) as well as the basis of allocation (i.e., hydrogen content, mass, market value, or energy content basis). Comparison of overall energy requirements in the refinery (calculated by adding the embedded energy in all the refinery final products which account for process unit throughputs on a mass unit basis) versus total energy requirements from all process units verifies the energy and material balance in the system.

To run the model, a user must select the crude, the configuration, and the allocation method desired. Default values can be used to represent the crude properties (by selecting a crude from the crude assay inventory in the model) and process units. Alternatively, a user can input a new crude assay or can modify any of the model parameters either by selecting a value in the range of values available in the model for each parameter or by inputting their own parameter value(s). To characterize the whole crude and its fractions, a total of 62 parameters are input to the model, accounting for five crude oil quality properties: crude distillation curve (i.e., information in terms of mass and volume yields of each fraction, and single fraction characteristic boiling point), API, sulphur content, hydrogen content as well as carbon residue Table 6 highlights the parameters). Two additional crude properties (aromatic content and crude light ends content) impact refinery GHG estimates and are modelled indirectly in PRELIM (sections 4.2.4, 4.2.6, and 4.3.7).

4.2.2 Configuration and model boundaries

Every refinery is configured differently and every crude can be processed in a range of refinery configurations. The interconnection of process units adopted in PRELIM (Figure 2) is consistent with many general energy petroleum refinery flow structures (see for example Robinson (2006), Energetics (2007), Wiley (2007), and Gary et al. (2007) for refinery configuration representations and for general to detailed descriptions of refinery processes and their interconnections). For the purposes of obtaining a generalized tool, the configuration is simplified based on discussions with refinery operation experts. For example, PRELIM uses a hydrotreating process unit to process the FCC feedstock. Refineries can meet gasoline sulphur content specifications either by using a hydrotreating process unit of FCC feedstock (hydrotreating of heavy gas oil) or a hydrotreating process unit of FCC gasoline product (gasoline desulphurization). Each of these process units is present in 39% of U.S. refineries, and their installed capacities are comparable (Table 3). A second example is that the current version of PRELIM does not model recycling of intermediate products among FCC, delayed coking, and hydrocracking process units. (e.g., FCC processing heavy material derived from the gas oil hydrocracking process unit [Robinson, 2006], hydrocracking or delayed coking processing medium to heavy fractions derived from the FCC process unit [Gary et al., 2007]). However, processing of recycled intermediate products among these process units is only operating in 17% of U.S. refineries (EIA, 2008) and the installed capacity of process units to process the recycled feed is low (Table 3).

Table 3: Capacity of the major refining processes in U.S. petroleum refineries and distribution as share of atmospheric crude distillation capacity.

Refinery Process	***Downstream Charge Capacity (BPSD)[a]***	***Distribution Share of Crude Distillation Unit capacity***	***Included within PRELIM***
Atmospheric Crude Oil Distillation	18,581,089	100.0%	Yes
Vacuum Distillation	8,542,643	46.0%	Yes
Thermal Cracking	2,631,676	14.2%	
Thermal Cracking, Coking	2,605,076	14.0%	
Delayed Coking	2,500,676	13.5%	Yes
Fluid Coking	104,400	0.6%	No
Thermal Cracking, Visbreaking	16,000	0.1%	No
Thermal Cracking, Other (including Gas Oil)	10,600	0.1%	No
Catalytic Cracking, Fresh Feed	6,140,121	33.0%	Yes
Catalytic Cracking, Recycled Feed	91,840	0.5%	No
Catalytic Hydrocracking	1,819,700	9.8%	
Catalytic Hydrocracking, Distillate	595,200	3.2%	Yes
Catalytic Hydrocracking, Gas Oil	1,079,500	5.8%	Yes
Catalytic Hydrocracking, Residual	145,000	0.8%	Yes
Catalytic Reforming	3,700,463	19.9%	Yes
Catalytic Reforming/Low Pressure	2,322,700	12.5%	
Catalytic Reforming/High Pressure	1,377,763	7.4%	
Desulphurization (including Catalytic Hydrotreating)	16,023,206	86.2%	
Catalytic Hydrotreating, Naphtha/Reformer Feed	4,281,046	23.0%	Yes
Desulphurization, Gasoline	2,394,882	12.9%	Yes[b]
Catalytic Hydrotreating, Heavy Gas Oil	2,796,798	15.1%	Yes
Catalytic Hydrotreating, Distillate	5,676,032	30.5%	
Kerosene/Jet Fuel	1,339,150	7.2%	Yes
Diesel Fuel	3,647,211	19.6%	Yes
Other Distillate Fuel	689,671	3.7%	
Catalytic Hydrotreating, Other/Residual Fuel Oil	874,448	4.7%	
Residual Fuel	246,200	1.3%	No
Other Oils	628,248	3.4%	No
Fuels Solvent Deasphalting	383,250	2.1%	No

[a] BPSD: Barrels Per Stream Day. It is the maximum number of barrels of input that a refinery can process within a 24-hour period, running at full capacity under optimal conditions, with no allowance for downtime.

[b] Naphtha and gas oil hydrotreating fulfill gasoline desulphurization requirements.

> Source: U.S. Energy Information Administration Data at January 1st, 2010.

4.2.2.1 Configurations available in the coking refinery

Figure 3 displays the coking refinery PFD as modeled in PRELIM. A PFD for each configuration is available in section 4.4.3 for all configurations common to both refinery types and in section 0 for configurations specific to the coking refinery.

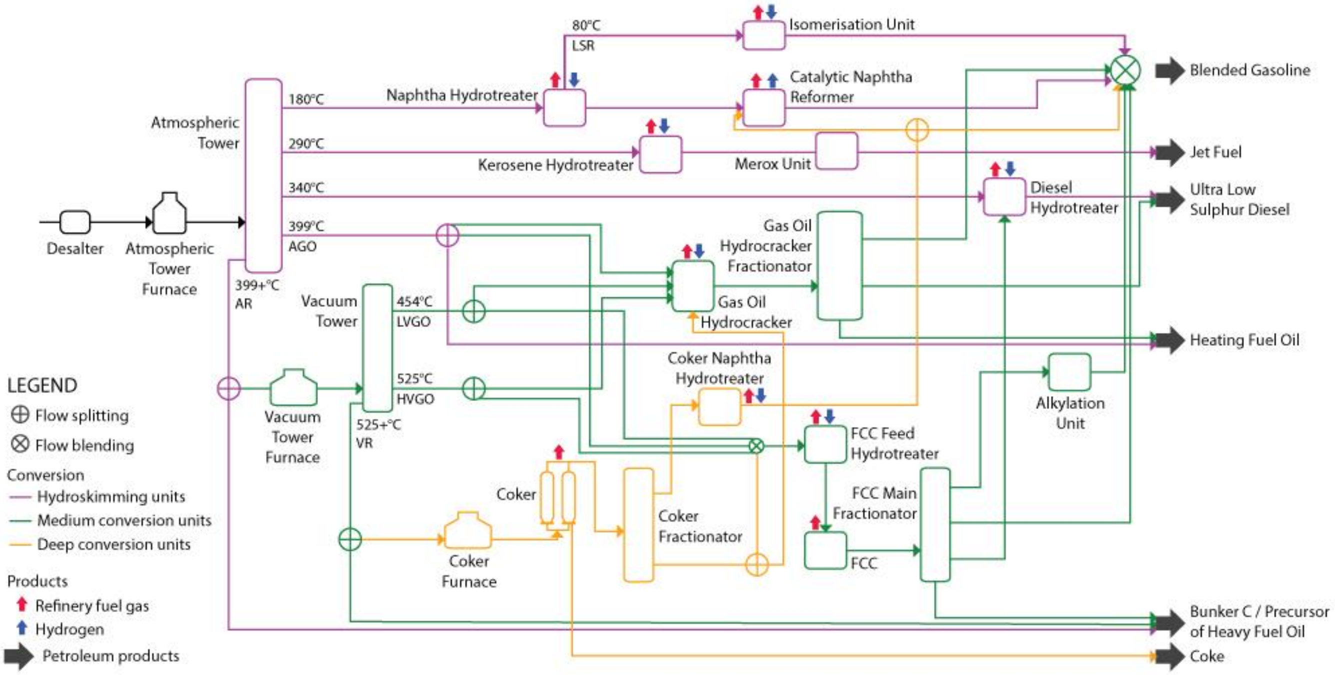


Figure 3: Coking refinery process flow diagram in PRELIM

The coking refinery consists of 21 process units that are enabled or disabled depending on the selected configuration. All refinery configurations include crude distillation, hydrotreating, and naphtha catalytic reforming processes. The configurations can be categorized in three types:

- **The hydroskimming configuration** is a basic configuration that processes the crude oil from the atmospheric tower into refined products without additional transformation (units in purple in Figure 3) (configuration `0`).
- **The medium conversion** configuration comprises the hydroskimming process units but also processes the heaviest component of the stream further using additional process units (units in green in Figure 3). The medium conversion can be run using one of these three configurations:
    - Using the fluid catalytic cracking only (configuration `1`);
    - Using the gas oil hydrocracker only (configuration `2`); or
    - Combining the fluid catalytic cracking and the gas oil hydrocracker (configuration `3`).
- When enabled, **the deep conversion** configuration includes additional process units to the medium conversion configuration, allowing for further processing of the heaviest fraction exiting the bottom of the atmospheric tower using higher temperatures to crack heavier compounds into higher quality

products (units in orange in Figure 3). The deep conversion configuration can be run using one of these three configurations:

- Using the fluid catalytic cracking only (configuration `4`);
- Using the gas oil hydrocracker only (configuration `5`); or
- Combining the fluid catalytic cracking and the gas oil hydrocracker (configuration `6`).

The three configurations are not independent--the medium conversion includes the hydroskimming configuration, and the deep conversion requires both the hydroskimming and medium conversion process units.

A default refinery configuration is assigned for each crude oil assay, using API gravity and sulphur content of the whole crude as the criteria. Figure 4 illustrates how PRELIM determines the most suitable configuration to process the crude among configurations 1, 3, 6, or 9.

PRELIM cannot automatically assign configurations 2, 4, 5, 7, and 8 based on its current selection criteria. That is, the medium conversion always uses configuration 3, and the deep conversion uses configuration 6 for the coking refinery and configuration 9 for the hydrocracking refinery. These configurations have both the fluid catalytic cracker and the gas oil hydrocracker enabled. The user can override these selections to explore the impact of using one of the other refinery configurations that are available.

The user has the ability to override the default configuration and pick another one in the `Process unit configuration` option available in the `Main Input & Output` worksheet.

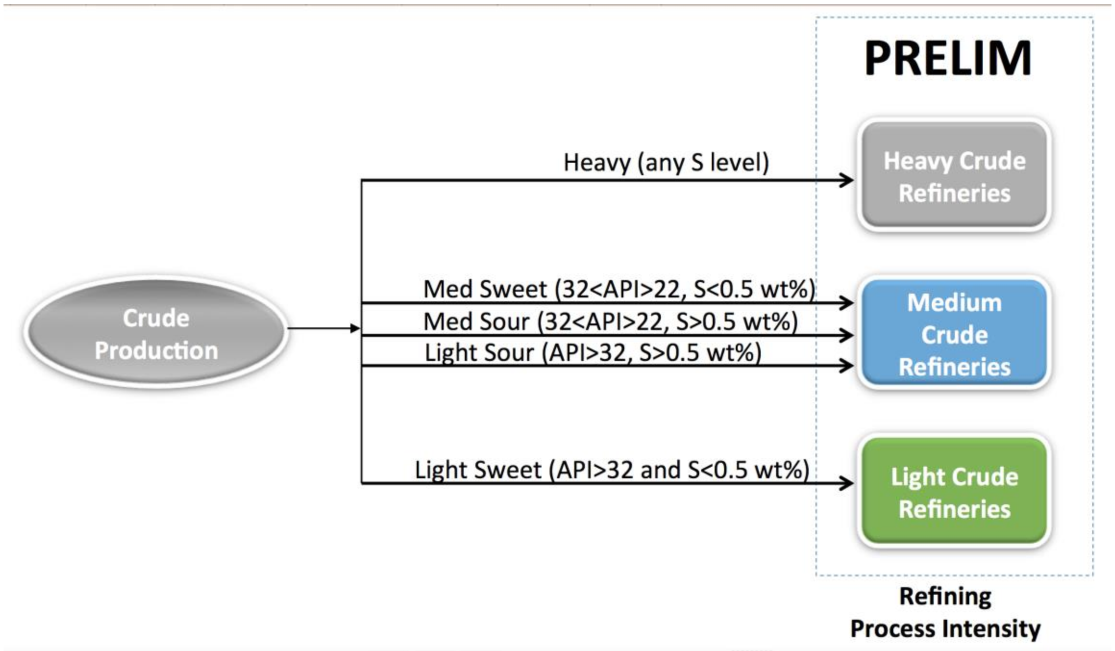


Figure 4: How PRELIM determine the refinery default configuration

4.2.2.2 Configurations available in the hydrocracking refinery

Figure 5 displays the hydrocracking refinery PFD as modeled in PRELIM. A PFD for each configuration is available in section 4.4.3 for all configurations common to both refinery types and in section 4.4.5 for configurations specific to the hydrocracking refinery.

The hydrocracking refinery consists of 21 process units that are enabled or disabled depending on the selected configuration. All refinery configurations include crude distillation, hydrotreating, and naphtha catalytic reforming processes. The configurations can be categorized in three types:

- **The hydroskimming configuration** is a basic configuration that processes the crude oil from the atmospheric tower into refined products without additional transformation (units in purple in Figure 5) (configuration `0`).
- **The medium conversion** configuration comprises the hydroskimming process units but also processes the heaviest component of the stream further using additional process units (units in green in Figure 5). The medium conversion can be run using one of these three configurations:
  - Using the fluid catalytic cracking only (configuration `1`);
  - Using the gas oil hydrocracker only (configuration `2`); or
  - Combining the fluid catalytic cracking and the gas oil hydrocracker (configuration `3`).
- When enabled, **the deep conversion** configuration includes additional process units to the medium conversion configuration, allowing for further processing of the heaviest fraction exiting the bottom of the atmospheric tower using higher temperatures to crack heavier compounds into higher quality products (units in orange in Figure 5). The deep conversion configuration can be run using one of these three configurations:
  - Using the fluid catalytic cracking only (configuration `7`);
  - Using the gas oil hydrocracker only (configuration `8`); or
  - Combining the fluid catalytic cracking and the gas oil hydrocracker (configuration `9`).

The three configurations are not independent--the medium conversion includes the hydroskimming configuration, and the deep conversion requires both the hydroskimming and medium conversion process units.

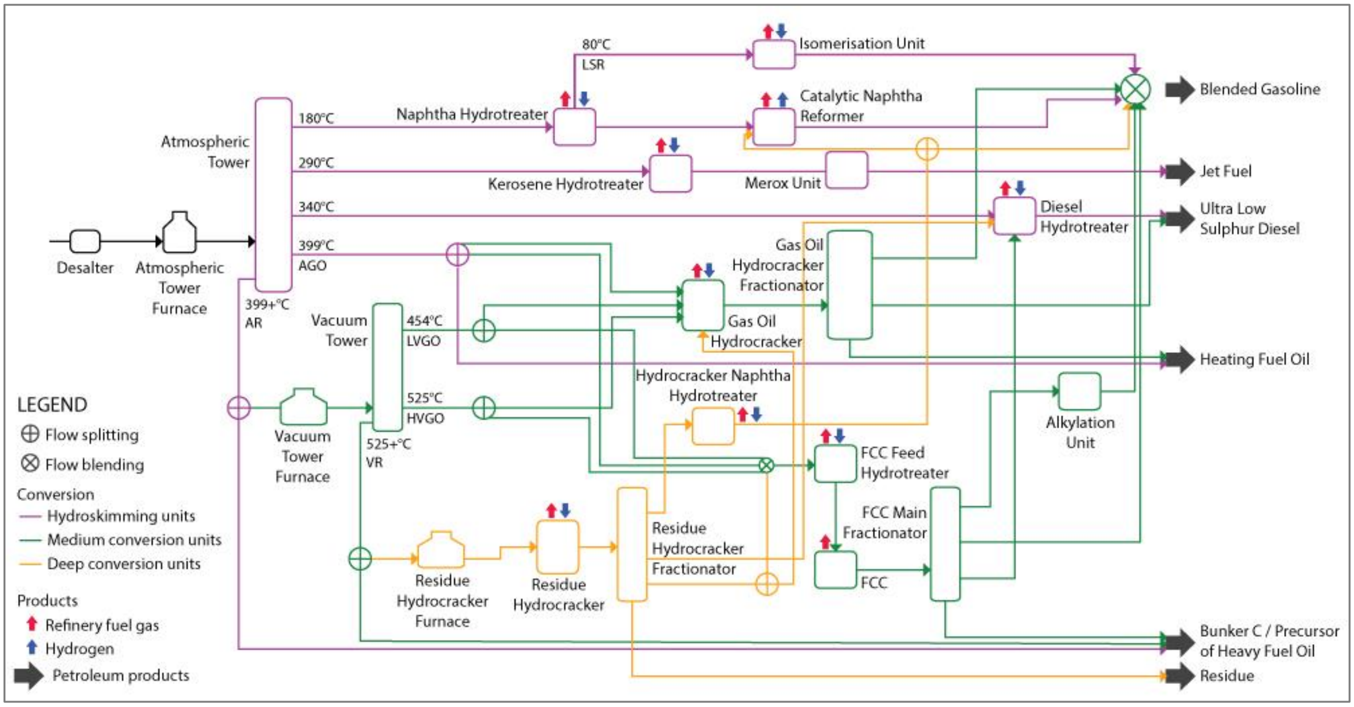


Figure 5: Hydrocracking refinery process flow diagram in PRELIM

The method used to determine the default refinery configuration is similar to the one used for the coking refinery and is explained in the previous section. The user has the ability to override it and pick another configuration in the `Process unit configuration` option available in the `Main Input & Output` worksheet.

4.2.3 Process energy requirements and data interpretation

Refinery process units require electricity, heat, and steam (referred to hereafter as "process energy requirements"). Electricity can be purchased from the power grid or produced on site at the refinery. Heat and steam can be obtained by process heat recovery and heat integration systems. The most common system uses pumparound of effluent streams for feed/effluent heat exchanging and/or for steam generation. Fuel gas produced on site and/or natural gas supply the process energy requirements after heat integration. Refineries also may burn fuel oil if the equipment is available and air emissions regulations permit it.

4.2.3.1 Process energy requirements data

PRELIM calculates total process energy requirements using information from the crude distillation curve (i.e., distribution of the whole crude material into its fractions).

For the distillation process units, two types of energy requirements are calculated: 1) energy for feed preheating, and 2) energy for crude separation (steam requirement). The energy to preheat the distillation process units feed is calculated based on a balance of enthalpies using a correlation from Moharam et al. (1998) for characterization of enthalpy of the crude fractions. The enthalpy of each crude fraction is calculated at the input and output temperatures of the preheater; the input temperature is assumed to be previously increased by a pumparound system while the output temperature is associated with an operating condition (both temperatures are input parameters in the model). Moharam et al.'s correlation is recommended (that considers the API and characteristic boiling point of a crude fraction) for light and medium crude fractions (naphtha to gas oil fractions), but it is applied across all fractions in PRELIM. For the light and medium fractions an average standard deviation of ±2.5% is expected (Moharam et al., 1998). The error of using the correlation for heavier fractions is unknown. However, the correlation helps to differentiate energy requirements for feed preheating among crudes. To the knowledge of the authors, there is no empirical correlation or simple method (based on little input data or commonly available parameters) that could be used for this purpose. Moharam et al. also suggest that more complex correlations will not necessary be more accurate for the prediction of the enthalpy properties of petroleum fractions (Moharam et al., 1998). In addition, the estimate of the error in the energy estimates for the crude distillation process unit is overestimated in this model in comparison with an industry accepted proprietary model (Baker & O'Brien). Though, it would be expected an accelerated growth in the heat capacity for heavy fractions above what is estimated for the lighter fractions. This implies that the use of the correlation is a conservative calculation in the model. Further work could improve the representation of energy requirements associated with the heavier fractions. The energy required to separate the crude into its fractions is calculated based on the volume of each crude fraction that is produced. The default values for the energy required for separation (the amount of steam per volume of crude fraction produced; input parameters in the model) is informed by industry experts (and literature presented in Table 3) and implies the energy efficiency in the distillation process unit (see Table 3).

Table 4: PRELIM default process energy requirements

Data are given on a per barrel of process unit volume feed basis unless otherwise specified (Szklo et al., 2007).

Refinery Process	Fuel (LHV) MJ/bbl	Electricity kWh/bbl	Steam [a] Lb/bbl	Calculated Energy PRELIM [b] MJ/bbl	Estimated Range U.S.2007 MJ/bbl [i]
Desalting	-	1.5x10^{-2}	-	5.4x10^{-2}	3.6-7.2x10^{-2} [ii]
Atmospheric Distillation	57 - 67[c]	0.9	4.4 - 8.8[d]	67 - 85	87 - 196
Vacuum Distillation	32 - 42[c]	0.3	0.8 - 10.8[d]	34 – 60	54 - 119
Hydrotreating [e,f]					64 - 173
H make-up Scf/bbl					
<150	105	2.0	6.0	122	
150-400	158	3.0	8.0	182	
>400	211	6.0	10.0	249	
Naphtha Catalytic Reformer [e]	317	3.0	30.0	317	225 - 361
Isomerization (Isopentane/Isohexane)		1.0	211.0	343	108 - 249
Merox Unit	-	0.1	-	0.36	
Gas Oil Hydrocracker [e,g]					168 - 339
H make up (Scf/bbl)					
<2000	106	8.0	50.0	216	
2000 – 3000	311	13.0	75.0	480	
>3000	217	18.0	100.0	445	
Fluid Catalytic Cracking [e]	106	- [h]	- [h]	106	221
Alkylation (H_2SO_4)	0	4.1	179.0	306	348 - 359
Delayed Coking	148	30.0 kWh/t coke [i]	5.0lb/bbl coker GO [j]	162 - 176	120 - 243
Steam Production [a,e]	3,502/t steam	4.8/t steam	186/t steam		
Amine Gas Treating [k]	280/m^3A	2.6/m^3 A	-		
Claus Sulphur Recovery [l]	-	98/t S	-1,215/t S		
Claus Tail Gas Treatment [l]	-	463/t S			
Steam Methane Reforming [m]					66–167/kgH
Estimated energy efficiency					
62% efficiency	203/kg H	0.33/kg H	-	204/kg H	
91% efficiency	183/kg H	0.20/kg H	-27/kg H	139/kg H	

[i] Energetics. *Energy and Environmental Profile of the US Petroleum Refining Industry* Prepared by Energetics Incorporated Columbia, Maryland for U.S. Department of Energy Industrial Technologies Program: November 2007; pp 39,40.

[ii] Worrell, E.; Galitsky, C. *Energy efficiency improvement and cost saving opportunities for petroleum refineries.*; LBNL-56183; Ernest Orlando Lawrence Berkeley National Laboratory: 2005; pp 10-16.

Base Case refinery energy requirements for processing a crude and GHG estimates are based on data given in Table 4. Most data are obtained from Gary et al. (2007); however, discussion of the data with refinery experts and comparison with confidential data and other literature sources was used to supplement or modify some values:
[a] Gary et al. (2007) suggest a steam LHV 2.79 MJ/kg (1200 Btu/lb) of steam. Refineries produce steam of different qualities using different energy efficiencies. In this study, it is assumed energy consumption to produce high pressure (900 psig) steam. It is high energy demand to produce steam of higher LHV (3.59 MJ/kg; 1542 Btu/lb); however, a high energy efficiency of 85% is also assumed (Parkash, 2003).
[b] No energy consumption for cooling systems is included. The ranges of total calculated energy in distillation and delayed coking process units are for the crudes included in this study.
[c] Atmospheric and vacuum distillation's furnace duty is a function of crude API and of the amount of products or fractions to distillate. PRELIM uses a correlation from Moharam et al. (1998) to determine enthalpy of petroleum fractions based on temperature, crude fraction API and Tb point (see below Approximated Watson characterization factor). This study assumed heating the feed of atmospheric distillation from 288-399 °C (stream of reflux and distillation product streams are used to preheat a desalted crude, see note d), and the feed of vacuum distillation (i.e. atmospheric residuum) from 399-454 °C. Though theoretical calculations of this energy requirement are considered low in comparison to real distillation energy consumption (Energetics. *Energy Bandwidth for Petroleum Refining Processes*; Prepared by Energetics Incorporated for the U.S. Department of Energy Office of Energy Efficiency and Renewable Energy Industrial Technologies: 2006; p 17.), the correlation is used to reflect differences on energy requirements due to crude quality; however, this is an approximation since the correlation is derived from a light fractions' data base (20).
[d] Atmospheric and vacuum distillation stripping steam depends of the boiling range of the feed and the type of fraction to vaporize; Gary et al. (2007) suggest a range of 10 to 50 lb/bbl of feed. PRELIM assumes 6, 4, 2, and 10 lb/bbl for Kerosene, Diesel, AGO, and AR fractions respectively at the Atmospheric distillation, and 15 lb/bbl for VR fraction at the Vacuum Distillation.
[e] Process energy exports can be expected as Energetics (2007) reported for U.S. Refinery industry. This study uses data from Gary et al. (2007) which does not show such values; therefore, there is not credit in this study for that. Besides that, process total calculated energy use is among the U.S. industry range (Energetics. *Energy and Environmental Profile of the US Petroleum Refining Industry* Prepared by Energetics Incorporated Columbia, Maryland for U.S. Department of Energy Industrial Technologies Program: November 2007; pp 39,40). (See note h for FCC unit).
[f] Gary et al. (2007) suggest that hydrotreating energy requirements vary based on hydrogen consumption. Data are available for consumption of the following ranges: 100-150, 150-400, 400-800 scf H/bbl. Hydrogen consumption for each case is determine by global hydrogen mass balance as difference in hydrogen content of hydrotreating feed and products and a factor for hydrogen losses. Additional hydrogen requirements are estimated for sulphur removal. PRELIM's hydrogen consumed for desulphurization reaction is based on stoichiometric quantities to transform sulphur into H2S.
[g] Gary et al. (2007) suggest that hydrocracking energy requirements vary based on hydrogen consumption. Data are available for consumption of 1000, 2000, and 3000 scf H/bbl. In this study, 80% of electricity requirements are allocated to reactor and the other 20% to fractionators. Also, hydrogen requirements in PRELIM application are derived from assuming a hydrocracking severity of 1500 scf H/bbl.
[h] FCC regenerator produces flue gas of important embodied energy. Gary et al. (2007) give data of power consumption of 6.9 kWh/bbl accounting for electric drive for air blower and off gas compressors and does not provide steam consumption data taking into account that FCC usually generates excess of steam by approximately 30 lb of steam per bbl of feed. Refiners may utilize the flue gas to drive a gas expander turbine that could generate the required power for the air blower and

to allow export of electricity. This study assumes that there is not steam export, and that the embodied energy content of the flue gas supplies the steam and electricity demand of the FCC.

[i] PRELIM uses an additional 0.5 kWh/bbl total coker liquids.

[j] Stripping steam depends of the boiling range of the feed and the type of fraction to vaporize. Gary et al. (2007) give a steam consumption of 700 lb/t of coke. PRELIM uses 5 lb/bbl coker gas oil; it is equivalent to 9.5 to 924 lb of steam/t coke for the assay inventory in this study.

[k] Energy requirements are based on amine solution circulation (A). The amine solution circulations is estimated assuming amine ratio of 3.0 moles amine per mole H2S, 100% H2S absorbed in amine, and 20% wt solution (Jones et al., 2008). Gary et al. (2007) give fuel requirements to obtain steam of low pressure (60 psig) for this process unit.

[l] Gary et al. (2007) give energy requirements as function of sulphur recovered. The authors suggest exports of steam of low pressure steam (250 psig) for the sulphur recovery process unit. In this study, it is assumed high pressure (900 psig) steam (3.59 MJ/kg; 1542 Btu/lb) (see note a); however, for consistency, in this process unit, steam is assumed to have an enthalpy of 2.79 MJ/kg (1200 Btu/lb).

[m] Energy requirements for the production of hydrogen via steam methane reforming (SMR) are given in a per kg of hydrogen basis. Fuel requirement includes natural gas used as feedstock and fuel. Estimated energy efficiency is calculated as the ratio between energy content in hydrogen and SMR process net energy requirement (i.e. fuel requirements for heating, steam production, and electricity plus energy content of natural gas used as a feedstock minus energy content of excess of steam produced). This study uses data from Gary et al. (2007) and NETL report (NETL *Development of Baseline Data and Analysis of Life Cycle Greenhouse Gas Emissions of Petroleum-Based Fuels* DOE/NETL-2009/1346.; National Energy Technology Laboratory: 2008.) as good approximations to current average industry practices (base case) and the case where modern purification technology is used (scenario of improvement of SMR process unit) respectively. Both studies supply the data in energy units and per scf or kg of H basis. This study used GREET version 1.8c default assumptions for fuel specifications; therefore, energy efficiencies were calculated using hydrogen low heating values (LHV) on mass basis: 127.06 MJ/kg and density 2.55 g/ft3. Different assumptions lead to a different estimated energy efficiency (see NETL 2008 report for a range of reported energy use in SMR in the literature and vendors, also NERL (Spath et al., 2001) for different assumptions about hydrogen specifications and energy requirements).

For other process units in the model (e.g., hydrotreating, naphtha catalytic reforming, and SMR process units), PRELIM uses information about the quantity and type of energy required from an individual refinery process unit and assumes that the process energy requirement is linearly related to the process unit volume feed flow. This reflects the process unit level approach that allows the flexibility to scale requirements up and down depending on the quality of the crude. This approach is needed to reflect differences in refining crudes with different distillation curves, which determine the subsequent process unit feed flows, and therefore the processing capacity and energy requirements for each subsequent process unit. This approach coincides with the idea that energy use in refineries is driven by the volume of material processed (Szklo et al., 2007). However, it only represents the case where processing the crude fractions and their derived intermediate products is not constrained by the size or installed capacity of individual processes. Using this approach, energy-intensity (in terms of energy use per barrel of input crude) will be a differentiator in the refinery energy use and GHG emissions estimates for a particular crude. PRELIM could be modified to reflect process unit capacity constraints but is not included in the current version of the model.

For the purposes of transparency and completeness, the data available in the model for process energy requirements is presented as a range of plausible values derived from the literature (see Table 5). The ranges of process energy requirements are wide in particular for hydroprocessing and the FCC process (e.g., 106 to 498 MJ of fuel/bbl in hydrocracking; 0 to 34 MJ of fuel/bbl in FCC). The data are compared with confidential information and discussed with experts from industry to conclude that such values and their ranges are feasible. The ranges in fuel and steam requirements arise from desired product yields and heat integration systems (see operation of delayed coking or FCC Catalyst regeneration in section 4.2.5 for examples). The range of electricity required is associated with the process unit operating conditions and layout of a unit operation. For example, in the case of the hydrotreating process unit, the range of plausible electricity requirements is wide due to variability in pressure, hydrogen consumption, and whether the makeup compressors are onsite or offsite (Karpe, 2010).

Table 5: Summary of range of energy requirements from literature

Process Unit	***Hydrogen*** kg/bbl[a]	***Fuel Gas*** MJ/bbl	***Electricity*** MJ/bbl	***Steam*** MJ/bbl[b]	***Source***
Desalting			0.00720-0.216		1, 2
Atmospheric Distillation		52.9-95.3	1.80-3.24	16.1-40.7	1, 2
Vacuum Distillation		31.8-95.3	1.08	16.1-81.4	1, 2
Hydrotreating					1, 2, 3
Naphtha	0.0602-0.337	0.0491-105	4.32-7.20	9.77-45.6	
Kerosene	0.0602-1.34	159-240	6.12-10.8	4.23-13.0	
Diesel	0.120-0.963	34.8-158	6.12	11.1	
Gas Oil	0.241-2.17	35.8-212	3.24-21.6	11.7-16.3	
Fluid Catalytic Cracking		0.00-105	2.70-7.67	4.70-17.3	1, 2, 3
Alkylation			10.1-39.6	58.6-293	1, 2, 3
Gas Oil Hydrocracking	2.41-7.22	106-498	12.2-64.8	81.4-163	1, 2, 3
Delayed Coking		114-178	4.32-13.0	-29.6-65.1	1, 2, 3
Naphtha Catalytic Reforming		2.64-286	2.16-10.8	48.8-65.1	1, 2, 3
Isomerization	0.0963	190	2.88-3.60	0.00-94.1	1, 2
	MJ chemical feedstock/kg H_2	MJ/kg H_2	MJ/kg H_2	MJ/kg H_2	
Steam Methane Reforming	97.8-139	16.3-102	0.777-1.26	(0.0505)-0.00	1, 2, 3, 4, 5

[a]- Factor to convert in mass basis 0.0024 kg of hydrogen per scf at 14.7 psi (1 atm) and 60 °F (15.6 °C).

[b]- Factor to convert in energy basis 3.59 MJ/kg of steam at 750 psi (5171 kPa) pressure and 1050 °F (565°C) temperature.

[1] Gary, J.; Handwerk, G.; Kaiser, M., *Petroleum Refining Technology and Economics* Fifth ed.; CRC Press: New York, 2007.

[2] Maples, R., *Petroleum Refinery Process Economics.* Second ed.; PennWell Corp: 2000.

[3] Parkash, S., Refining Processes Handbook. Elsevier: Burlington, 2003.

[4] Skone, T.; Gerdes, K. *Development of Baseline Data and Analysis of Life Cycle Greenhouse Gas Emissions of Petroleum-Based Fuels* DOE/NETL-2009/1346; National Energy Technology Laboratory (NETL): November 26, 2008.

[5] Spath, P. L.; Mann, M. K. *Life Cycle Assessment of Hydrogen Production via Natural Gas Steam Reforming*; NREL/TP-570-27637; National Renewable Energy Laboratory: 2001.

PRELIM default values for process energy requirements are from Gary et al. (2007). The data are described as "average typical energy requirements" suitable for conducting economic analysis of different configurations close to the year of publication. As in the case of process unit yield correlations (section 4.2.5), the data applies for some refineries but not all. This reference is considered a good representation of basic performance indicators in industry based on discussion with industry experts (Karpe, 2009). However, users are encouraged to input their own data if available for these parameters in the model. Table 4 details the default process energy requirements for each unit. The table aggregates the data to also include the range of energy requirements reported for the U.S. refinery industry (Energetics, 2007) for comparison.

4.2.4 Hydrogen addition processes and global hydrogen mass balance method

One of the main functions of a refinery is to increase the hydrogen to carbon ratio of a crude, and hence, convert it into more valuable products. Therefore, differences in hydrogen content between feedstock and refined products are significant factors that drive refinery GHG emissions. PRELIM uses a global hydrogen mass balance method to determine the hydrogen requirements for each hydroprocessing unit, taking also into account the hydrogen produced by the naphtha catalytic reforming process unit. Differences in the feedstock's hydrogen content are considered, as well as the assumption that all crudes are to be processed to meet intermediate and final product hydrogen specifications.

Hydrotreating and hydrocracking processes increase the hydrogen to carbon ratio of the feedstock by means of hydrogen addition. Hydrogen is added to the molecules at elevated temperature and pressure in the presence of a catalyst while sulphur, nitrogen, and metals are removed. Several chemical reactions occur and result in a hydrotreated liquid product and fuel gas. The main distinction between hydrotreating and hydrocracking processes is the severity of conversion associated with their operating conditions. Hydrotreating occurs under milder operating conditions (lower pressure and temperature) compared to hydrocracking. Therefore, in a hydrotreating process unit, the boiling range and hydrogen content of the process unit feed is only slightly altered through the process unit. Conversely, the operating conditions in hydrocracking process units contribute to breaking the large hydrocarbon molecules of the process unit feed, increasing the yield of lighter products, and saturating aromatics and olefins (i.e., breaking the double or triple bonds between two carbon atoms present in these types of hydrocarbon molecules, and attaching the hydrogen to the carbon atom). Figure 2 shows the inputs and outputs as well as the subsequent process unit of the output for the naphtha, kerosene, diesel, and gas oil hydrotreating process units and for the gas oil and vacuum residue hydrocracking process units present in the model.

4.2.4.1 Global hydrogen mass balance method at the process unit level

In PRELIM, a global hydrogen mass balance method is used to determine hydrogen requirements in the hydrotreating and hydrocracking process units. Using this method, the hydrogen requirement for each process unit is calculated by taking the difference in hydrogen content between the mass of the process unit feed input (liquid feed) and the mass of the hydrotreated liquid product and fuel gas (Figure 6).

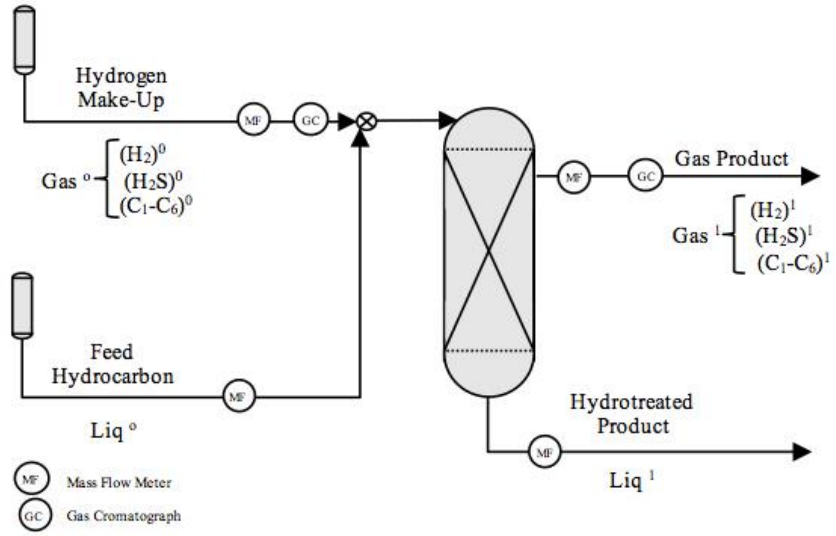


Figure 6: Global Hydrogen Mass Balance Method at the Process Unit Level

> Figure modified from Castañeda et al. (2011)

This method is adopted because it accounts for the hydrogen content of each fraction and is a good representation of the hydrocarbon molecules present in any particular crude fraction. Also, it allows for a simple method to identify the destination of the hydrogen supplied (i.e., the hydrogen flow through the refinery and the identification of the source of the associated energy requirements and GHG emissions). Although the global hydrogen mass balance method is relatively simple, in PRELIM several additional assumptions are required and are outlined below.

4.2.4.2 Hydrotreating process units assumptions

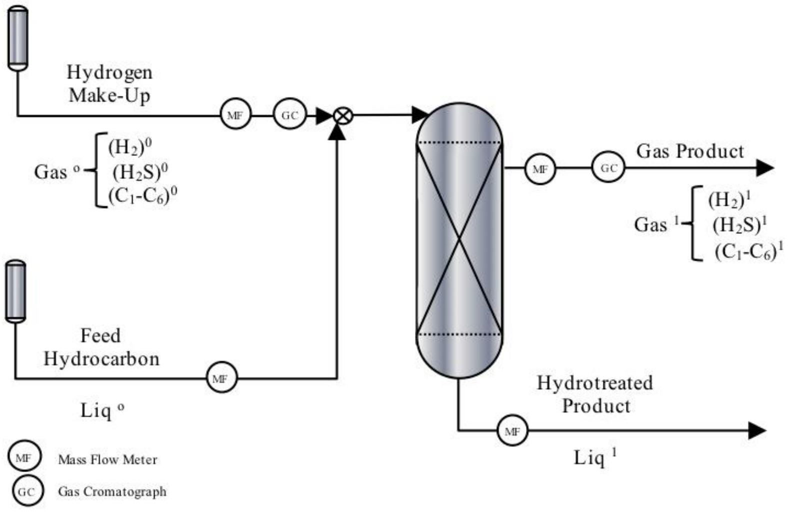
An important assumption is the hydrogen content of the hydrotreated liquid, which is defined based on the type of crude fraction that is hydrotreated. For example, the hydrogen content for hydrotreated diesel is assumed to be 12.8 wt% while the hydrogen content for hydrotreated FCC feed (gas oil fractions) is assumed to be 12.5 wt%. The former is derived from a diesel fuel carbon coefficient estimated by the U.S. Energy Information Administration and assuming the content of other elements to be negligible (%wt hydrogen equals 100% minus %wt carbon)(EIA, 2008). The latter represents the hydrogen content used to obtain high gasoline yields from the FCC process unit (Brierley et al., 2006). By using assumptions about the hydrogen content of the hydrotreated liquid, it is assumed that all refinery crude feedstock is processed to meet the same intermediate product specifications. However, because PRELIM does not distinguish between the structural compositions of the crude fractions (hydrogen content is an aggregated representation of the hydrocarbon molecules in the crude fraction), it is not feasible in the current version of PRELIM to track the quality of the final products to ensure they meet fuel aromaticity specifications.

In real operations, if a crude of high aromaticity is processed in a configuration without a hydrocracking process unit and milder operating conditions (i.e., lower pressure and temperature), the aromatics do not get destroyed and they end up in the diesel (Karpe, 2011). However, in hydrotreating process units, aromatics saturation is facilitated by operating variables such as hydrogen purity of recycled gas, pressure in products separator, type of catalyst, and ratio of volume feed to volume catalyst. All of these variables are related to the hydrogen partial pressure in the reactor. These variables are defined prior to the process unit operation by economic analysis and process unit design (Jones et al., 2006). PRELIM does not model these parameters and assumes that the hydrotreating units operate under the appropriate operating conditions to comply with the fuel specifications and that the hydrogen content of the final product represents the structural composition expected.

Another important assumption is the amount and quality of the fuel gas produced in the hydrotreating units which define the process unit product yields (i.e., hydrotreated liquid product and fuel gas). As the fuel gas produced in refineries is a mixture of streams generated in various refinery processes, its composition varies constantly. Usually, this fuel gas contains hydrogen, methane and ethane, some propane and butane, and higher molecular weight gases (Grover et al., 2007; Márquez-Riquelme et al., 2010). The ideal calculation to determine fuel gas production as well as its composition is refinery and unit operation specific: "Flash calculations for each unit operation (not each type of unit) to determine the offgas composition. There is no rule of thumb. Depending on design, the feedstock, and the severity, the hydrogen content could be anywhere from 10 to 60% of the combined offgases" (Karpe, 2010). Therefore, in PRELIM, the estimates of the mass of fuel gas produced are a first approximation and will differ somewhat from real operations. The amount of fuel gas produced in the hydrotreating process units is assumed to be composed of a hydrocarbon fuel gas free of sulphur (Figure 6, mass of H and (C1-C6) in stream Gas^1) and hydrogen sulphide gas (Figure 6, H2S in stream Gas^1). The hydrocarbon fuel gas free of sulphur is assumed to be 0.2wt% of the process liquid feed (Parkash, 2003). Also, the hydrogen content of this fuel gas is assumed to be 22wt% (holding this assumption constant throughout the refinery), which represents a distribution of the hydrogen both in the hydrocarbons as well as the hydrogen present as H in the fuel gas (Grover et al., 2007). The mass of hydrogen sulphide (also known as acid gas) is calculated using the sulphur content of the liquid feed (i.e., sulphur content of the crude fraction), a percentage of sulphur removal through hydrodesulphurization (every mole of sulphur uses 2 moles of hydrogen to convert it into H2S). The hydrogen needed to produce the hydrogen sulphide is in addition to the hydrogen requirements from the fuel gas free of sulphur. The hydrogen consumption due to hydrodenitrogenation is accounted for by including the hydrogen content of the liquid product in the calculation. Hydrogen consumption to remove nitrogen is negligible compared to the hydrogen needed to saturate the molecules from which this element is removed (see Figure 8). These assumptions are needed to determine (by mass balance) the amount of liquid product coming out of the hydrotreating process units. The mass and volume yield estimates of liquid product from the hydrotreating process units neglect the slight change in the boiling point range of the hydrotreating process unit feed. The liquid product in real operations is separated into different intermediate products based on their boiling range (as crude is separated into its fractions). PRELIM assumes it to be a single product in the same boiling point range.

Figure 7 explains these assumptions in more detail and illustrates the steps in the hydrogen mass balance for the hydrotreating process unit of the FCC feed (gas oil hydrotreating process unit). In addition

Figure 8 shows the calculated values for this combination of assumptions for a specific bitumen crude.



Hydrotreating of FCC Feed

Global Mass Balance:

$$\mathbf{Gas^0 + Liq^0 = Gas^1 + Liq^1}$$

inlets (^{0}) and oulets (^{1})

Gas^0, Gas^1, and Liq^1 are unknown, then

Gas^1 Flow

Assumption

1. Yield of Fuel Gas $[(C1\text{-}C6)+H2]^1$: 0.2 wt% of process liquid feed

$$\rightarrow Gas^1 = 0.002\, Liq^0 + H_2S$$

Liq^1 Flow

Assumptions

2. Hydrogen Make-up purity: 100%

$$Gas^0 = H^0$$

3. Fuel Gas Hydrogen Content $[(C_1\text{-}C_6)+H2]^1$: 22 wt%
4. Hydrotreated Liquid Product (FCC Feed) Hydrogen content: 12.5 wt%
5. Hydrotreated Liquid Product Sulphur and Nitrogen content negligible

$\rightarrow Liq^1 = (Liq^0\ (1\text{-}\%H\text{-}\%S\text{-}\%N)\ \text{-}\ (Fuel\ Gas^1\ (1\text{-}0.22))/(1\text{-}0.125)$

Gas^0 Flow or Hydrogen Requirements

Global Balance of Hydrogen :

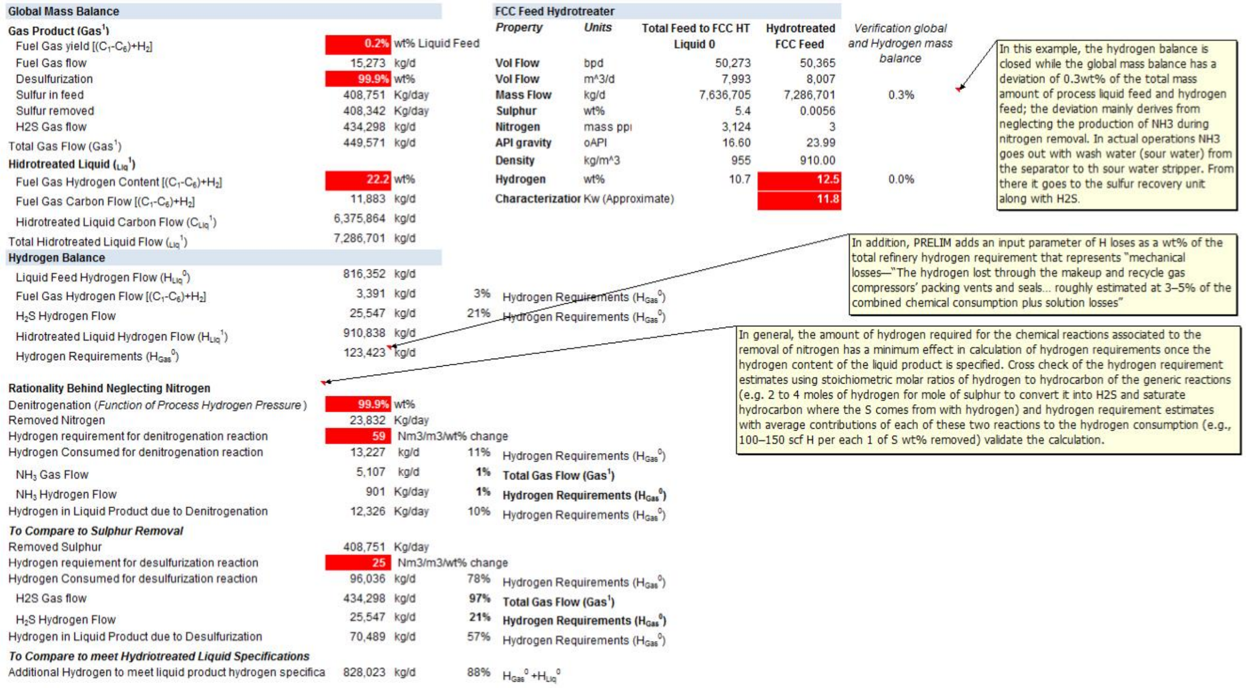
$$\mathbf{H^0_{Gas} + H^0_{Liquid} = H^1_{Gas} + H^1_{Liquid}}$$

$H^0_{Liquid} = 0.22\, Liq^1$
$H^1_{Gas} = 0.22\, Gas^1 + H^1_{H_2S}$
$H^1_{Liquid} = 0.125\, Liq^1$

$$\rightarrow H^0_{Gas} = H^0_{Make\text{-}up} = Gas^0 = H^1_{Gas} + H^1_{Liquid} - H^0_{Liquid}$$

Figure 7: PRELIM Hydrogen Balance Calculation Method

Figure modified from Castañeda et al. (2011)



Global Mass Balance				
Gas Product (Gas^1)				
Fuel Gas yield $[(C_1\text{-}C_6)+H_2]$	0.2%	wt% Liquid Feed		
Fuel Gas flow	15,273	kg/d		
Desulfurization	99.9%	wt%		
Sulfur in feed	408,751	Kg/day		
Sulfur removed	408,342	Kg/day		
H2S Gas flow	434,298	kg/d		
Total Gas Flow (Gas^1)	449,571	kg/d		
Hidrotreated Liquid ($_{Liq}$^{1})				
Fuel Gas Hydrogen Content $[(C_1\text{-}C_6)+H_2]$	22.2	wt%		
Fuel Gas Carbon Flow $[(C_1\text{-}C_6)+H_2]$	11,883	kg/d		
Hidrotreated Liquid Carbon Flow (C_{Liq}^1)	6,375,864	kg/d		
Total Hidrotreated Liquid Flow ($_{Liq}$^{1})	7,286,701	kg/d		
Hydrogen Balance				
Liquid Feed Hydrogen Flow (H_{Liq}^0)	816,352	kg/d		
Fuel Gas Hydrogen Flow $[(C_1\text{-}C_6)+H_2]$	3,391	kg/d	3%	Hydrogen Requirements (H_{Gas}^0)
H_2S Hydrogen Flow	25,547	kg/d	21%	Hydrogen Requirements (H_{Gas}^0)
Hidrotreated Liquid Hydrogen Flow (H_{Liq}^1)	910,838	kg/d		
Hydrogen Requirements (H_{Gas}^0)	123,423	kg/d		
Rationality Behind Neglecting Nitrogen				
Denitrogenation (*Function of Process Hydrogen Pressure*)	99.9%	wt%		
Removed Nitrogen	23,832	Kg/day		
Hydrogen requirement for denitrogenation reaction	59	Nm3/m3/wt% change		
Hydrogen Consumed for denitrogenation reaction	13,227	kg/d	11%	Hydrogen Requirements (H_{Gas}^0)
NH_3 Gas Flow	5,107	kg/d	**1%**	**Total Gas Flow (Gas^1)**
NH_3 Hydrogen Flow	901	Kg/day	**1%**	**Hydrogen Requirements (H_{Gas}^0)**
Hydrogen in Liquid Product due to Denitrogenation	12,326	Kg/day	10%	Hydrogen Requirements (H_{Gas}^0)
To Compare to Sulphur Removal				
Removed Sulphur	408,751	Kg/day		
Hydrogen requiement for desulfurization reaction	25	Nm3/m3/wt% change		
Hydrogen Consumed for desulfurization reaction	96,036	kg/d	78%	Hydrogen Requirements (H_{Gas}^0)
H2S Gas flow	434,298	kg/d	**97%**	**Total Gas Flow (Gas^1)**
H_2S Hydrogen Flow	25,547	kg/d	**21%**	**Hydrogen Requirements (H_{Gas}^0)**
Hydrogen in Liquid Product due to Desulfurization	70,489	kg/d	57%	Hydrogen Requirements (H_{Gas}^0)
To Compare to meet Hydriotreated Liquid Specifications				
Additional Hydrogen to meet liquid product hydrogen specifica	828,023	kg/d	88%	$H_{Gas}^0 + H_{Liq}^0$

FCC Feed Hydrotreater				
Property	***Units***	**Total Feed to FCC HT Liquid 0**	**Hydrotreated FCC Feed**	*Verification global and Hydrogen mass balance*
Vol Flow	bpd	50,273	50,365	
Vol Flow	m^3/d	7,993	8,007	
Mass Flow	kg/d	7,636,705	7,286,701	0.3%
Sulphur	wt%	5.4	0.0056	
Nitrogen	mass ppı	3,124	3	
API gravity	oAPI	16.60	23.99	
Density	kg/m^3	955	910.00	
Hydrogen	wt%	10.7	12.5	0.0%
Characterizatior	Kw (Approximate)		11.8	

In this example, the hydrogen balance is closed while the global mass balance has a deviation of 0.3wt% of the total mass amount of process liquid feed and hydrogen feed; the deviation mainly derives from neglecting the production of NH3 during nitrogen removal. In actual operations NH3 goes out with wash water (sour water) from the separator to th sour water stripper. From there it goes to the sulfur recovery unit along with H2S.

In addition, PRELIM adds an input parameter of H loses as a wt% of the total refinery hydrogen requirement that represents "mechanical losses—"The hydrogen lost through the makeup and recycle gas compressors' packing vents and seals… roughly estimated at 3–5% of the combined chemical consumption plus solution losses"

In general, the amount of hydrogen required for the chemical reactions associated to the removal of nitrogen has a minimum effect in calculation of hydrogen requirements once the hydrogen content of the liquid product is specified. Cross check of the hydrogen requirement estimates using stoichiometric molar ratios of hydrogen to hydrocarbon of the generic reactions (e.g. 2 to 4 moles of hydrogen for mole of sulphur to convert it into H2S and saturate hydrocarbon where the S comes from with hydrogen) and hydrogen requirement estimates with average contributions of each of these two reactions to the hydrogen consumption (e.g., 100–150 scf H per each 1 of S wt% removed) validate the calculation.

Figure 8: Illustration of PRELIM hydrogen balance calculation for hydrotreating of fluid catalytic cracking feed

4.2.4.3 Hydrocracking assumptions

The level of conversion in hydrocracking processes and yields of process unit products depend on the type of catalyst and specific design of the process unit (Parkash, 2003). PRELIM hydrocracking product yields (mainly gasoline, medium and heavy gas oils, and fuel gas) are correlated to three parameters: 1) process unit feed API, 2) crude fraction characteristic boiling point, and 3) an approximated hydrogen requirement that can represent different levels of severity of the process unit operating conditions (i.e., the level of conversion sought). PRELIM uses correlations from Gary et al. (2007) that provide data for two feeds of extreme quality (paraffinic and highly naphthenic/aromatic) and three different levels of hydrogen requirements (500, 1500, and 2500 scf hydrogen/bbl). The correlations also provide a method to estimate the hydrogen content of the hydrocracking process unit products. The hydrogen requirements of the hydrocracking process unit are then calculated by the global hydrogen mass balance method. However, these correlations do not capture variation in process unit product yields due to changes in the type of catalyst, which varies among refineries.

4.2.4.4 Origin of hydrogen supplies and greenhouse gas emissions associated with its production

In PRELIM, the global hydrogen mass balance method is also applied to determine the yield of produced hydrogen and fuel gas from the naphtha catalytic reforming process unit. Basically, this process unit rearranges the carbon and hydrogen bonds of the hydrocarbon molecules to increase the octane of naphtha fractions by means of dehydrogenation and production of aromatic components. In this case, issues with aromatic content of the process unit feed and yields of fuel gas and hydrogen due to process unit operating conditions exist as well. The difference between hydrogen requirements for hydroprocessing and hydrogen production from the naphtha catalytic reformer determines SMR hydrogen needs from which offsite refinery energy use can be determined. In PRELIM, the fuel gas is prioritized to be used first in supplying heat, second in steam production, and finally as a feedstock for hydrogen production (similar scheme to actual refinery operations). Natural gas is only used to offset energy requirements that are not supplied by the fuel gas and as the main feedstock for hydrogen production. The amount and energy content of the fuel gas produced on site is subtracted from the total amount of energy required for all the refinery operations to estimate the amount of natural gas that is required from offsite and determine the upstream GHG emissions associated with this. Also, the amount of hydrogen produced from the SMR is the main determinant of GHG emissions from hydrogen in the refinery. The emissions are mainly CO_2 that is produced during the chemical transformation of natural gas into hydrogen (chemical reaction in which a mole of CO_2 is formed for every mole of carbon in the natural gas), in addition to the combustion emissions from supplied fuel and steam used to satisfy the SMR process energy requirements. Using PRELIM default values, direct refinery emissions from either using natural gas or refinery fuel gas are very similar as it is assumed that the hydrogen content of both feedstocks are similar. Preliminary results show that the heating value, the amount of refinery fuel gas and the range of possible emissions factors for the refinery fuel gas does not have a significant effect on the refinery GHG emissions (see sections 5.2 and 5.3.1 from Abella [2012] for details).

The hydrogen balance is the most challenging task in refinery operations and modelling. In real operations, the hydrogen balance of the whole refinery can be affected by a cumulative error resulting from varied levels of accuracy in the measurement of flow rate and hydrogen content of several refinery streams (e.g., purge gas from a high-pressure hydrocracker)(Stratiev et al., 2009). At the process unit level, the most common method used by refinery operators – based on the hydrogen balance of the gas streams (streams Gas^0 and Gas^1 in Figure 6) can underestimate hydrogen consumption up to 6% (Castañeda et al., 2011). In modelling, there is no method more accurate for predicting hydrogen consumption. When the process unit streams (liquid feed, hydrotreated liquid product, and fuel gas) are experimentally characterized, the global hydrogen mass balance method is considered to be more accurate than simple and quick calculation methods used by refinery operators (e.g., based on the type of crude fraction processed and process unit volume feed or based on the hydrogen balance of the gas streams). When the global hydrogen mass balance method is adopted based on empirical correlations, the hydrogen requirement estimates can have a standard deviation that ranges from 9 to 15% compared with experimental data for hydrotreating processes (Castañeda et al., 2011). Several other methods exist to determine the hydrogen requirements of hydrotreating processes (see for example Castaneda et al. [2011] and Stratiev et al., [2009] for a description and comparison of such methods). However, they require a high level of complexity in modelling (more detailed representation of the chemical reactions that take place) or additional data collection that is not desirable for the purposes of policy analysis. Also, they do not perform better than a global hydrogen mass balance based on empirical correlations. Deviations from experimental data for all methods are specific to the type of crude fraction hydrotreated, but standard deviations can be as high as 50% (Castañeda et al., 2011). The PRELIM global mass hydrogen balance approach (i.e., the use of approximations for hydrogen content instead of empirical correlations associated with the structural composition of the molecules) is evaluated against a more detailed and different modelling approach (sections 5.1.1 shows the methods and 5.2.4 shows the results).

4.2.4.5 Surplus Hydrogen

Some crudes have more hydrogen in certain fractions then what is needed to meet the specifications of the intermediate or final products. In a refinery this would be dealt with by blending crudes in such a way to meet specifications with minimal amounts of additional hydrogen required. Due to the fact that PRELIM can estimate energy and GHG emissions for an individual crude, this needs to be handled in a slightly different way. This surplus can occur in the hydrotreaters throughout the refinery or in the naphtha catalytic reformer. The type of surplus is different for these two types of units. That is, hydrotreater hydrogen surplus is simply a higher hydrogen content of the hydrocarbon molecules. Therefore, the hydrogen is not readily available to be used in other process units in the refinery; instead, the stream exiting the unit is higher than the intermediate product specifications. This is different for the surplus hydrogen provided in the NCR. This hydrogen is in a form that can be readily used in a variety of process units throughout the refinery. Therefore, the hydrogen produced by the NCR is used to satisfy hydrogen requirements in the refinery. If this hydrogen is not sufficient to meet the refinery demands, the SMR will be used to supplement the hydrogen from the NCR. If there is a surplus of hydrogen in the NCR then the SMR will not be used and more hydrogen is produced by the NCR than is needed by the refinery. Again, in a refinery this would be used to process other crudes in the refinery. In order to calculate the energy and GHG emissions associated with a crude that produces a surplus of hydrogen, this must be taken into account. This can be done in several ways. Below we describe the simple way in which PRELIM handles this surplus for the two main functional units currently available in PRELIM.

4.2.4.5.1 Total refinery emissions

If the functional unit of per bbl of crude input is selected, any surplus hydrogen produced in the NCR is considered a product. Ultimately, this hydrogen could be used to process other crudes, sold outside of the refinery etc. It is possible to consider a credit for this hydrogen if it offsets another product (e.g., SMR produced hydrogen), however, what is being offset must be determined in order to do this. Therefore, the total refinery emissions will include the emissions associated with producing this product and PRELIM reports the amount of surplus hydrogen that is produced within the product slate output tabs. If surplus hydrogen occurs in the hydrotreaters, the hydrogen is simply carried into the output product stream. The value of this additional hydrogen is uncertain. A future version of PRELIM could explore ways to credit this surplus.

4.2.4.5.2 Emissions per final product

If the functional unit of per MJ of final product is selected, any surplus hydrogen produced by NCR will be considered a final product and will have emissions allocated to it. This will result in a reduction of emissions for the rest of the product slate. However, to date, any crudes that produce surplus hydrogen have altered product emissions by negligible amounts. If surplus hydrogen is present in any of the hydrotreaters, the hydrogen will be passed on to the output products.

4.2.5 Carbon rejection processes and product yields

FCC and delayed coking processes increase the hydrogen to carbon ratio of the feedstock by means of carbon rejection. The heavy material is broken into molecules of varied hydrogen to carbon ratio under pressure and high temperature. The vapours of the molecules with the lowest hydrogen to carbon ratio condense to produce coke (“large polynuclear aromatics precipitate to form crystalline liquids and ultimately solidify to form coke”, Robinson [2006]); the remaining material is separated into desired process unit products by fractionation. Figure 2 shows the inputs and outputs as well as the destination of the outputs for FCC and delayed coking process units in the model.

4.2.5.1 FCC process unit

The FCC process upgrades crude gas oil or medium fractions (atmospheric and vacuum gas oils) in the presence of a powdered catalyst whereby coke formation is minimized during the cracking of the heavy hydrocarbons. During the process unit operation, the coke is deposited on the catalyst, and the catalyst is later recovered to be recycled in the process unit, which requires the coke to be burned off (i.e., catalyst regeneration process). The energy from the combustion of the coke supplies the heat of reaction and heat required to vaporize the FCC process unit feed (Parkash, 2003). In addition, the gases resulting from coke combustion have energy content that can be recovered for use in the process unit (e.g., production of electricity using a turbo expander or steam generation using a waste heat boiler).

In PRELIM, FCC product yields (mainly gasoline, medium and heavy gas oils, unsaturated LPG, fuel gas, and coke) are correlated to two parameters: 1) conversion of process unit feed into products (PRELIM input parameter) that can represent process unit operating conditions (i.e., temperature, pressure, and catalyst to oil ratio), and 2) a characterization parameter called Watson characterization factor (Kw) that combines a crude fraction characteristic boiling point and specific gravity to represent the structural composition of the crude fraction (Watson, 1933). The structural composition is a key feed characteristic for the FCC process unit operation. Aromatics crack less easily than paraffins; therefore, increasing aromatic content in the FCC feed increases yields of coke and fuel gas and decreases overall conversion and yields of gasoline (Parkash, 2003). PRELIM uses correlations from Gary et al. for a zeolite catalyst and for two Kw values (Gary et al., 2007)(11.8 and 12.4) that represent only half of the scale of Kw values that can be expected. Highly paraffinic crudes will have a Kw of 12.5 while highly naphthenic or aromatic materials will approach 10 as a minimum value (Watson, 1933). The use of these correlations does not capture variation in process unit product yields due to changes in the type of catalyst that varies among refineries or due to use of highly naphthenic/aromatic feeds. (PRELIM includes an alternative calculation method that assumes a constant distribution of products yield if specific yields are known by the user).

PRELIM's structure assumes that all FCC feed has to be hydrotreated. PRELIM allows the choice of upgrading heavy gas oil products resulting from the delayed coking process unit in the FCC process unit. That gas oil may be highly naphthenic/aromatic (based on the quality of the crude), and the expected Kw for such gas oil can be lower than 11.8 (e.g., Fisher [1990] presents Kw values for different FCC feedstocks that range from 10.7 from a fluid coking-derived vacuum gas oil to 11.5 for a Canadian conventional crude). Hydrotreating the FCC feed saturates some of the hydrocarbon molecules present, decreasing the relative amounts of aromatics and napthenes in the gas oil fractions to be represented for a high Kw value. It is assumed that the Kw curve of 11.8 applies in such cases.

The application of PRELIM showed that the Kw factor calculated for the blend of gas oil fractions of the crudes included in PRELIM crude assay inventory (without including delayed coking gas oils and hydrotreating) ranges from 11.1 to 11.9. The correlation for a Kw of 11.8 is used as a default, and the correlation for Kw 12.5 is used to explore the effects of differences in FCC process unit product yields due to changes in the Kw value. Additionally, a conversion of 75% is used as a default value as it is recommended to be used for heavy crude fractions by Gary et al. (2007).

4.2.5.2 Delayed coking

Delayed coking can upgrade a variety of feedstocks; typically the heaviest fraction resulting from the vacuum distillation process is upgraded (vacuum residue). The delayed coking process occurs in the absence of a catalyst and the conversion of the residue feed into lighter products occurs by means of heat alone; high residence time favours the cracking reactions and the amount of coke produced is considerable (e.g., for the current assay inventory, coke yield can be up to 40%wt of a crude vacuum residue fraction). Variation in the operating conditions such as temperature and pressure, in addition to process unit feed quality, can affect the amount of coke produced as a refinery final product.

In PRELIM, the delayed coking process unit product yields (i.e., coke, fuel gas, coking heavy naphtha, and [indirectly by means of mass balance] coking gas oil yields) are linearly correlated to the amount of carbon residue in the process unit feed (Gary et al., 2007). "The carbon residue is the residue that remains after evaporation and pyrolysis of crude oil under given conditions..., it is indicative of the coke-forming tendency of the crude under thermal degradation conditions" (Hassan et al., 2009). The use of such a correlation is important because it accounts for the quality of the heaviest fractions of the crude and uses a parameter that is easy to measure. For example, a technique such as "Micro Carbon Residuum" uses small amounts of sample and simple laboratory instruments (Hassan et al., 2009). PRELIM uses correlations from Gary et al. (2007) for coke and liquid yields based only on the carbon residue. However, in the delayed coking process unit, temperature, pressure, and product recycling ratio are used to control delayed coking yields and product quality (Parkash, 2003). Using the Gary correlation, PRELIM will not capture variations in delayed coking product yields due to changes in these operating conditions.

4.2.6 Liquefied petroleum gases

PRELIM assumes that propane and butane, derived from different process units, are used as a refinery fuel gas and blended into gasoline respectively. However, this represents only one possible destination for these intermediates products. Refineries can opt for recovering the propane and butane to be sold as petrochemical feedstock or as a combination of gases to be sold as LPG. Some refineries consider gasoline a more economically desirable product than LPG and blend most butanes into gasoline, as n- butane or as alkylate after being isomerized (isobutene) and transformed in an alkylation process unit (Gary et al., 2007). PRELIM calculation methods group lighter gases (i.e., it does not distinguish between methane, ethane, propane and butanes) derived from the crude distillation process unit or from fuel gas produced on site. This simplified approach does not allow for considering a scenario where LPG is produced and sold as a transportation fuel. However, this is a planned expansion for a future version of PRELIM.

To model the alternative production pathways of LPG in a way that reflects changes in refinery crude feedstock, more detailed modelling and data are needed. It requires light ends crude assay data (volume percent distribution of the low molecular weight compounds that are present in the crude and include, but are not limited to, methane, ethane, propane, and butanes), and an estimate of the mass fraction of these components for each crude assigning/using molecular weight and density to each component (i.e., pseudo-components method [Parkash, 2003]). In addition, it is necessary to include a material balance component that allows for tracking the different sources of propane and butane through the model. For example, currently the model routes C3 and light ends in the hydrocracking process unit to the refinery fuel gas and the C4 to gasoline, while it sends the C3 and C4 in the FCC process unit to the alkylation process unit. Finally, a light ends recovery plant has to be added to the PRELIM configuration. It is mostly distillation process units that separate these gases in the same way that the crude is separated into its fractions.

These modelling components could be incorporated into the current PRELIM structure for the purposes of modelling LPG as a final product. However, the level of complexity associated with modelling LPG production will not necessary result in a better differentiation of the refinery energy use and GHG emissions associated with a particular crude. A rough estimate, based on runs of a proprietary model, indicates that less than 5%wt of the whole crude can end in a light ends recovery plant, and less than 2wt% of the whole crude can be transformed into LPG in a refinery with similar structure as represented in PRELIM (Baker & O'Brien). Basically, overall refinery energy use and GHG emissions would be affected by the energy use linked directly to processing this amount of material in the light ends recovery plant. Also, refinery products energy and GHG emissions intensity will vary depending on the process-based allocation method used to assign these to each crude.

4.3 PRELIM crude assay inventory

The PRELIM Crude Assay Inventory is developed to allow a user to select from a predetermined list of crude assays. If a user does not have access to their own assay, they can select a crude that is close to the crude they are interested in investigating without having to collect or measure this sensitive data themselves. However, any petroleum-based crude assay can be input and run in the model. The construction of the inventory requires transformations of simplified data in the public realm and demonstrates a method that can be used by others. The current PRELIM crude assay inventory includes 51 publicly available crude assays from different fields in various countries obtained from the websites of different major oil companies (BP, Chevron, ExxonMobil, and Statoil) as well as from the Knovel database and the Canadian Crude Quality Monitoring Program (CCQMP, http://www.crudemonitor.ca), with permission from these sources. The inventory thus includes a comprehensive range and diversity of qualities. Currently, at least two crude assays represent each of these general crude classification categories in the PRELIM crude assay inventory. Western Conventional Canadian crudes are well characterized using the data available in the public realm.

PRELIM requires characterization of the crude properties for nine crude fractions (Figure 2, section 4.2.1). The scheme of separating the crude into nine fractions is selected to get the flexibility to model different configurations. For example, PRELIM provides the flexibility to route each of the three crude gas oil fractions to hydrocracking and/or FCC process units in a different proportion (e.g., route 50% of the crude atmospheric gas oil fraction to FCC and 50% to hydrocracking). This requires that the assay data obtained be transformed prior to use in PRELIM. CCQMP provides information for only four crude fractions and does not include hydrogen information. Confidential data provide more detailed information, but the crude fractions are narrower than the data required by PRELIM (up to 15 crude fractions can be analyzed with standard techniques). This section details how the assays are transformed and the assumptions that are required in order to obtain the complete set of information needed (i.e., 62 parameters associated with the five crude oil properties). The methods used for validation/verification/evaluation of the final data are also explained. Table 6 shows the property ranges (presented as minimums and maximums) for each crude oil fraction of the PRELIM crude assay inventory and illustrates the 62 parameters needed (white dotted cells). As mentioned in section 2.3.5 several new assays from different companies (including BP, Chevron, ExxonMobil, Statoil, and Knovel) have been added to the assay inventory of the current version of the model with the companies' permission. For the sake of demonstration, crude monitor assays that were first added to the early versions of the model are discussed in section 4.3. A similar process is used to transform the assay data from other sources.

Table 6: Property ranges for each crude oil fraction of the PRELIM's crude assay inventory

Description	***Range***	***Whole Crude***	***LSR***	***Naphtha***	***Kerosene***	***Diesel***	***AGO***	***LVGO***	***HVGO***	***VR***	***AR***
Sulphur (wt%)	Min	0.0900	0.000	0.000	0.0100	0.0500	0.0900	0.180	0.310	0.100	0.220
	Max	5.14	0.310	0.980	2.17	2.98	3.54	4.18	4.90	8.55	7.47
Nitrogen (ppm)[a]	Min	350	0.00	0.00	0.00	35.0	194	514	1002	321	872
	Max	4600	0.00	9.00	152	733	1390	2203	3116	7077	5709
API gravity	Min	7	35	35	28	22	17	12	7	-1	1
	Max	39	105	76	41	33	29	25	22	14	40
Density (kg/m3)	Min	828	598	682	819	860	882	901	921	969	824
	Max	1019	848	848	887	924	953	988	1022	1111	1111
Hydrogen (wt%)	Min	10.1	12.2	12.2	12.0	11.6	11.1	10.3	9.6	8.0	8.7
	Max	13.2	18.9	15.5	13.3	13.4	12.9	12.6	12.2	13.8	12.8
MCR (wt%)	Min	0.02								1.72	
	Max	14.7								32.0	
Approximated Kw	Min	11.0	10.7	10.9	11.1	11.1	11.0	10.9	10.9	10.6	10.6
	Max	12.2	13.9	12.4	11.8	11.8	11.9	11.0	12.0	11.8	12.0
Tb(50%) weight basis (°C)	Min	296	26	111	221	302	360	404	452	534	203
	Max	467	214	214	276	326	377	431	493	687	700
Mass fraction yield(%)	Min	100	0.00	0.00	1.70	4.80	6.00	7.00	5.00	1.00	19.0
	Max	100	8.00	21.0	26.4	20.0	26.0	26.0	15.9	59.3	83.7
Volume fraction yield(%)	Min	100	0.00	0.00	2.00	5.00	6.00	6.76	4.48	0.881	17.3
	Max	100	12.2	22.0	28.8	19.5	25.6	25.0	16.4	56.7	82.0

[a] Note: Current version of PRELIM uses nitrogen only for information purposes. White cells highlight the 62 parameters needed and associated with the five crude properties. Atmospheric Residue: AR. Vacuum Residue: VR. Atmospheric Gas Oil: AGO, Light Vacuum Gas Oil: LVGO, and Heavy Vacuum Gas Oil: HVGO

4.3.1 Transformation methods

Four sets of calculations are used to estimate the crude quality parameters from publicly available assay data are used. 1) Average crude distillation curves, 2) Regression analysis between the fraction properties and a single fraction characteristic boiling point (i.e., a single value of boiling point that represents the boiling temperature range specific to each crude fraction) to determine crude fraction API and sulphur, 3) Empirical correlations to determine hydrogen content of crude fractions, and 4) Approximations for the characterization of the heaviest crude fractions that include determining carbon residue content. Five years of average data for each crude are used to account for seasonal variation in the quality of conventional crudes and OS products. The transformation methods are evaluated using more than 50 confidential assays (assays include crudes which sulphur content and API of the whole crude range from 0.023 wt% to 5.4 wt% and API range from 10.3 to 44.9 respectively) and the final parameter values are evaluated in a assay co-validation exercise (section 4.1.2 provides the assay co-validation methods and section 4.3 provides their results and analysis).

4.3.2 Canadian crude quality monitoring program data

CCQMP offers two types of assay data: it provides simple (less costly/easy measurement) assay information that includes distillation curves determined by a gas chromatography method (High Temperature Simulated Distillation - HTSD) and the assessment of the whole crude API, sulphur, nitrogen, and MCR content. It also has more detailed assay information that includes crude fraction yield analysis by using real distillation methods (ASTM D2892/D5236) and subsequent analysis of sulphur content, nitrogen content, and API properties of the crude fractions. A set of cut temperatures (i.e., the boiling temperature range that have to be specified to separate the crude into its fractions) has been standardized by CCQMP to analyze only four fractions: Naphtha at 190°C, Distillate at 343°C, Gas Oil at 527°C, and Residue at a temperature beyond 527°C (i.e., 527+°C) (CCQMP): the data result from analyzing monthly samples for each crude. Most crudes are tested to obtain the simple assay information, but not all of them get the more detailed analysis. At the time of validation described in section 5 (2010-2012), the PRELIM assay inventory used the data for 22 crudes where both types of assay data were provided at the time of the data collection (November 2009).

4.3.3 Average crude distillation curves

PRELIM crude assay inventory uses the distillation curve information derived from the HTSD method. The information is used for the purposes of determining specific crude fraction yields and the single characteristic boiling point for the range within each fraction. The data obtained by the HTSD method are selected over the real distillation information due to its level of resolution; specifically, it reports the temperature at which each incremental wt% of the crude is recovered. The data therefore allow the flexibility to determine the crude fraction yields at any set of cut temperatures. In addition, it allows for the determination of the single fraction characteristic boiling point. The latter is required in further characterization of the crude (i.e., use of empirical correlations to determine hydrogen content and regression analysis methods to derive API and sulphur content of each fraction).

4.3.3.1 Crude fraction yields

PRELIM uses information about crude fraction yields on mass and volume units at nine cut temperatures (Figure 4). The cutting scheme is not unique, and in real operations the boiling temperature ranges of each crude fraction vary based on desired refinery products (Gary et al., 2007). The mass yield of each fraction is determined after average HTSD temperature data at each 1wt% incremental mass yield, and the cumulative mass yield of the low end of the fraction boiling temperature range is subtracted from the cumulative mass yield of the high end of the fraction boiling temperature range. The volume yield of each fraction is calculated as the fraction mass yield times the crude fraction density. In industry, there are several empirical correlations that convert distillation curve data to different measurement units. Ideally, the distillation curve data on a mass basis would be transformed to a volume basis using one of these correlations, because it would have dealt with the issues associated with predicting crude fraction density (section 4.3.4). However, to the knowledge of this author, there is no empirical correlation that relates HTSD data to other methods of measurement that report the crude fraction yields and boiling points on a volume basis (empirical correlations among other distillation curves are available in Riazi [2007]). A reason for this may be the fact that though the cumulative statistical error of the HTSD method compared with ASTM methods (D2892/D5236) is acceptable ("the relative SDs of the total percent recoveries of material in the range <720°C ... ranged from about 1% to 5% for the different crude oils tested"), the HTSD method is still under investigation to be accepted as a standard in industry (Villalanti et al., 2000).

4.3.3.2 Single fraction characteristic boiling point

In the construction of the PRELIM assay inventory, a single fraction characteristic boiling point is consistently used in the empirical correlations available for crude fraction hydrogen content and enthalpies as well as for calculating the Kw factor and conducting the regression analysis. The use of a single value boiling point that represents the boiling temperature range of a crude fraction is a common approach in industry. This approach can be applied in different ways that differ in how the characteristic boiling point of a crude fraction is calculated. Ideally, the characteristic boiling point should account for differences in the ratio of specific gravity to molecular weight among hydrocarbons (molal average boiling point) (Watson et al., 1933) and have additive characteristics in a mixture (i.e., account for both the weight fraction/contribution of each component in the mixture and the molal average boiling point known as mean average boiling point) (Smith et al., 1937). In practice, several definitions for a single fraction characteristic boiling point appear based on the type of information available. For example, one fraction characteristic boiling point can be the fraction volume average boiling point. This boiling point on a volume basis can be calculated by distilling the crude fraction using a standard distillation test (ASTM D86/ ASTMD1160), and averaging the temperatures at 10, 30, 50, 70, and 90% volume yields of the fraction (Riazi, 2007). In the documentation, the single fraction characteristic boiling point corresponds to the temperature that represents 50% of the mass yield of each fraction ($Tb_{wt50\%}$ on mass basis). There is a need to recognize that because the HTSD represents the whole crude distillation curve, this approach may neglect the deviations that exist between each crude fraction distillation curve and the whole crude distillation curve. However, the measurement of the effects of this approach was out of the scope of the documentation.

4.3.4 Regression analysis

Regression analysis between the fractions properties and the single fraction characteristic boiling point is recognized as a method in industry to predict properties of the crude at different cut temperatures (Riazi, 2007; Maples, 1997). Regression analysis is carried out in order to determine sulphur content and API of each fraction based on its $Tb_{wt50\%}$. A specific regression analysis is conducted for each crude and crude property. For example, for Albian Heavy Synthetic crude, the sulphur content of a fraction is calculated by the expression:

$$S\ wt\% = 5.65x10^{-08}\ (Tb_{wt50\%})^3 - 5.33x10\text{-}^{05}(Tb_{wt50\%})^2 + 2.10x10\text{-}^{02}(Tb_{wt50\%}) - 1.72.$$

The expression results from using the property values of each fraction assessed from the real distillation analysis and the single fraction characteristic boiling point derived from the HSTD. The third polynomial regression form results from plotting the API and sulphur values for each crude fraction against its $Tb_{wt50\%}$, where the data exhibit a polynomial trend. The third order polynomial regression fits for most crudes (coefficient of determination with a value above 0.99), except for synthetic crude oil API (section 4.3.6). The average of the properties of the whole crude from samples analyzed by HTSD is checked against the average and standard deviation of such properties from samples analyzed by the real distillation analysis to analyze that the data are consistent.

4.3.5 Empirical correlations for determining hydrogen content of crude fractions

Crude fraction $Tb_{wt50\%}$ and API properties are used to predict hydrogen content of each crude fraction. The hydrogen content of the lighters fractions of the crude (i.e., LSR, Naphtha, and Kerosene) are predicted using the Goossens correlation (Goossens et al., 1997). The correlation requires density, refractive index, oxygen content, and molecular weight data for the crude fractions; current assay inventory neglects effects of oxygen content (an alternative when using the correlation) and combined the Goossens hydrogen correlation with the Goossens molecular weight correlation (Goossens et al., 1997; Goossens et al., 1996) to determine (by trial and error calculation) the hydrogen content using only crude fraction $Tb_{wt50\%}$ and API. The hydrogen content of the remaining heavier fractions is predicted using the Choudhary correlation (Choudhary et al., 2008), which also only requires the crude fraction $Tb_{wt50\%}$ and API. There is a concern in using Goossens hydrogen correlations for the lighters fractions since most of the fractions that Goossens used to develop the correlations are heavy gas oils, extra heavy gas oils, or hydrocracked vacuum gas oils. Also, the fractions that Goossens used for correlation development are low in sulphur, relative to fractions from bitumen or bitumen-containing crudes. However, the correlations outlined in Goossens are used since other simple methods are not found to estimate hydrogen content of the lighters fractions. The Choudhary correlation is tested using 22 confidential assays that included hydrogen content of heavy fractions. It is confirmed that the Choudhary correlation works well for most of the heavy fractions, and underestimates hydrogen content of the heaviest fractions (565°C+) by approximately 5%. The co-validation process confirmed the appropriateness of using both Goossens and Choudhary correlations (section 5.5.1).

4.3.6 Approximations for characterization of heaviest crude fractions

The main challenge in characterizing the heaviest crude fractions (i.e., distillation residue fractions: atmospheric and vacuum distillation residues) is to determine API or density and carbon residue. Characterization of crude fractions is not a straightforward procedure. Sophisticated methods such as use of pseudocomponents and/or probability distributions can be used. For the heaviest fractions, "these methods are more accurate than the use of bulk properties for the estimation of various properties" (Riazi, 2007). For current assay inventory, the mass yield of atmospheric and vacuum distillation residues is determined from the HTSD data. The data are suitable to be used because the HTSD method is able to determine boiling range distribution of hydrocarbons to a final boiling point of about 750°C (Villalanti et al., 2000); PRELIM final cut temperature is below that value (i.e., 525+°C). The sulphur content of the heaviest fractions is estimated through mass balance using whole crude sulphur content and the estimates of sulphur content in the light and medium crude fractions. In turn, these latter estimates are calculated using the polynomial regression analysis between the sulphur content of the crude fractions and their single fraction characteristic boiling point (section 4.3.4). In addition, the use of Choudhary correlation based on $Tb_{wt50\%}$ and API to determine hydrogen content is found to underestimate hydrogen content of heaviest fractions by 5%. It is considered an acceptable margin of error in hydrogen content estimates.

4.3.6.1 API of heaviest fractions (atmospheric and vacuum distillation residues)

Alternative approximation methods are sought to determine the API or volume yield of the distillation residue fractions. For most crudes, the methods involve neglecting volume changes that arise from mixing and approximating the fraction volume yield to the whole crude volume minus the volume yield of other crude fractions. They also include changing or approximating PRELIM final cut temperature using the CCQMP final cut, and characterizing the vacuum residue fraction with the average real distillation data without any transformation. Differences between the alternative calculations are found for the sulphur and API estimates specific to each crude. The deviation between the use of the regression coefficients and the alternative calculations in the estimates of density, mass yield, and hydrogen are not higher than 8%, 9%, and 15% respectively. These results are comparable with results from the assay co-validation method (section 5.5.1).

4.3.6.2 Approximation for carbon residue content of the heaviest crude fraction

McKetta (1993) states that 90% of the total MCR of the whole crude is present in non-distillable residue fractions or fractions with a characteristic boiling point over 690°C. In PRELIM assay inventory the vacuum residue is defined as the fraction of the crude that boils above 525+°C. Using the HTSD data, it is estimated that the "$Tb_{wt50\%}$" of the vacuum residue fraction is around 600°C (the final boiling point of the fraction is assumed to be the final temperature reported for each crude by the HTSD method). Therefore, for current assay inventory it is assumed that most of the MCR of the whole crude (approximately 99.9%) is present in the vacuum residue fraction. The review of the 57 additional confidential assays helps to confirm that the assumption is reasonable (i.e., the percentage of MCR of whole crude in the vacuum residue fraction is comparable to the percentage reported in the assay inventory for a crude with similar whole crude API and sulphur content that the cut fraction). The assay co-validation exercise shows that the approximation is appropriate for most crudes (section 5.5.1).

4.3.6.3 Bottomless SCO

Most of the light SCO produced in oil sands (OS) upgrading operations is "bottomless" (do not have any vacuum residue material in it). However, CCQMP HSTD data report that up to 6wt% of the whole crude is above the cut temperature specified in the PRELIM crude assay inventory for the vacuum residue (525+°C) (this material may be associated with the material remaining in transportation pipelines). A third data point, the detailed assay information from CCQMP real distillation, does not report properties for this fraction. Therefore, it is difficult to determine whether characterization of the light SCO crudes should include vacuum residue yields and properties. Confidential assays report a fraction of material that boils over 490°C, but they do not report how much boils over 525°C (the PRELIM cut temperature for vacuum residue). Using PRELIM cut temperatures to define the presence of vacuum residue, the industry assay database used in the assay co-validation exercise (section 5.1.2) reports a vacuum residue fraction for light SCO assays.

Therefore, PRELIM light SCO assays include a vacuum residue fraction. Because there are few data points available from the assays in the public realm, it was not possible to get a good fit of the data using the polynomial regression method for the purposes of predicting API and sulphur content of the fractions. Therefore, an exponential regression form is applied. The comparison of the estimates using the exponential form versus a polynomial regression derived from the SCO confidential assay (API and $Tb_{wt50\%}$ data are available for 15 narrower cut temperatures) shows that the API of the first six SCO fractions is underestimated by 2 to 9%

and the API of the heavy vacuum gas oil fraction is overestimated by 16%. The assumption about MCR content of the heaviest fraction is also applied to the light SCO assays. The confidential assay shows that this approximation may provide a value for the MCR of the SCO vacuum residue fraction close to the measured value for all the fraction of material that boils over 490°C of the light SCO (underestimated by only in one percentage unit). The assay co-validation shows a large deviation in the MCR value of the same fraction. Effects of these assumptions are discussed in section 5.3.

4.3.7 Approximated Watson characterization factor

Kw definition uses the "mean average boiling point" as a single fraction characteristic boiling point instead of the $Tb_{wt50\%}$ to represent the structural composition of a crude fraction (as discussed in sections 4.2.5 and 4.3.3). Several alternative calculation methods are used to explore the effects of this approximation which included mainly: 1) crosschecking the estimated Kw values with values reported in confidential assay information, and 2) using confidential assay information to calculate the sensitivity of the Kw parameter to using a characteristic boiling point on mass or volume basis. The estimated Kw value may change in the second or first decimal place due to changes in the use of a mean average boiling point, a $Tb_{wt50\%}$, or a $Tb_{50\%}$ on volume basis. However, the estimated Kw value may change by one unit (e.g. 11 to 12) when accounting for the standard deviation in the $Tb_{wt50\%}$ resulting from the five-year average HTSD distillation data. This suggests that the approximation may have a negligible effect when compared to the variation that could derive from upstream blending decisions that affect the crude distillation curves. The assay co-validation exercise shows that the estimated Kw values in PRELIM crude assay inventory are consistent with the values reported from a more comprehensive crude assay database (section 5.5.1).

4.4 Process unit modelling

A refinery is defined as a set of interconnected process units that convert relatively low value hydrocarbon material into more valuable products by increasing its hydrogen to carbon ratio. This section details how PRELIM models the process units in the coking and the hydrocracking refineries in the calculations worksheets. These have blue-coloured tabs in PRELIM.

4.4.1 Associated worksheets in PRELIM

4.4.1.1 The process flow diagram worksheets

The `CokingRefineryPFD` and `HydroRefineryPFD` worksheets presents the process flow diagram (PFD) of the refinery as modelled in PRELIM. The PFD displays the relationship between the process units as well as results for key performance indicators and volumetric flow rate for each process unit (calculated in the calculations worksheet).

A box in the top left sums up the currently enabled configuration. Note that the box on the `CokingRefineryPFD` worksheet contains configuration options that apply to both refineries.

4.4.1.2 Calculation worksheets

The `CokingRefineryCalcs` and `HydroRefineryCalcs` worksheets are where most of the calculations take place. PRELIM models the volumetric flow rate, the energy use and requirement of each of the process units of the refinery. The worksheet has two boxes:

- The `Process unit level calculations` box on the left details all calculations for each process unit; and
- The `System-level calculations` displays results aggregated at the refinery level.

Calculation worksheets are based on a set of constants derived from peer-reviewed literature (as described in sections 4.1 and 4.2). Constants used in the calculations have a red background and can be overridden by expert users in the `Constants` worksheet.

PRELIM models the swings that allow splitting the streams between process units in the refinery. Swings are flow splitters that distribute flows between process units. These swings are modelled in the calculations worksheets (`CokingRefineryCalcs` and `HydroRefineryCalcs`). Default values (typically 0, 50%, or 100%) shouldn't be overridden, as the model is very sensitive to these values.

4.4.1.3 Control worksheets

The `CokingRefineryControls` and `HydroRefineryControls` worksheets are used to gather data that are used by macros for advanced features from the `Expert Input` worksheet. It is recommended that this worksheet not be modified as this may result in inaccurate results or the model becoming unstable.

4.4.2 Summary of description of process units' operating characteristics in PRELIM

The following table presents a summary of the process units' purpose and specifications per type.

Table 7: Summary of description of process units' operating characteristics in PRELIM

Process	Feed	Purpose	Products	Parameters that define actual yield and products distribution	PRELIM Assumptions for yield and products distribution estimates[a]	Origin of energy requirements and particular considerations[b]
Crude distillation	Whole crude to atmospheric operations, atmospheric residuum to vacuum operations	Separate crude in fractions of different boiling range	Straight-run fractions (SRF): naphtha, kerosene, diesel, gas oils, residue.	Boiling curve of whole crude Cut temperatures	Average TBP for each crude at a specified cut temperature Sulphur distribution on SRF and estimates of SRF API unique for each crude	Heating crude until required temperature to cause vaporization of products and stripping steam to separate light ends from each distillation products. Heat exchanges between feed, products, and reflux increase energy efficiency and reduce energy requirements.

Reforming and isomerization	Naphtha fractions boiling above 204oC, previously hydrotreated for catalyst protection.	Modify the structure of the hydrocarbons in the lighter fractions to increase gasoline octane by isomerization and cyclization reactions: Parafines to naphthenes, naphthenes to aromatics	Reformate: hydrocarbons components of high octane for gasoline Hydrogen Light gases from some hydrocracking reactions	Process severity: Temperature, pressure, catalyst, and feed properties Correlations based on RON number and Kw or RON number and aromatics and naphthenic content.	Feed hydrotreated to same hydrogen content and no change in boiling point; therefore, similar Kw and similar yields. Yield of light gas production (22wt%H content) 10 wt% of the hydrocarbon feed in reformer and 1%wt in Isomerization. Reformate calculated by carbon and hydrogen balance.	Endothermic dehydrogenation reactions. Negligible hydrogen to minimize carbon deposits on catalyst
Hydrotreating	Straight run fractions from crude distillation processes	Reduce content of S and N and saturate olefins or aromatic rings of distillate fuels without change their boiling range to meet specifications of feedstock for further processing, or specifications of end products (i.e. increase H/C ratio).	Saturate hydrocarbon, hydrogen sulphide, light gases	Product yield expected from 95 to 98% volume on feed.	Yield 0.2%wt liquid feed rate and refinery fuel gas hydrogen content of 22%wt.	Preheating feedstock Stripping steam hydrogen rich gas
Fluid catalytic cracking	Gas oils	Increase the yield of lighter products from heavier gas oil fractions. Mostly benefit gasoline yields.	Light gases: C1 to C4 with high olefin content. High octane Gasoline Light and heavy cycle gas oils.	Reaction temperature, type and activity of the catalyst, ratio of catalyst mass per feed mass, and contact time Also hydrogen content of process feed.	Correlation based on 75% conversion and 11.8 Kw factor using zeolita catalyst. Full hydrotreating of FCC feed to 12.5 wt% hydrogen[c].	Heat balance is possible due to endothermic cracking reactions and exothermic catalyst regeneration Steam stripping
Hydrocracking	Kerosene, diesel, Gas oils or residuum	Increase the yield of lighter products from heavier fractions. Mostly benefit diesel yields.	Light gases: C1 to C4 Gasoline and or kerosene, and or diesel	Reactor pressure, catalyst contact time, type and activity of catalyst, and type of feed	Correlation based on feed Kw and approximated hydrogen consumption	Hydrogen rich gas Excess of heat may be produce due to high exothermic hydrogenation reactions versus

					Products are routed as follow: C3 and lighters to refinery fuel gas, C4 and fractions below 204 oC (400 oF) to gasoline, and the rest of the material that boils above the gasoline cut temperature, can be used either as jet fuel or diesel	low endothermic cracking reactions
Delayed coking	Vacuum residuum (VR) or FCC heavy gas oils	Increase the yield of lighter products from heavier fractions. Prepare FCC and HC feedstock. FCC heavy gas oils are use to produce needle coke.	Coke Light gases: C1 to C4 Naphtha Gas oil	Heater outlet temperature, fractionators' pressure, vapours' temperature, and "free" carbon content	Correlation based on "free" carbon content (measured by micro carbon residuum) and API of the feed. Correlation was derived for feed under 18 API and straight run products (VR)	Thermal cracking process Steam stripping Decoking system

S: Sulphur content; content; H: Hydrogen content; ~Kw Watson characterization factor; wt: weight basis.

[a] Products specifications assumptions in Table 8

[b] Energy requirements assumptions in Table 5 and Table 4

[c] FCC Conversion: 100 (volume of feed - volume of effluent not converted to naphtha and lighter products)/ volume of feed. The model assumes conversion of 75% suggested for high boiling feed.

Table 8: PRELIM assumptions on refinery intermediate products specifications

Intermediate Product	API / Density (kg/m^3)	Sulphur wt%	Hydrogen wt%
Distillated Fractions	Crude assay inventory	Crude assay inventory	Crude assay inventory
Hydrotreated Naphtha	CAI[a] +1 API [1]	0	15.7
Hydrotreated Kerosene	41 / 820	0	13.8
Hydrotreated Diesel	40 / 825	11 ppm	13.8
Keromix Product	41 / 808	0	13.8
Coker naphtha	52 / 770	S, FCDP [b]	12.0
Coker gas oil	20 / 934	S, FCDP [b]	11.0
Coke	n.a.[c]	n.a.[c]	5.9
Hydrotreated Coker Naphtha	60 / 740	0	15.7
Hydrotreated Hydrocracking Naphtha	65 / 720	0	15.7
Hydrotreated FCC Feed	24 /910	0	12.5
FCC LPG	FC [d]	S, FCDP [b]	16.1
FCC Gasoline	FC [d]	S, FCDP [b]	14.5
FCC LGO	FC [d]	S, FCDP [b]	9.8
FCC HGO	FC [d]	S, FCDP [b]	8.0
FCC Coke	n.a [c]	S, FCDP [b]	5.9
Reformate	52 / 770	n.a [c]	12.3
Hydrogen from Naphtha Catalytic Reformer	n.a [c]	n.a [c]	100
Alkylate	73 / 693	n.a [c]	n.a [c]
HC Products	FWF [e]	Feed's S 100% to HC Fuel oil	FWF[e] and 17.2 for iC4&nC4

[1] Maples, R., *Petroleum Refinery Process Economics.* Second ed.; PennWell Corp: 2000.

[a] CADI: Crude Assay Inventory
[b] FCDP: Process Feed Content of sulphur (S) Distributed in process's Products. Gary et al. (2007) give figures that show S distribution in process's products as function of the S present in the process' feed.
n.a [c] No applicable to PRELIM model calculations.
[d] FC: Function of Conversion. Gary et al. (2007) give figures that shows FCC product's density as function of conversion: 100 (volume of feed - volume of effluent not converted to naphtha and lighter products)/ volume of feed. This study, assumed conversion of 75% suggested for high boiling feed (see Sensitivity FCC Performance Assumptions section for further details).
[e] FWF: Function of Watson characterization Factor. Gary et al. (2007) give figures that show characterization factor and hydrogen content of hydrocracking products as function of average mid boiling points. The density was calculated (see section Approximated Watson characterization factor). and hydrogen specified from these factors and assumptions on average mid boiling points This study, assumed Gary et al. suggested average mid boiling points of 55, 138, and 238 °C for the hydrocracking products and uses figures for zeolite catalyst. Gary et al. (2007) give figures that show yields as function of API and hydrocracking severity. This study uses yields derived from assuming a hydrocracking severity of 1500 scf H/bbl.

4.4.3 Configurations common to the coking and the hydrocracking refinery

4.4.3.1 Process flow diagrams

The following figures provide a process flow diagram and a short description for each of the four refinery configurations common to the two refinery types modelled in PRELIM.

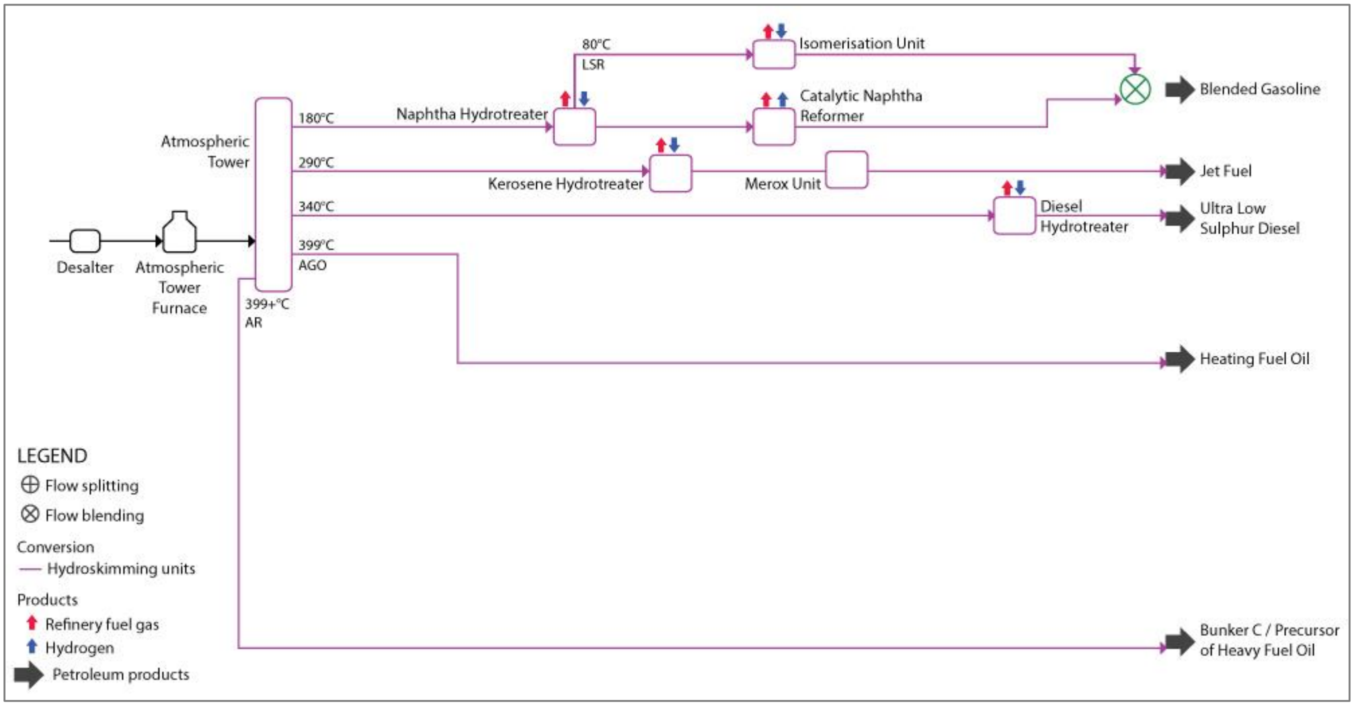


Figure 9: Configuration 0

> Only the hydroskimming process units are enabled in configuration 0.

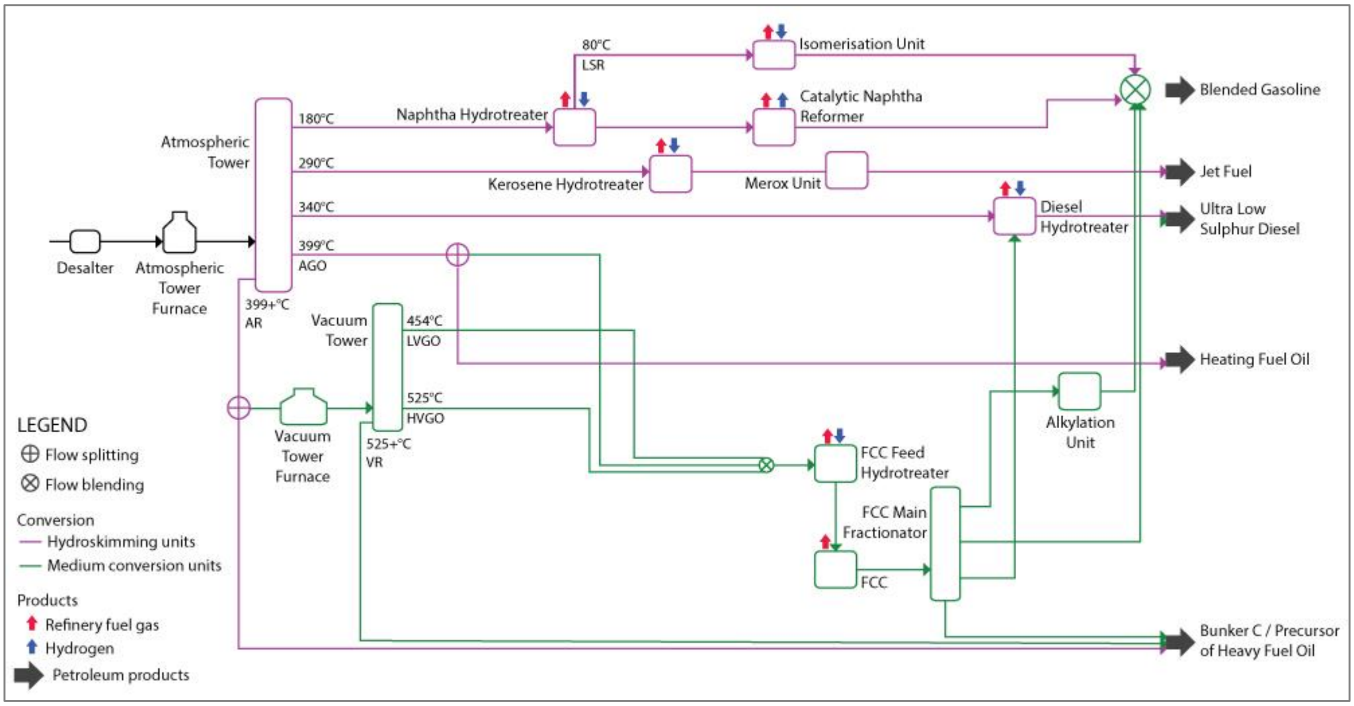


Figure 10: Configuration 1

> In the configuration 1, the hydroskimming process units as well as the process units associated with the fluid catalytic cracker (FCC) are enabled to provide a medium conversion.

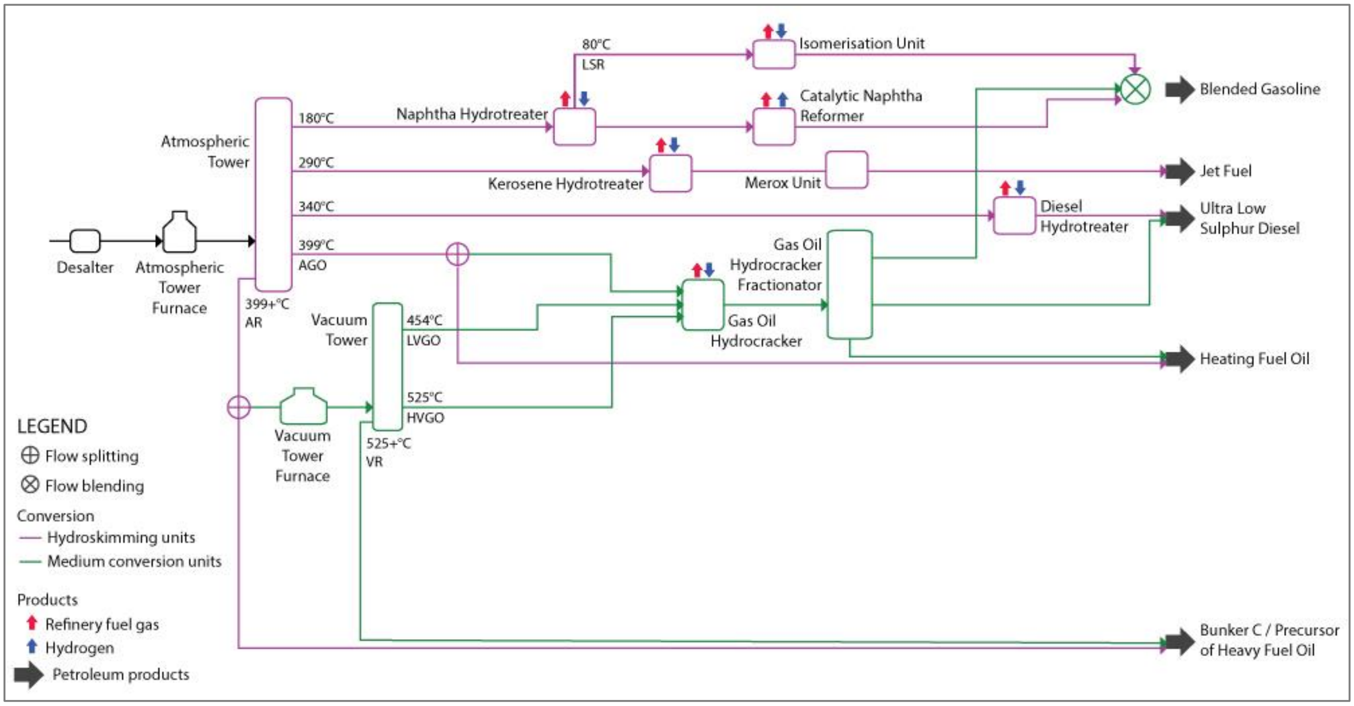


Figure 11: Configuration 2

> In the configuration 2, the hydroskimming process units as well as the process units associated with the gas oil hydrocracker are enabled to provide a medium conversion.

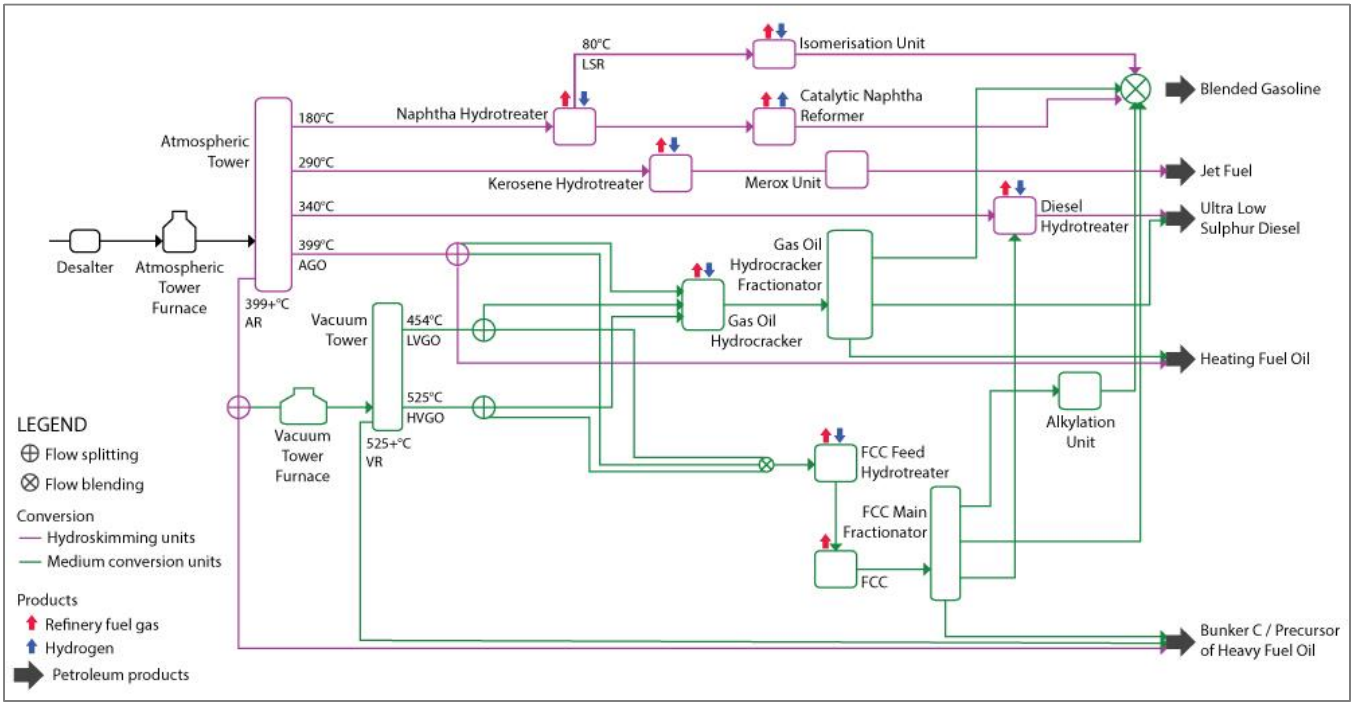


Figure 12: Configuration 3

> In the configuration 3, the hydroskimming process units, the process units associated with the gas oil hydrocracker, and the process units associated with the fluid catalytic cracker (FCC) are enabled to provide a medium conversion.

4.4.3.2 Process unit description

This subsection provides the user with an overview of each process unit used in the configurations common to the two main refinery types, including:

- A general description of the process unit purpose and function;
- The list of all (active and potential) input and output streams – this includes the swings that can be modified to change the destination of streams (note: power is necessary for operation of all process units, and is not specifically mentioned as an input); and
- Calculations in PRELIM specific to each process unit, including the assumptions tied to the calculations and the equations used. These processes are detailed in the order they are presented in both the `CokingRefineryCalcs` and `HydroRefineryCalcs` worksheets.

4.4.3.2.1 Desalter

4.4.3.2.1.1 Process unit description

This unit is the first unit that the crude oil passes through in a refinery. Its purpose is to remove the salt present in the crude oil.

4.4.3.2.1.2 Output

The desalted crude oil is sent to the Atmospheric Tower Furnace.

4.4.3.2.1.3 Calculations

4.4.3.2.1.3.1 Stream processing

PRELIM does not take into account the mass of the salt that is removed, as the value and effect on the calculations are negligible. This explains the fact that the output stream has exactly the same properties as the input stream that are considered in the model. However the energy used for desalting the crude is considered.

4.4.3.2.2 Atmospheric Tower Furnace

4.4.3.2.2.1 Process unit description

This unit preheats the crude stream before it enters the atmospheric tower.

4.4.3.2.2.2 Input

The stream comes directly from the desalter unit.

4.4.3.2.2.3 Output

Once preheated, the stream is sent to the atmospheric tower.

4.4.3.2.2.4 Calculations

The energy consumption of the unit is calculated based on the volume of gas required to heat the volume of crude oil passing through the unit.

4.4.3.2.2.4.1 Equation

The calculation is performed based on the enthalpy of the input and output streams, using the following equation (Moharam et al., 1998):

$$H_L = [0.03181T + 0.00001791Kw^{4.693}]^{2.2916}$$

Where:

H_L is the enthalpy of the stream (kJ/kg)
T is the temperature in K
Kw is the characterization factor

4.4.3.2.3 Atmospheric Tower

4.4.3.2.3.1 Process unit description

The atmospheric tower is the first major unit met by the crude and the most important one in the refinery. In this unit, the molecules of the crude entering the tower are separated based on their boiling point. The lighter molecules evaporate and travel to the top portion of the atmospheric tower where they are collected, while the heavier ones are collected at the bottom of the tower.

4.4.3.2.3.2 Input

The stream comes from the atmospheric tower furnace.

4.4.3.2.3.3 Output

There are five straight-run fractions (SRF) coming out of the atmospheric tower. Each fraction is sent to a different process unit for further processing, based on the new properties of the fraction that are different from the original whole crude oil.

The light straight-run fractions are sent to different sections of the refinery for further processing based on their distillation cut temperature:

- Naphtha (distillation cut temperature of initial boiling point (IBP) to 180°C) is sent to the naphtha hydrotreater;
- Kerosene (distillation cut temperature of 180 to 290°C) is sent to the kerosene hydrotreater; and
- Diesel (distillation cut temperature of 290 to 340°C) is sent to the diesel hydrotreater.

The atmospheric tower also produces two heavy fractions:

- The atmospheric gas oil (AGO, distillation cut temperature of 340 to 399°C); and
- The atmospheric residue (AR, distillation cut temperature of 399+°C).

In the hydroskimming-only configuration, these two heavier fractions are considered final products (heating fuel oil and coke). If the medium or the deep conversion configuration is selected, two swings are activated to process these streams further to produce higher quality products.

4.4.3.2.3.4 Calculations

The whole crude assay's properties are used to calculate the flow rate of the output to each subsequent process unit for each fraction as a mass balance. The following assumptions are used by PRELIM to estimate yield and product distribution:

- Average temperature boiling point (TBP) at a specified cut temperature;
- Sulphur distribution of the SRF and estimates of SRF API are unique for each crude.

4.4.3.2.4 Naphtha hydrotreater

Process unit description

This hydrotreater unit uses gas, electricity and hydrogen to reduce to reduce sulphur and nitrogen content, as well as to saturate olefins or aromatic rings of distillate fuels without changing the boiling range of the fraction to meet specifications of feedstock for further processing, or specifications of end products (i.e., increase H/C ratio).

Input

The stream contains the light straight run naphtha (SRN) from the atmospheric tower.

Output

This process unit produces desulphurized light gases of three types:

- The light straight run (LSR, distillation cut temperature of 80°C) is sent to the isomerization unit;
- The rest of the naphtha stream is sent to the catalytic naphtha reformer unit;
- Refinery fuel gas that can be reused within the refinery or sold as a product since it has properties close to natural gas.

4.4.3.2.4.1 Calculations

PRELIM assumes a product yield of 0.2%wt for liquid feed rate and refinery fuel gas hydrogen content of 22%wt.

4.4.3.2.5 Isomerization unit

Process unit description

The isomerization unit modifies the structure of the hydrocarbons in the lighter fractions to increase gasoline octane by isomerization and cyclization reactions (i.e., paraffins to naphthenes, naphthenes to aromatics).

Input

Input to this process unit is the desulphurized stream coming from the naphtha hydrotreater.

Output

This process unit produces two streams:

- Reformates, hydrocarbon components with high octane content for gasoline processed stream;
- Hydrogen light gas that can be reused as RFG within the refinery.

4.4.3.2.5.1 Calculations

PRELIM uses the following assumptions to process the stream:

- There is no change in boiling point; therefore the input and output streams from this unit have similar Kw and yields.
- Yield of light gas production is 1%wt of the hydrocarbon (Gary et al. (2007)). The output stream is calculated using carbon and hydrogen balance.

4.4.3.2.6 Catalytic naphtha reformer

Process unit description

The catalytic naphtha reformer further processes the stream from the naphtha hydrotreater and breaks it into lighter fractions that can be added to the gasoline pool. One of the byproducts of this unit is the associated hydrogen production.

Input

The desulphurized stream comes from the naphtha hydrotreater in the hydroskimming-only configuration, and may be associated with a stream coming from the heavy naphtha hydrotreating unit if the deep conversion is selected.

Output

This process unit produces three streams:

- The processed stream is sent to the gasoline pool;
- Hydrogen; and
- Refinery fuel gas that can be reused within the refinery or sold as a product since it has properties close to natural gas.

4.4.3.2.6.1 Calculations

PRELIM uses the following assumptions to process the stream:

- The feed is hydrotreated to the same hydrogen content as the input stream and there is no change in boiling point; therefore the streams have similar Kw and yields.
- Yield of light gas production (22wt%H content) is 10 wt% of the hydrocarbon feed (Gary et al. (2007) and input from industry experts). Reformate stream is calculated using a carbon and hydrogen balance.

4.4.3.2.7 Kerosene hydrotreater

4.4.3.2.7.1 Process unit description

The kerosene hydrotreater unit uses gas, electricity and hydrogen to reduce sulphur and nitrogen content, as well as to saturate olefins or aromatic rings of distillate fuels without changing their boiling range to meet specifications of fraction for further processing, or specifications of end products (i.e., increase H/C ratio).

4.4.3.2.7.2 Input

The stream consists of the kerosene straight run fraction coming from the atmospheric tower (distillation cut temperature of 290°C).

4.4.3.2.7.3 Output

This process unit produces two streams:

- A desulphurized stream of the kerosene fraction; and
- Refinery fuel gas that can be reused within the refinery or sold as a product since it has properties close to natural gas.

4.4.3.2.7.4 Calculations

PRELIM assumes a product yield of 0.2%wt for liquid feed rate and refinery fuel gas hydrogen content of 22%wt (Gary et al. (2007) and input from industry experts).

4.4.3.2.8 Kerosene Merox unit

4.4.3.2.8.1 Process unit description

The Merox unit allows additional treatment to transform the hydrotreated kerosene stream into jet fuel. Merox is an acronym for mercaptan oxidation. It is a catalytic chemical process used to remove mercaptans from the kerosene stream.

4.4.3.2.8.2 Input

The desulphurized stream comes from the kero hydrotreater.

4.4.3.2.8.3 Output

The processed stream is sent to the jet fuel pool. The mercaptans are not included in the characteristics of the crude but the energy required to remove them is estimated in the model.

4.4.3.2.9 Diesel hydrotreater

4.4.3.2.9.1 Process unit description

The diesel hydrotreater unit uses gas, electricity and hydrogen to reduce to reduce sulphur and nitrogen content, as well as to saturate olefins or aromatic rings of distillate fuels without changing their boiling range to meet specifications of feedstock for further processing, or specifications of end products (i.e. increase H/C ratio).

4.4.3.2.9.2 Input

The stream consists of the kerosene straight run fraction coming from the atmospheric tower (distillation cut temperature of 340°C). Another stream coming from the fluid catalytic cracking (FCC) feeds the diesel hydrotreater if the medium or the deep conversion is active. An additional stream coming from the coking or the hydrocracking unit feeds the diesel hydrotreater if the deep conversion is active.

4.4.3.2.9.3 Output

This process unit produces two streams:

- The desulphurized stream is sent to the ULSD pool;
- Refinery fuel gas that can be reused within the refinery or sold as a product since it has properties closed to natural gas.

4.4.3.2.9.4 Calculations

PRELIM assumes a product yield of 0.2%wt for liquid feed rate and refinery fuel gas hydrogen content of 22%wt.

4.4.3.3 Process units added in the medium conversion configuration

The following process units are used in addition to the preceding ones when the medium conversion or the deep conversion configuration is enabled.

> Note: PRELIM automatically chooses the “most suitable” configuration to process crude oil as a default. However, the user can override the refinery configuration on the ‘Main Inputs and Outputs’ worksheet.

4.4.3.3.1 Gas oil hydrocracker

4.4.3.3.1.1 Process unit description

The gas oil hydrocracker further cracks the heaviest molecules from the atmospheric tower into molecules that can be made into higher quality products. That is, the process increases the yield of lighter products from heavier fractions. In general, it increases diesel yields.

4.4.3.3.1.2 Input

The input stream can have up to four origins depending on the selected configuration:

- The atmospheric gas oil (AGO, distillation cut temperature of 399°C) coming from the atmospheric tower (all configurations);

- The light vacuum gas oil (LVGO, distillation cut temperature of 454°C) coming from the vacuum tower (medium and deep conversion);
- The heavy vacuum gas oil (HVGO, distillation cut temperature of 525°C) coming from the vacuum tower (medium and deep conversion); and
- The coking or hydrocracking residue coming from the coking or hydrocracking unit (deep conversion).

4.4.3.3.1.3 Output

This process unit produces two streams:

- The processed stream is sent to the gas oil hydrocracker fractionator; and
- C3 and lighters are routed to refinery fuel gas, to be reused within the refinery or sold as a product since it has properties close to natural gas.

4.4.3.3.1.4 Calculations

The required assumptions for hydrogen consumption and yield and product distribution calculations are taken from Jones (2008) and Gary et al. (2007), respectively.

4.4.3.3.2 Gas oil hydrocracker fractionator

4.4.3.3.2.1 Process unit description

The gas oil hydrocracker fractionator is similar to the atmospheric tower in that it separates the input stream into three new streams based on their quality parameters.

4.4.3.3.2.2 Input

The stream comes from the gas oil hydrocracker.

4.4.3.3.2.3 Output

This process unit produces three streams:

- The light stream consists of C4 and fractions with boiling points below 204 °C. This stream goes to the gasoline pool;
- The medium stream boils above the gasoline cut temperature and goes to the ULSD pool;
- The heavy stream goes to the heating fuel oil pool.

The calculations of the gas oil hydrocracker fractionator yields are based on the method proposed by Gary et al. (2007).

4.4.3.3.3 Vacuum tower furnace

4.4.3.3.3.1 Process unit description

The vacuum tower furnace is similar to the atmospheric tower furnace in that it preheats the fuel that goes to the vacuum tower.

4.4.3.3.3.2 Input

The input stream is the atmospheric residue coming from the atmospheric tower.

4.4.3.3.3.3 Output

The processed stream is sent to the vacuum tower.

4.4.3.3.3.4 Calculations

4.4.3.3.3.4.1 Equation

The calculation is performed based on the enthalpy of the input and output streams, using the following equation (Moharam et al., 1998):

$$H_L = [0.03181T + 0.00001791Kw^{4.693}]^{2.2916}$$

Where:

H_L is the enthalpy of the stream (kJ/kg)
T is the temperature in K
Kw is the characterization factor

4.4.3.3.3.4.2 Assumptions to calculate the petroleum fraction enthalpy

This equation uses the difference between the inlet and outlet temperatures to calculate the difference in enthalpy for all fractions of the crude oil.

4.4.3.3.4 Vacuum tower

4.4.3.3.4.1 Process unit description

The vacuum tower is similar to the atmospheric tower but operates at low pressures and high temperatures to further crack the molecules present in the stream.

4.4.3.3.4.2 Input

The atmospheric residue stream comes from the vacuum tower furnace, where it is preheated.

4.4.3.3.4.3 Output

This process unit produces three streams:

- Light vacuum gas oil (LVGO, distillation cut temperature of 454°C) is sent to a swing that distributes it to the gas oil hydrocracker and/or to the fluid catalytic cracker;
- Heavy vacuum gas oil (HVCO, distillation cut temperature of 525°C) is sent to a swing that distributes it to the gas oil hydrocracker and/or to the fluid catalytic cracker;
- Vacuum residue (VR, distillation cut temperature of 525+°C) is sent to the heavy fuel oil pool. If the deep conversion is selected, a swing allows for the rerouting of a share of the VR to the coking furnace or the residue hydrocracker furnace, depending on the configuration.

4.4.3.3.5 Fluid catalytic cracking feed hydrotreater

4.4.3.3.5.1 Process unit description

This hydrotreater unit uses gas, electricity and hydrogen to reduce to reduce sulphur and nitrogen content, as well as to saturate olefins or aromatic rings of distillate fuels without changing the boiling range to meet specifications of the stream for further processing, or specifications of end products (i.e., increase H/C ratio).

4.4.3.3.5.2 Input

A swing allows mixing streams from up to four sources, depending on the selected configuration:

- LVGO from the vacuum tower (medium and deep conversion);
- AGO from the atmospheric tower (medium and deep conversion);
- HVGO from the vacuum tower (medium and deep conversion);
- Coking or gas oil residue hydrocracker from the coking or the residue hydrocracker fractionator (deep conversion).

> Note: all swing values can be overridden in the calculations worksheet.

4.4.3.3.5.3 Output

This process unit produces two streams:

- The desulphurized stream passes through to the fluid catalytic cracker;
- Refinery fuel gas that can be reused within the refinery or sold as a product since it has properties closed to natural gas.

4.4.3.3.5.4 Calculations

PRELIM assumes a product yield of 0.2%wt for liquid feed rate and refinery fuel gas hydrogen content of 22%wt.

4.4.3.3.6 Fluid catalytic cracker

4.4.3.3.6.1 Process unit description

The fluid catalytic cracker (FCC) cracks large molecules from the heavy stream into smaller molecules. It therefore increases the yield of lighter products from heavier gas oil fractions and mostly produces a stream that can be used to increase gasoline yields.

4.4.3.3.6.2 Input

The FCC is fed by the gas oils coming from the fluid catalytic cracker feed hydrotreater unit.

4.4.3.3.6.3 Output

This process unit produces two streams:

- Light gases and light and heavy cycle gas oils are directed to the FCC main fractionator;
- Refinery fuel gas that can be reused within the refinery or sold as a product since it has properties close to natural gas.

4.4.3.3.6.4 Calculations

Yields and products distribution estimates are calculated based on the method proposed by Gary et al. (2007) with input of industry experts. Full hydrotreating of FCC feed to 12.5wt% hydrogen is also assumed.

4.4.3.3.7 Fluid catalytic cracking main fractionator

4.4.3.3.7.1 Process unit description

The FCC main fractionator is similar to the atmospheric tower as it separates the incoming stream into three streams based on the properties of the fractions.

4.4.3.3.7.2 Input

The stream of light gases and light and heavy cycle gas oils comes from the FCC unit.

4.4.3.3.7.3 Output

This process unit separates the stream into four streams:

- Light gases (C1 to C4 with high olefin content) are sent to the alkylation unit;
- High octane gasoline (medium stream) is sent to the gasoline pool where it is mixed to lighter streams;
- Light and heavy cycle gas oils (heavy stream) is sent to the diesel hydrotreater where the sulphur is removed and the stream is then added to the ULSD pool;
- The heaviest stream is sent to the heavy fuel oil pool.

4.4.3.3.8 Alkylation unit

4.4.3.3.8.1 Process unit description

This unit converts isobutene and low-molecular-weight alkenes coming from the fluid catalytic cracking main fractionator into alkylate, a high quality gasoline component.

4.4.3.3.8.2 Input

The stream of light gases (C1 to C4 with high olefin content) comes from the fluid catalytic cracker main fractionator.

4.4.3.3.8.3 Output

The processed stream is sent to the gasoline pool where it is mixed to lighter streams and process unit calculations are based on energy consumption assumptions from the literature (Gary et al., 2007; Maples, 2000; Parkash, 2003).

4.4.3.3.9 Gasoline blending

Although this process unit is not explicitly displayed on the PFDs it is modelled and detailed in the calculation worksheets.

4.4.3.3.9.1 Process unit description

The gasoline pool gathers and mixes gasoline streams coming from various process units.

4.4.3.3.9.2 Input

Gasoline streams may come from up to five process units, depending on the selected configuration:

- The isomerization unit (all configurations);
- The gas oil hydrocracker fractionator (medium and deep conversion);
- The catalytic naphtha reformer (all configurations);
- The alkylation unit (medium and deep conversion); and
- The fluid catalytic cracking main fractionator (medium and deep conversion).

4.4.3.3.9.3 Output

The output is blended gasoline.

4.4.3.3.9.4 Calculations

4.4.3.3.9.4.1 Stream processing

Incoming streams (iC5, reformate, HT naphtha product, FCC gasoline, HC gasoline, and alkylate) are blended. Blend properties are calculated based on the mass balance equation.

4.4.3.3.10 Fuel gas treatment, sulphur recovery and pollution control

Although these process units are not displayed on the PFDs it is modelled and detailed in the calculation worksheets.

4.4.3.3.10.1 Process unit description

These units are responsible for treating the fuel gas to remove acid gas and sulphur.

4.4.3.3.10.2 Input

Streams are coming from all process units generating fuel gas.

4.4.3.3.10.3 Output

The output is a fuel gas that is compliant with environmental regulations associated with emissions of sulphur.

4.4.3.3.10.4 Calculations

4.4.3.3.10.4.1 Amine treatment

Acid gas is removed using amine treatment. Calculations are based on Gary et al. (2007) and Jones (2008).

4.4.3.3.10.4.2 Sulphur removal

Sulphur is removed using the Claus tail gas treatment.

> Source used for the sulphur recovery data: *Refining Processes Handbook*, Chapter 8 p.221 to 241

4.4.3.3.11 Steam generation

Although this process unit is not displayed on the PFDs it is modelled and detailed in the calculation worksheets.

4.4.3.3.11.1 Process unit description

This unit generates steam for the refinery, using natural gas as the source of primary energy.

4.4.3.3.11.2 Input

Natural gas is the only input to this process unit.

4.4.3.3.11.3 Output

This process unit produces steam that is circulated throughout the refinery.

4.4.3.3.11.4 Calculations

Sources used to calculate the steam generation energy requirements are:

- Wang 2008, Spreadsheet (File Refinery Efficiency Calculations-Wang-10-07-v4-1)
- Petroleum Refining Technology and Economics p.356
- Refining Processes Handbook, p. 302

4.4.3.3.12 Steam methane reformer

Although this process unit is not displayed on the PFDs it is modelled and detailed in the calculation worksheets.

4.4.3.3.12.1 Process unit description

The steam methane reformer produces hydrogen for the refinery.

4.4.3.3.12.2 Input

The steam methane reformer requires two inputs: steam, and natural gas.

4.4.3.3.12.3 Output

This process unit produces hydrogen for seven process units, depending on the active configuration:

- Naphtha hydrotreater (all configurations);
- Kerosene hydrotreater (all configurations);
- Diesel hydrotreater (all configurations);
- Gas oil hydrocracker (medium and deep conversion);
- Coking naphtha hydrotreater (deep conversion);
- Fluid catalytic cracking feed hydrotreater (medium and deep conversion); and
- Isomerization unit (all configurations).

4.4.3.3.12.4 Calculations

PRELIM first calculates the hydrogen balance for all of the process units. It then subtracts the hydrogen supplied by the naphtha catalytic reformer. Lastly, the energy required to produce the supplemental hydrogen in the SMR unit is calculated based on the specific natural gas, steam, and power consumption (Gary et al., 2007; Maples, 2000; Parkash, 2003; Skone et al., 2008; Spath et al., 2001).

4.4.4 Configurations specific to the coking refinery

4.4.4.1 Process flow diagrams

The following figures provide a process flow diagram and a short description for each of the three refinery configurations specific to the coking refinery configuration when the deep conversion is selected.

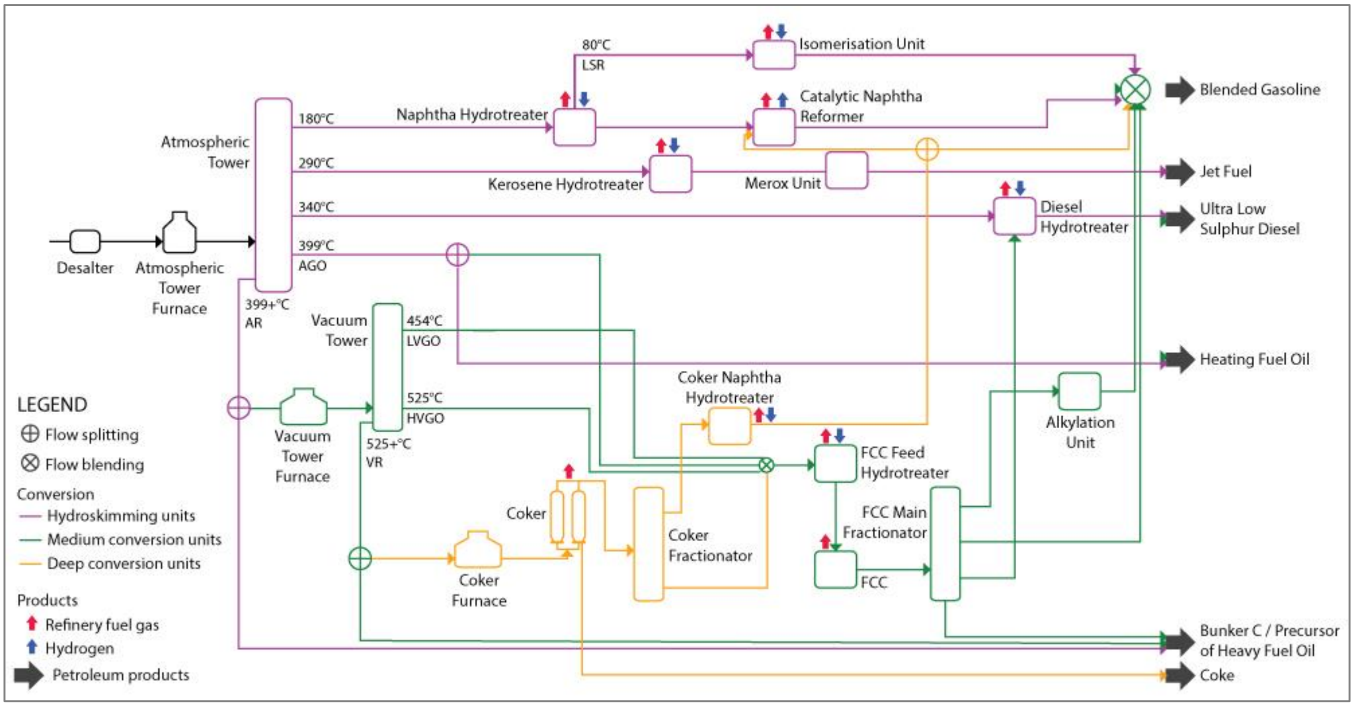


Figure 13: Configuration 4

> In the configuration 4, the hydroskimming process units, the process units associated with the fluid catalytic cracker (FCC), and the process units associated with the coking are enabled to provide a deep conversion.

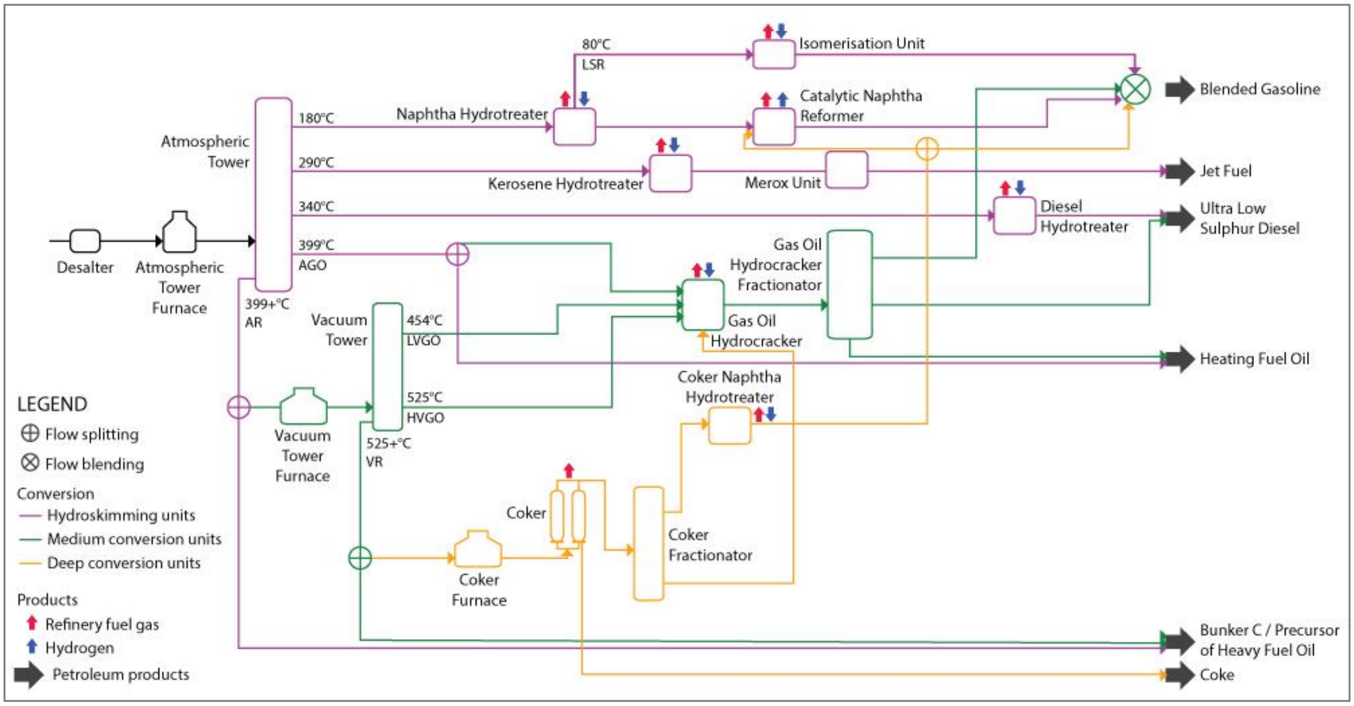


Figure 14: Configuration 5

> In the configuration 5, the hydroskimming process units, the process units associated with the gas oil hydrocracker, and the process units associated with the coking are enabled to provide a deep conversion.

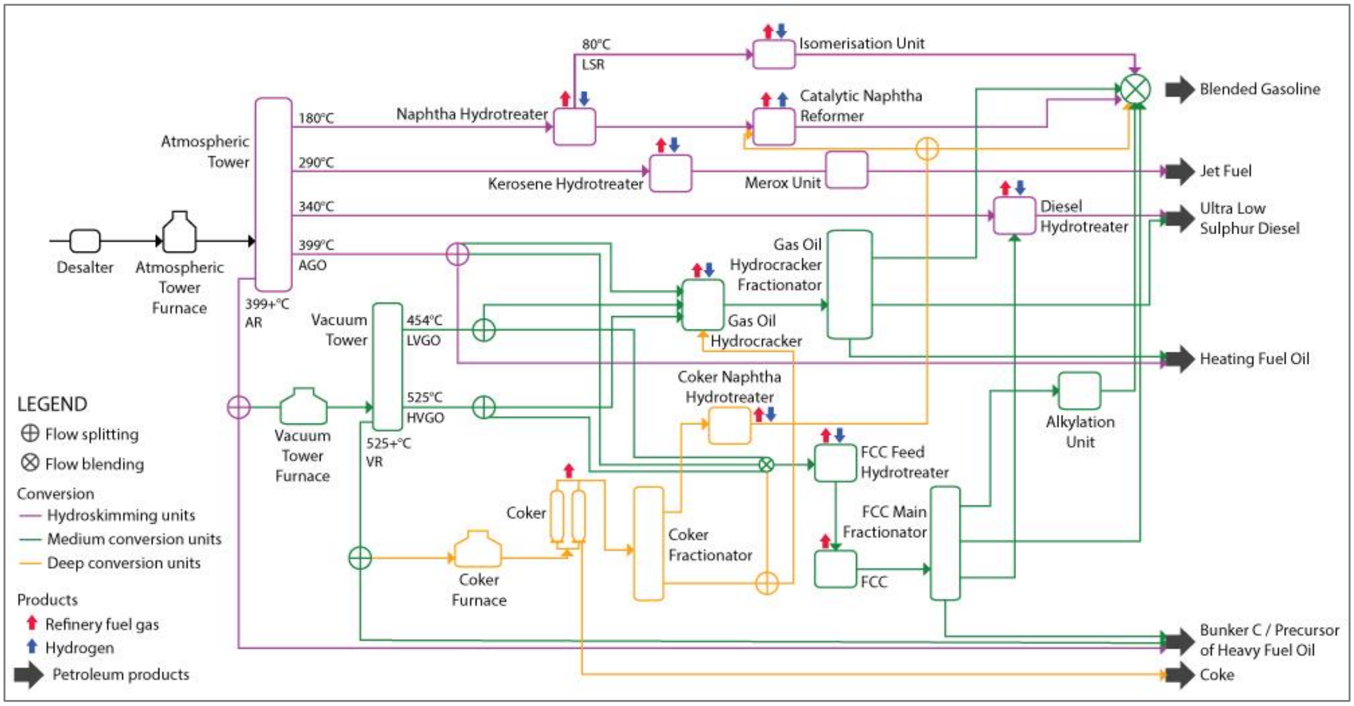


Figure 15: Configuration 6

> In the configuration 6, the hydroskimming process units, the process units associated with the fluid catalytic cracker (FCC), the process units associated with the gas oil hydrocracker, and the process units associated with the coking are enabled to provide a deep conversion.

4.4.4.2 Process unit description

This subsection provides the user with an overview of each process unit used in the deep conversion configuration in the coking refinery, including:

- A general description of the process unit purpose and function;
- The list of all (active and potential) input and output streams – this includes the swings that can be modified to change the destination of streams; and
- Calculations in PRELIM specific to each process unit, including the assumptions tied to the calculations and the equations used. These processes are detailed in the order they are presented in the `CokingRefineryCalcs` worksheet.

4.4.4.2.1 Coking furnace

4.4.4.2.1.1 Process unit description

The coking furnace preheats the stream before it is processed in the coking unit.

4.4.4.2.1.2 Input

The coking furnace is fed by the vacuum residue stream (VR) originating in the vacuum tower.

4.4.4.2.1.3 Output

The heated vacuum residue is sent to the coking unit.

4.4.4.2.2 Coking (or delayed coking unit)

> Note: calculations for the `Coking` and the `Coking Fractionator` are gathered in the same section of the `CokingRefineryCalcs` worksheet. However, they are presented separately in this documentation.

4.4.4.2.2.1 Process unit description

The coking unit brings the input stream to a higher temperature to crack the molecules. It therefore increases the yield of lighter products from heavier fractions and prepares the coker naphtha hydrotreater, the FCC hydrotreater, and gas oil hydrocracker feedstock.

4.4.4.2.2.2 Input

The VR comes from the vacuum tower furnace where it is preheated.

4.4.4.2.2.3 Output

This process unit produces three streams:

- Light gases such as C1 to C4 and naphtha gas oil are sent to the coking fractionator;
- Coke is sent to the coke pool;
- Refinery fuel gas that can be reused within the refinery or sold as a product since it has properties close to natural gas.

4.4.4.2.2.4 Calculations

The correlation is based on “free” carbon content (measured by micro carbon residuum, MCR) and API of the feed. The correlation was derived for feed under 18 API and straight run products (VR) and uses the following equation (Gary et al., 2007):

$$\text{Coker yield} = 11.29 + 0.343 \times MCR$$

4.4.4.2.3 Coking fractionator

4.4.4.2.3.1 Process unit description

The coking fractionator separates the light gases coming from the coking unit into two streams based on the fraction properties.

4.4.4.2.3.2 Input

Light gases such as C1 to C4 and naphtha gas oil come from the coking unit.

4.4.4.2.3.3 Output

The coking fractionator produces two streams:

- The coker naphtha (light fraction) is sent to the gas oil hydrocracker for further processing; and

- The coker gas oil (heavy fraction) is sent to a swing that distributes the stream to the FCC feed hydrotreater and/or the gas oil hydrocracker for further processing.

4.4.4.2.4 Coking naphtha hydrotreater

4.4.4.2.4.1 Process unit description

The coking naphtha hydrotreater uses gas, electricity and hydrogen to reduce to reduce sulphur and nitrogen content, as well as to saturate olefins or aromatic rings of distillate fuels without changing the boiling range to meet specifications of the stream for further processing, or specifications of end products (i.e., increase H/C ratio).

4.4.4.2.4.2 Input

The stream consists of the light fraction coming the coking fractionator.

4.4.4.2.4.3 Output

This process unit produces two streams:

- The desulphurized stream is sent to a swing that delivers the stream to the naphtha catalytic reformer or directly to the gasoline pool depending on the selected `Naphtha catalytic reformer options` on the `Main Input & Output` worksheet. If `SR Naphtha` is selected, the output of the coker naphtha hydrotreater goes straight to the gasoline pool, and if `SR Naphtha + Heavy Naphtha` is selected, it is sent to the naphtha catalytic reformer;
- Refinery fuel gas that can be reused within the refinery or sold as a product since it has properties close to natural gas.

4.4.5 Configurations specific to the hydrocracking refinery

4.4.5.1 Process flow diagrams

The following figures provide a process flow diagram and a short description for each of the three refinery configurations specific to the hydrocracking refinery when the deep conversion is selected.

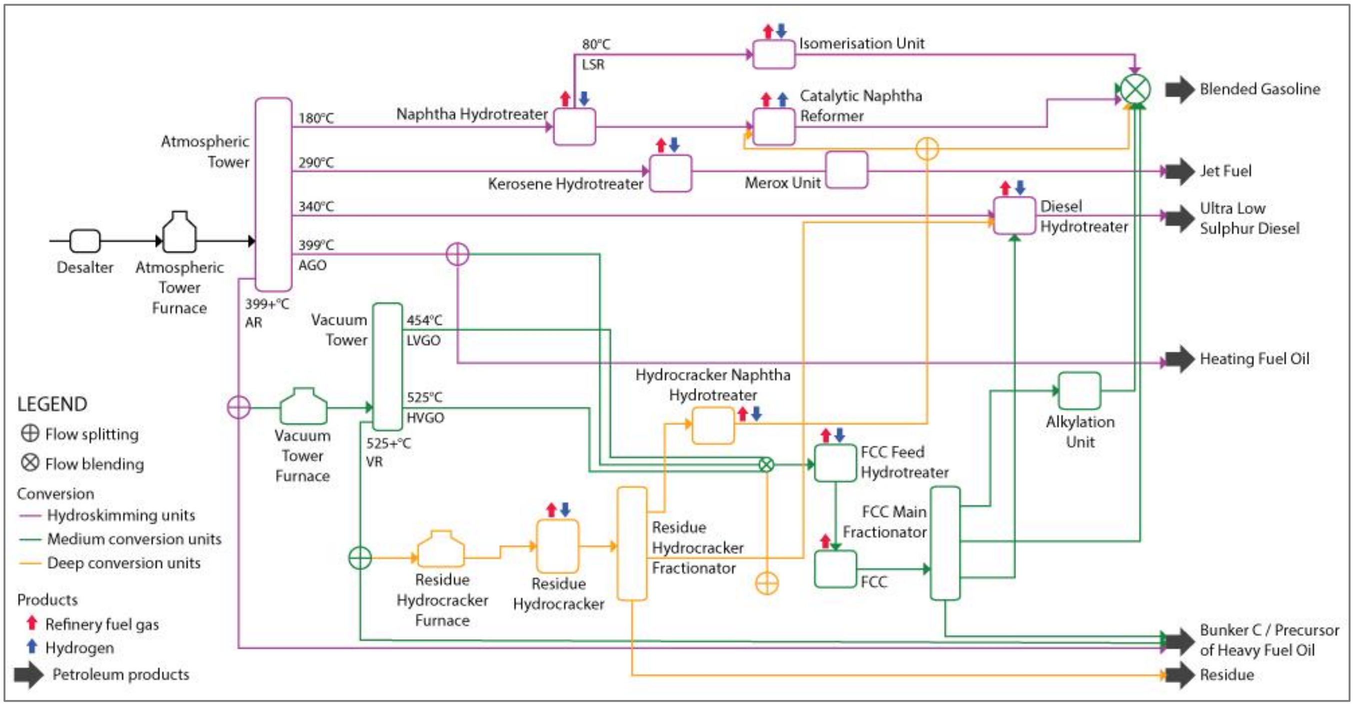


Figure 16: Configuration 7

> In the configuration 7, the hydroskimming process units, the process units associated with the fluid catalytic cracker (FCC), and the process units associated with the residue hydrocracker are enabled to provide a deep conversion.

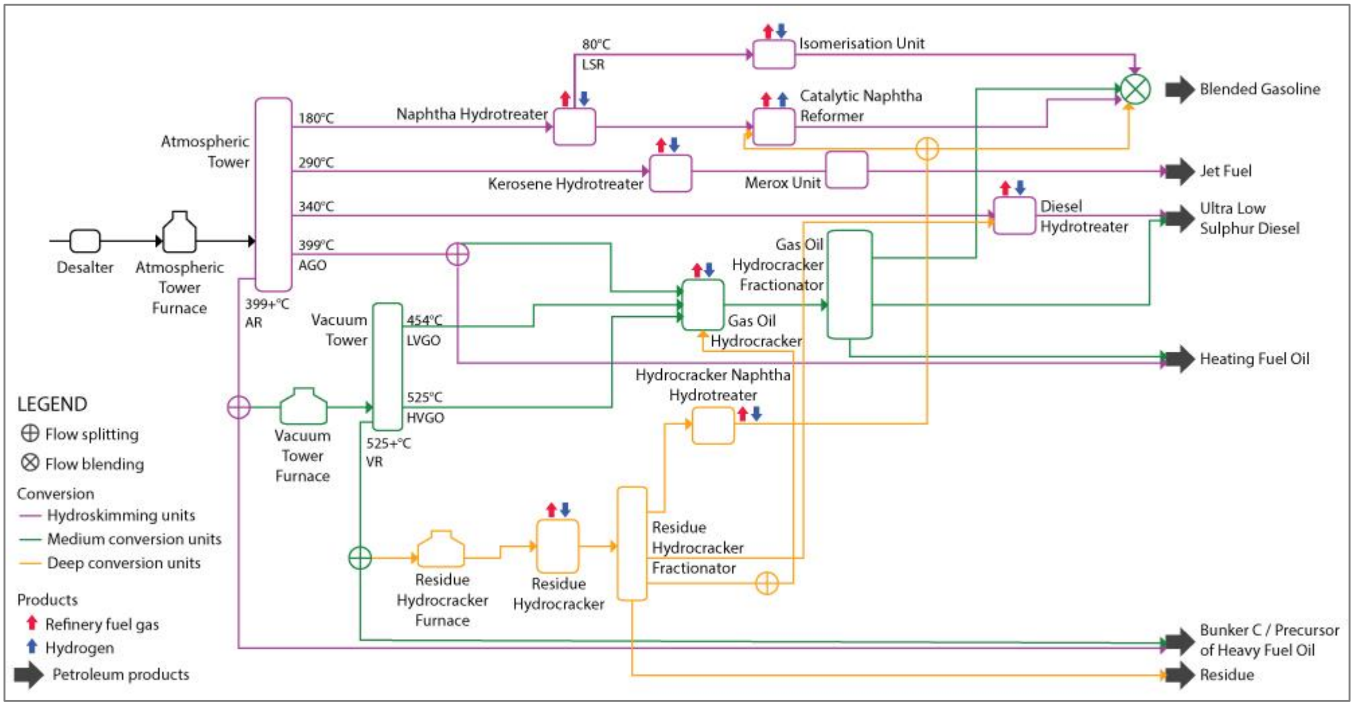


Figure 17: Configuration 8

> In the configuration 8, the hydroskimming process units, the process units associated with the gas oil hydrocracker, and the process units associated with the residue hydrocracker are enabled to provide a deep conversion.

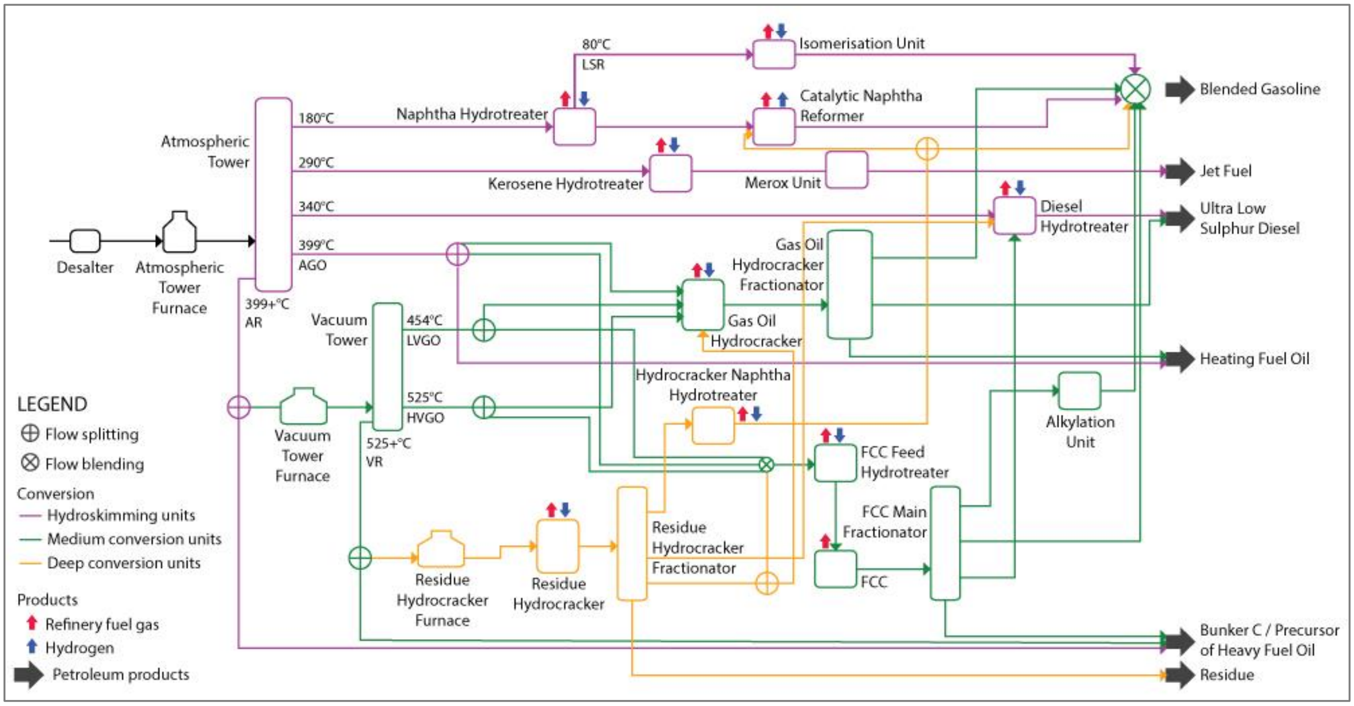


Figure 18: Configuration 9

> In the configuration 9, the hydroskimming process units, the process units associated with the fluid catalytic cracker (FCC), the process units associated with the gas oil hydrocracker, and the process units associated with the residue hydrocracker are enabled to provide a deep conversion.

4.4.5.2 Process unit description

This subsection provides the user with an overview of each process unit used in the deep conversion configuration in the hydrocracking refinery, including:

- A general description of the process unit purpose and function;
- The list of all (active and potential) input and output streams – this includes the swings that can be modified to change the destination of streams; and
- Calculations in PRELIM specific to each process unit, including the assumptions tied to the calculations and the equations used. These processes are detailed in the order they are presented in the `HydroRefineryCalcs` worksheet.

4.4.5.2.1 Residue hydrocracker furnace

4.4.5.2.1.1 Process unit description

The residue hydrocracker furnace preheats the stream before it is processed in the residue hydrocracker.

4.4.5.2.1.2 Input

The residue hydrocracker furnace is fed by a swing that distributes the vacuum residue (VR) coming from the vacuum tower.

4.4.5.2.1.3 Output

The preheated VR stream is sent to the residue hydrocracker.

4.4.5.2.2 Residue hydrocracker

4.4.5.2.2.1 Process unit description

The residue hydrocracker unit breaks the heavy petroleum fractions into simpler molecules, such as gasoline and kerosene, by addition of hydrogen under high pressure in the presence of a catalyst. It increases the yield of lighter products from heavier fractions and primarily increases diesel yields.

4.4.5.2.2.2 Input

The VR stream comes from the residue hydrocracker furnace.

4.4.5.2.2.3 Output

The residue hydrocracker produces two streams:

- The processed stream is sent to the residue hydrocracker fractionator;
- Refinery fuel gas that can be reused within the refinery or sold as a product since it has properties close to natural gas.

The yield and product distribution calculations are based on the method proposed by Gary et al. (2007) and modified by input from industry experts.

4.4.5.2.2.4 Calculations

Correlation is based on feed Kw and approximated hydrogen consumption.

4.4.5.2.3 Residue hydrocracker fractionator

4.4.5.2.3.1 Process unit description

The residue hydrocracker fractionator separates the stream into four streams depending on the properties of the fractions.

4.4.5.2.3.2 Input

The stream comes from the residue hydrocracker.

4.4.5.2.3.3 Output

The residue hydrocracker fractionator produces four streams:

- The light stream (naphtha) is sent to the hydrocracker naphtha hydrotreater for further process;
- The second light stream is sent to the diesel hydrotreater for further process;

- The heavy stream (gas oil) is sent to a swing that distributes this stream to the FCC feed hydrotreater's swing and/or the gas oil hydrocracker.
- The hydrocracking residue is not further processed and is sent to the residue pool.

4.4.5.2.4 Hydrocracker naphtha hydrotreater

4.4.5.2.4.1 Process unit description

The hydrocracker naphtha hydrotreater uses gas, electricity and hydrogen to reduce sulphur and nitrogen content, and to saturate olefins or aromatic rings of distillate fuels without changing the boiling range to meet specifications of stream for further processing, or specifications of end products (i.e. increase H/C ratio).

4.4.5.2.4.2 Input

The stream consists of the light fraction coming from the top of the residue hydrocracker fractionator.

4.4.5.2.4.3 Output

The hydrocracker naphtha hydrotreater produces two streams:

- The desulphurized stream is sent to a swing that delivers the stream to the naphtha catalytic reformer or directly to the gasoline pool depending on the selected `Naphtha catalytic reformer options` on the `Main Input & Output` worksheet. If `SR Naphtha` is selected, the output of the hydrocracker naphtha hydrotreater goes straight to the gasoline pool, and if `SR Naphtha + Heavy Naphtha` is selected, it is sent to the naphtha catalytic reformer;
- Refinery fuel gas that can be reused within the refinery or sold as a product since it has properties close to natural gas.

4.5 Data and constants worksheets

4.5.1 Constants

The `Constants` worksheet provides all the constants used in the calculation worksheets on a process unit basis. Each constant is presented with a unit, a minimum and a maximum value as well as a default value that can be overridden by advanced users. Some constants also include an average value, a median value, and a mode value.

The worksheet also includes the price of products used when the user selects the `Market Value Basis` as the allocation method.

> Source: product prices are obtained from historical North American data of Platts (www.platts.com), and CMAI (www.cmaiglobal.com).

4.5.2 Energy & Unit Conversions

The `Energy & Unit Conversions` worksheet gathers all the factors used to convert values in imperial units into metric units, and vice versa.

4.5.3 Process correlations

The `Process Correlations` worksheet includes calculations of the yields and densities that are required for the hydrocracking and the fluid catalytic cracking process units. All correlations used in PRELIM are based on Gary et al. (2007).

4.5.4 Emissions factors

The `Emissions Factors` worksheet includes the greenhouse gas emission factors associated with each process unit.

4.5.5 Assay inventory

The `Assay Inventory` worksheet displays all the crude oil assays available in PRELIM. It also displays the `Custom Assay` that a user can input on the `Expert Inputs` worksheet as well as the assay resulting from the `Crude Blender` tool at the bottom of the worksheet.

The crude oil assays presented in this inventory have been selected in attempt to provide examples of the range in quality of crudes produced and used globally. This also helps to show a range of possible energy requirements associated with this varying quality. However they are not exhaustive and this inventory will be expanded further in future versions of PRELIM.

This worksheet should not be modified as it is used by the macros used to blend crude assays.

5 Model evaluation

Since PRELIM attempts to balance ease of use and simplicity that informs policy analysis with the rigor required to produce reliable estimates, it is imperative that the methods, data, and results be evaluated against more detailed refinery models. This section presents the methods employed to evaluate the model. In particular, the section describes the approach used to assess the proximity of PRELIM estimates to a more complex proprietary refinery model and present a comparison of PRELIM against the other model estimates for overall refinery CO_2 emissions; product yields, process energy requirements; and hydrogen requirements. Also, a comparison is made between PRELIM estimates using the assay transformation methods described in section 4.3 compared to the assay data from a more comprehensive proprietary database. Finally, a comparison between the previous version of PRELIM (published in 2012) and the current version is made. The implications of differences found are discussed throughout.

5.1 Methods for model evaluation

PRELIM reduces the level of complexity in modelling refinery operations from the models used by industry to optimize their operations (See Parkash [2003] for a detailed description about refinery linear programming modelling). Confidential data (associated with crude assays, operating conditions, and energy estimates) and discussion with refining experts was necessary to assess the validity of PRELIM input data and assumptions. In addition, sensitivity analyses and/or alternative logic calculations to estimate hydrogen content of intermediate products, API of the heaviest fractions, and the Kw parameter are conducted. However, there is also a need to evaluate PRELIM outputs against those of a more detailed refinery model in order to assess its performance, identify any improvements required, and to specify the level of accuracy that can be expected when using the model to inform policy (referred to hereafter as the co-validation process).

Two industry standard tools are used, with input from industry experts, to co-validate two key aspects of PRELIM: 1) a detailed but generic proprietary refinery linear programming model (PRISM^{TM}) is used for estimates of refinery energy requirements and product yields based on PRISM^{TM} (Baker & O'Brien PRISM Overview, http://www.bakerobrien.com/services/PRISM) assumptions for a specific crude assay. PRISM^{TM} is a good basis of comparison as it focuses on very detailed energy requirement and product yield calculations (e.g., PRISM^{TM} uses alternative calculation methods which include operating conditions as modelling parameters in some process units) whereas PRELIM focuses on detailed GHG emissions estimates. 2) Haverly's Crude Assay Management System (H/CAMS) is used to evaluate the transformation of public assay data into data used as input to the current PRELIM crude assay inventory (Haverly Systems Inc. Haverly's Crude Assay Management System, http://www.haverly.com/main-products/13-products/10-hcams). H/CAMS includes a comprehensive proprietary assay database and applications that allow prediction of cut yields and properties for single or blends of crudes (Haverly Systems Inc.). The accuracy of these tools is accepted by industry, and they are commonly used for the analysis of industrial operations and business planning. Permission to use these tools for PRELIM evaluation was obtained and published in Abella (2012).

The model validation was conducted when the model was published in the academic literature in 2012. At that time, PRELIM's crude assay inventory included publicly available assay data that represented 22 Western Canadian Basin crudes tracked by the Canadian Crude Quality Monitoring Program (CCQMP). Small changes were made to the model since this version, however, the comparisons made during the validation are still valid.

5.1.1 Co-validation for estimates of refinery energy requirements and product yields

A total of 22 runs in PRISM^{TM} are used for the assessment of the differences between the models with respect to their estimates of refinery energy requirements and product yields. Three out of the 10 PRELIM configurations were replicated in PRISM^{TM}. One is the hydroskimming configuration suitable to process only light sweet crudes, and the other two are deep conversion configurations that can be applied to refining any crude: (1) delayed coking and FCC process units present, and (2) delayed coking, FCC, and gas oil hydrocracking process units present. Also, ten crudes of different quality are selected to be run in both the PRISM^{TM} and PRELIM models. These included a light sweet conventional crude and a light sweet SCO. Assays included OS products – bitumen, dilbit, syndilbit, synbit, heavy SCO – and Canadian conventional crudes – light sour, medium, and heavy. H/CAMS assay information is selected to be used over PRELIM crude assay inventory to decouple differences between the model outputs due to differences in the crude assay information and due to differences in modelling approaches. Similarly, in order to obtain comparable results, PRELIM assumptions about process energy requirements (which included steam exports from naphtha catalytic reforming, delayed coking, and FCC process units), and emission factors for natural gas (combustion, no upstream emissions) and electricity are set equal to the corresponding assumptions in PRISM^{TM}. Common outputs of the model such as refinery final product yields (i.e. gasoline, diesel, fuel gas and coke) and energy requirements (i.e. FCC coke-burned, on site produced gas, natural gas, electricity, and hydrogen requirements) as well as refinery CO_2 emissions are compared to assess overall proximity between model results.

Because PRISM^{TM} does very detailed energy requirement and product yield calculations using methods that are different from PRELIM, it is used as the basis to mathematically measure how well the models (PRISM^{TM} and PRELIM) outputs match (proximity criteria). Three measurements are employed as described here:

1) Coefficient of Variation of the Root-Mean-Square Deviation (CV (RMSD)) to quantify the magnitude of under or overestimates specific to an output. In this case, it calculates the square root of the variance between PRISM^{TM} and PRELIM estimates for a particular crude, normalized by the mean of the PRISM^{TM} estimates:

$$CVRMSD\left(\theta_{PRISM^{TM}}, \theta_{PRELIM}\right) = \frac{\sqrt{\frac{\sum_{i=1}^{n}\left(x_{PRISM^{TM},i} - x_{PRELIM,i}\right)^{2}}{n}}}{\overline{X_{PRISM^{TM}}}} \times 100\%; \quad \theta = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

Where,

$\theta = Model\ output\ such\ as\ MJ\ of electricity\ required\ per\ MJ\ of\ crude\ being\ processed$

$x = value\ estimated\ by\ a\ model\ in\ a\ run\ for\ a\ particular\ output$

$n = number\ of\ runs = 22$

$\overline{X_{PRISM^{TM}}} = average\ of\ \ values\ estimated\ by\ PRISM^{TM}$

$Numerator\ provides\ \ the\ variance\ between\ model\ outputs\ in\ the\ same\ units\ (e.g., MJ)$

$Denominator\ provides\ an\ estimate\ of\ the\ variance\ expresed\ as\ a\ percentage$

For example, over all runs and configurations, the deviation in CO_2 emissions between PRISM^{TM} and PRELIM is estimated to be 0.7 g CO2/MJ of crude, or 10% relative to PRISM^{TM} estimates. Under or overestimates are illustrated by using scatter diagrams where the x-axis is used to represent PRISM^{TM} estimates and the y-axis is used to represent PRELIM estimates. Data points over the diagonal line indicate where PRELIM overestimates values compared to PRISM^{TM} estimates. Data points under the diagonal line illustrate that PRELIM underestimates values compared to PRISM^{TM} estimates.

2) The coefficient of determination (r^2) to quantify proximity to reproduce variability in model outputs due to crude assay information ("natural" variability due to crude quality). In this case, it calculates the squared value of the coefficient of correlation or the combined variation against the single variation of the PRISM^{TM} estimates and PRELIM estimates for a particular model output:

$$r^2 = \left(\frac{\sum_{i=1}^{n} \left(x_{PRISM,i} - \overline{X_{PRISM}}\right)\left(x_{PRELIM,i} - \overline{X_{PRELIM}}\right)}{\sqrt{\sum_{i=1}^{n} \left(x_{PRISM,i} - \overline{X_{PRISM}}\right)^2} \sqrt{\sum_{i=1}^{n} \left(x_{PRELIM,i} - \overline{X_{PRELIM}}\right)^2}} \right)^2$$

Where,

$x = value\ estimated\ by\ a\ model\ in\ a\ run\ for\ a\ particular\ output\ (e.g., electricity)$

$\bar{X} = average\ of\ \ values\ estimated\ by\ a\ model$

$n = number\ of\ runs = 22$

The r^2 value describes how much of the variation in PRISM^{TM} estimates is represented by the variation in PRELIM estimates. The r^2 value may range from 0 to 1. A value of 0 represents no correlation while a value of 1 represents that the variation is similar in the estimates from both models. In other words a r^2 close to 1 indicates that PRELIM is able to reproduce the "natural" variability in model outputs (associated with a particular crude and configuration) predicted by PRISM^{TM} very well (Krause et al., 2005).

3) A weighted coefficient of determination (wr^2) to measure the "overall model match". This coefficient is an indicator that combines the model performance in reproducing the variability specific to an output/estimate as indicated above, measured by the coefficient of determination, and the magnitude of under- or over-estimates using the gradient of correlation (i.e., the slope of the regression on which r^2 is based. If the equation of a line is expressed as $y = bx + c$; the gradient of correlation (b) should be close to 1 if there is good agreement between the two estimates. If the intercept of the regression (c) is 0, the gradient of correlation indicates the magnitude of the under or overestimates. For example, in a scatter diagram in which the x-axis is used to represent PRISM^{TM} estimates and the y-axis is used to represent PRELIM estimates, a gradient of linear regression of 0.5 means that PRELIM underestimates PRISM^{TM} outputs by 50% if the intercept is 0. In this application, the intercept may not be 0, and therefore, the gradient of correlation is not used to indicate the magnitude of under or over estimates. The CV (RMSD) is used for this purpose as explained above. However, the weighted coefficient of determination is still meaningful to quantify the overall model match as it is based on the principles of least squares. The weighted coefficient of determination (wr^2) is proposed in Krause et al. (2005) to be calculated as follows:

$$wr^2 = \left\{ \begin{array}{c} |b| \times r^2\ for\ b \leq 1 \\ |b|^{-1} \times r^2\ for\ b > 1 \end{array} \right\}$$

Where,

$$b = slope\ or\ regression\ coefficient\ \ resulting\ from\ linear\ regression$$

$$between\ PRISM^{TM} and\ PRELIM\ estimated\ values\ for\ a\ particular\ output$$

The range of values for wr^2 is from 0 to 1; where a value of 0 means no proximity while a value of 1 means a perfect "match". Therefore, "overall model match" can be ranked based on the wr^2 value. The following rank was used to characterize the match between PRISM^{TM} and PRELIM estimates: Low match ($wr^2 < 0.5$) intermediate match ($0.5 < wr^2 < 0.7$), high intermediate match ($0.7 < wr^2 < 0.9$), and high ($0.9 < wr^2$). wr^2 values are also reported.

5.1.2 Co-validation for transformation of publicly available assay data in PRELIM

The quality of the crude assay data is evaluated based on how differences in the assay information can affect precision in PRELIM GHG estimates. There are a total of 99 runs in PRELIM for the assessment of the differences in PRELIM GHG estimates using both H/CAMS assays and PRELIM crude assay inventory data. Nine out of the 10 crude assays selected for co-validation are studied; the 10th is excluded based on completely dissimilar whole crude characteristics such as sulphur, API, and distillation curve between the H/CAMS and PRELIM assay data implying that the crudes considered were significantly different. Also, each crude is run in nine configurations, and in one configuration at two levels of energy use (a total of 11 refinery cases). Overall refinery GHG emissions as well as gasoline and diesel GHG emissions estimates are tabulated for the analysis (allocation only to transportation fuels is used). Measurement of the variation in PRELIM GHG estimates for each crude as well as the deviation in each individual quality parameter is used to gain information about quality of the PRELIM assay data, limitations of the transformation methods adopted, and needs for improvement of assay data. The Coefficient of Variation of the Root-Mean-Square Deviation (CV (RMSD)) is used to quantify the magnitude of the variance in PRELIM GHG estimates; the square root of the variance is normalized by the mean of PRELIM estimates when H/CAMS assay data are used.

5.2 Comparison of fit between PRISM^{TM} and PRELIM

PRELIM is able to estimate the energy use and GHG emissions associated with a particular crude in different configurations as it could be done from a more complex refinery model with a margin of error appropriate between the bounds of life cycle analysis and the transparency needed to inform policy. This section presents the results of the co-validation process that measures the difference between estimates of the two models. This process helps to highlight the difficulty in replicating estimates not only due to differences in modelling approaches but also due to the level of complexity and flexibility that exits in operating processes in refineries.

5.2.1 Overall model performance

Overall refinery emissions estimates are used as the first level of comparison of the models. These emissions estimates include CO_2 emissions that result from gas combustion, SMR emissions, FCC coke-burned, and indirect emissions due to electricity use. Figure 19a shows the refinery emissions estimates (g CO_2/MJ of crude) for a range of crudes with PRELIM model on the y axis and PRISM^{TM} model on the x axis. Figure 19b and Figure 19c show the same plot but per MJ of gasoline and diesel respectively (No allocation procedure is applied in PRELIM [see section 4.2.1] to be consistent with PRISM^{TM}).

The figure illustrates that there is a good agreement (match) between the models' estimates. PRELIM replicates 93% of the variability in CO_2 emissions due to crude quality and configuration, and the deviation calculated as a Coefficient of Variation of the Root-Mean-Square Deviation is low (CV(RSMSD) 10%). The deviation in the estimates is considered appropriate within the bounds of life cycle assessment. More generally, literature in the field of life cycle assessment suggests that standard deviations for variation in emissions range from a typical 20% (when assessing existing technologies and processes) up to 100% for estimating less certain technologies (e.g., emerging technologies and processes [Llyod et al., 2007]).

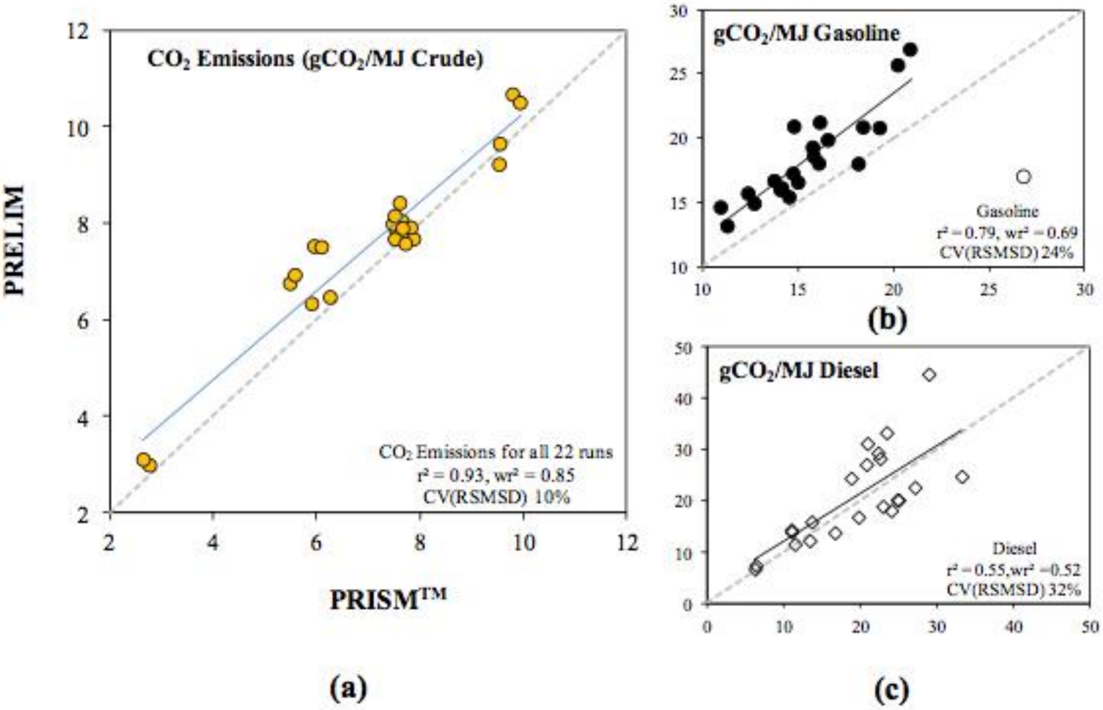


Figure 19: Comparison of Fit between PRISM^{TM} and PRELIM CO_2 Estimates

> The x-axis shows PRISM^{TM}'s CO_2 emissions (g CO_2/MJ Crude), and the y-axis shows PRELIM's CO_2 emissions (g CO_2/MJ Crude). Solid lines illustrate deviations that are due to variation in crude properties.
>
> It includes onsite emissions from gas combustion, hydrogen production via steam methane reforming, and indirect emissions due to electricity use. r^2: coefficient of determination, wr^2: weighted coefficient of determination accounting for gradient of correlation to quantify overestimates and variability together. CV(RSMSD): coefficient of variation of the root-mean-square deviation (normalized by the mean of PRISM^{TM} estimates). Diagonal dotted lines illustrate deviations that are due to variation in crude properties.

There are methodological compromises when the unit of measurement changes to a per product basis versus an overall refinery. The match rank goes from a high intermediate to intermediate value and the estimate deviation increases. However, such behaviour is more a reflection of the range of operating conditions possible (e.g., temperature and pressure) and the configuration being modelled rather than one model being more accurate than another. Further details are discussed in the following sections, which demonstrate that no simple calibration process can be followed to match the models' performance if the flexibility and variability that exist in real refinery operations is taken into account. This demonstrates the value of a simple and flexible tool. Nonetheless, the comparison of these models opens questions about potential improvements in PRELIM to model the refinery system. Despite using same assumptions in the basic options in both models, two types of source of uncertainty exist, those of which are derived from the level of detail in PRELIM modelling and those that are uncertain by their very nature. To explore the source of the variability observed between the models, intermediate model estimates or outcomes are explored in the following.

5.2.2 Products yields

One key element in comparing the models is the amount of each final product that results from processing a certain crude. Therefore, it is important to get agreement about the amount of refinery final products (e.g., gasoline and diesel) obtained from a specific crude in a particular configuration. Figure 20 shows the models' estimates of product yields for gasoline and diesel (MJ of product/MJ of crude processed) for the same set of crudes grouped by configuration. The comparison of the models' estimates of product yields demonstrates several points: a) The assessment of overall emissions on a per product basis is impacted by the type of configuration being modelled, b) PRELIM can replicate the "natural variability" in model outputs predicted by PRISM^{TM} due to the quality of the crude in a specific refinery configuration, c) the magnitude of the deviations in final product yields are mainly associated with deviations resulting from modelling the hydrocracking process unit, d) deviations may also result from the different level of detail in modelling process unit operating conditions between the two models or divergence in the accuracy in the process unit product yield correlations.

The assessment of overall emissions on a per product basis is impacted by the type of configuration being modelled. In Figure 19b and Figure 19c, agreement between the models' overall emissions estimates on a per product basis (i.e., overall emissions divided by the final product yield) are evaluated over all of the runs regardless of the configuration that is modelled. Figure 20 also helps to illustrate that the configuration plays an important role in the assessment of the magnitude of variability and deviations.

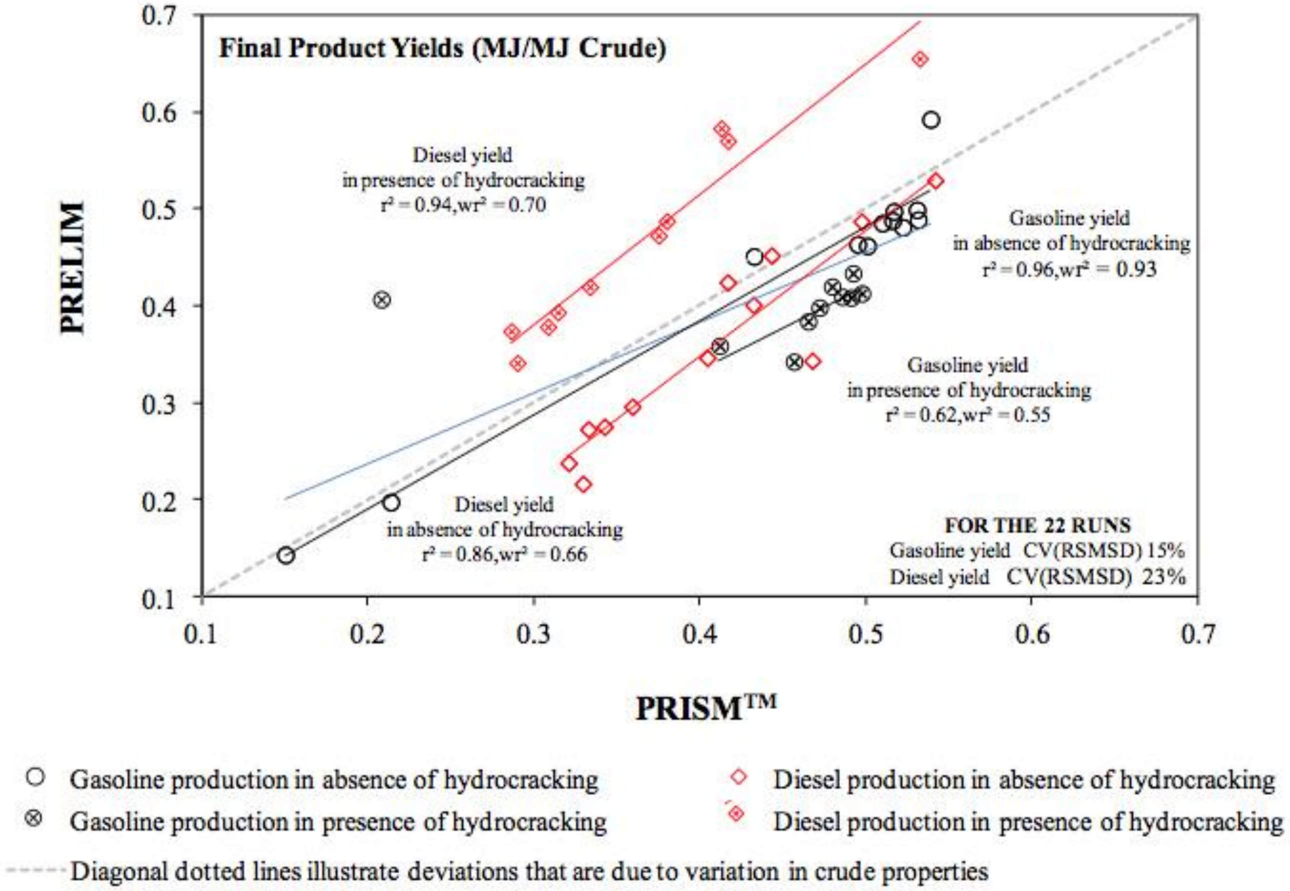


Figure 20: Comparison of fit between PRISM^{TM} and PRELIM final product yields estimates

> The x-axis shows PRISM^{TM}'s final product yields (MJ/MJ Crude), and the y-axis shows PRELIM's final product yields (MJ/MJ Crude). Solid lines illustrate deviations that are due to variation in crude properties.
>
> White series denotes: Gasoline and diesel productions in hydroskimming configuration or configuration where delayed coking and fluid catalytic cracking are present (in absence of hydrocracking). X series denotes: Gasoline and diesel productions in configuration where delayed coking, fluid catalytic cracking, and gas oil hydrocracking are present (in presence of hydrocracking). r^2: coefficient of determination, wr^2: weighted coefficient of determination accounting for gradient of correlation to quantify overestimates and variability together. CV(RSMSD): coefficient of variation of the root-mean-square deviation (normalized by the mean of PRISM^{TM} estimates).

Once there is an agreement on the type of refinery processes to include, Figure 20 shows that PRELIM can replicate the "natural variability" in model outputs predicted by PRISM^{TM} due to the quality of the crude. PRELIM is able to replicate most of the variability in gasoline and diesel yields for a refinery with hydroskimming and deep conversion configurations, without a gas oil hydrocracking process unit (r^2=0.95 for gasoline; r^2=0.86 for diesel). Also, in the presence of hydrocracking, there is an acceptable and good replication of variability in gasoline and diesel yields respectively (r^2=0.62 for gasoline; r^2=0.94 for diesel). If overall refinery emission estimates on a per product basis are analyzed in this way, it shows that PRELIM can replicate most of the variability of PRISM^{TM} estimates as well. The coefficient of determination that represents how much of the variation in PRISM^{TM} estimates is represented by the variation in PRELIM estimates improves from the aggregated coefficient of determination presented in Figure 19 for both products and the three configurations (Figure 20 shows that r^2 improves to a value of 0.85 for gasoline and to 0.97 for diesel). Therefore, PRELIM can reliably be used to simulate variability in resulting emissions estimates from processing different crudes in different configurations.

Also, Figure 20 illustrates that the magnitude of the deviations in final product yields (therefore in overall emissions on a per product basis) are mainly associated with deviations resulting from modelling the hydrocracking process unit. It is difficult to determine the exact source of the deviation considering the flexibility in operating conditions that exists for this specific process unit. The hydrocracking process unit can be used to produce more gasoline or more diesel depending on process operating conditions. At first glance, it seems that the PRELIM hydrocracking product yield correlations favours diesel production. When the hydrocracking process unit is not present, PRELIM underestimates diesel yields (i.e., Figure 20 shows that the data points associated with diesel production in absence of hydrocracking are under the diagonal dotted line). However, PRELIM hydrocracking product yield correlations should favour gasoline production (Gary et al., 2007), which is consistent with the basic modelling option that is selected in PRISM^{TM} for the purposes of the co-validation. This suggests that PRISM^{TM} may model more severe operating conditions that increase gasoline yield at the expense of diesel yield. For the purposes of co-validation, PRISM^{TM} is run at a 70% level of conversion of process unit feed to lighter products. In real operations, in a particular hydrocracking process unit of high efficiency, conversion could range from 50 to 70% (Gary et al., 2007). Therefore, correlations used in PRELIM are plausible and likely represent a process unit with less efficient conversion.

On the other hand, Figure 20 indicates that deviations may also result from the different level of detail in modelling process unit operating conditions between the two models. It is not clear if PRISM^{TM}'s capability to account for process unit operating conditions such as pressure or temperature could be internally used by PRISM^{TM} to determine product yields specific to each crude. For example, PRELIM estimates of coke yield from the delayed coking unit are consistently high compared with PRISM^{TM} estimates for all crudes whose crude quality is below the quality of a conventional light sour crude in opposition to coke yield from the sweet light crudes (coke yield 40% CV(RSMSD)). Operating conditions in the delayed coking process unit do change coke yields. An increase in coke yield can result in consistently underestimating both gasoline and diesel yields when the hydrocracking process is absent (Figure 20). Another example is the outlier in Figure 20 for gasoline yield (when the hydrocracking process unit is present). It corresponds not only to the conventional light sweet crude, but also to a case where refinery final gasoline yield is influenced by changes in the extent of hydrocracking (i.e., amount of hydrogen added). Because PRISM^{TM} is consistently run at a 70% conversion, it could represent a low extent of hydrocracking for this crude that is easy to be processed. On the other hand, PRELIM is consistently run assuming the same level of hydrocracking (approximately 1,500 standard cubic feet of hydrogen per barrel of feed) to process all crudes; a more intense level of hydrocracking compared to the level that PRISM^{TM} could have assumed for this crude. It is possible to run PRELIM at a level of hydrocracking to be comparable to PRISM^{TM}; however, a relationship between conversion (input parameter in PRISM^{TM}) and approximately hydrogen requirement (input parameter in PRELIM) would have to be determined. Therefore, PRELIM appears to overestimate gasoline production specific to this crude as opposed to the underestimates of other crudes. When PRELIM is run with decreased level of hydrocracking (e.g., change from adding 1,500 to 500 standard cubic feet of hydrogen per barrel of feed), the finals refinery gasoline yield estimated for this crude is reduced by

12%. Similar to the delayed coking process unit, it is unknown how PRISM^{TM} internally models and links variables such as the extent of hydrocracking to feed quality.

Moreover, the condition of over or under estimating final product yields as well as the magnitude of the deviations partially results from divergence in the accuracy in the process unit product yield correlations. Similar to PRELIM, PRISM^{TM} correlations have been derived from a set of process unit operating conditions, including a set of crude runs, and it is unknown to what extent the correlations in both models can be generalized to all crude of different quality. This includes the crudes derived from bitumen (crude of largest deviation in final product yield estimates). Both, PRELIM and PRISM^{TM} correlations could be correct with some margin of error (difficult to determine), and therefore their process yields are likely to be equally valid but different with some uncertainty inherent to the modelling process.

Considering the points above, over all of the runs, PRELIM deviations in gasoline and diesel yield are acceptable (15% and 23% CV(RSMSD) respectively) and can be explained by differences in model approaches. The overall model match on these outputs ranks at a high intermediate and intermediate value (average $wr^2=0.74$ on gasoline yield; average $wr^2=0.68$ on diesel yield) and is mostly affected by process unit operating conditions that could be modelled by establishing a clear link between them and the feedstock quality as further development of PRELIM.

5.2.3 Gas requirement

The proximity of the models in estimating the gas required by the refinery to process a crude is presented in Figure 21. Gas requirement is the single most important process energy requirement in refining crude oil. It is used to supply heat, steam, and hydrogen. PRELIM and PRISM^{TM} estimates show that on an energy basis, the gas requirement estimates are up to ten times higher than the estimates for electricity and five times higher than the estimates for FCC coke-burned. Estimates of the gas requirement will affect how much gas is purchased from offsite and CO_2 emissions associated with the gas combustion and its chemical transformation into SMR hydrogen. Also, the gas requirement affects upstream impacts of purchased gas production, processing, and transport.

Figure 21 shows the comparison of gas requirement estimates from both models in terms of total energy requirement as well as energy required from offsite. The comparison implicitly compares the models' proximity in three outputs: 1) match in gas requirement due to hydrogen demand, 2) proximity in gas requirement due to process energy requirements, and 3) match in onsite fuel gas production estimates. The latter compares two different levels of aggregation by modelling the amount and quality of the fuel gas. Conversely to PRISM^{TM}, PRELIM calculation methods group lighter gases; i.e. they do not distinguish between methane, ethane, propane, and butanes, and generalize fuel gas production yields in all hydrotreating process units.

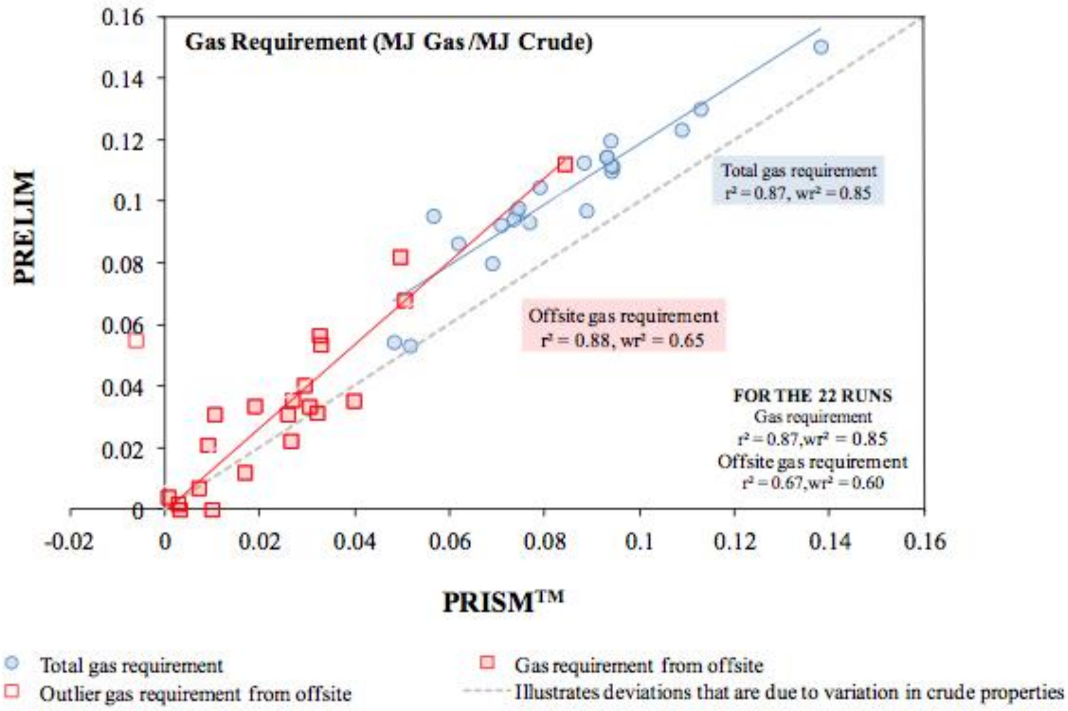


Figure 21: Comparison of Fit between PRISM^{TM} and PRELIM Gas Requirement Estimates

> The x-axis shows PRISM^{TM}'s gas requirement (MJ Gas/MJ Crude), and the y-axis shows PRELIM's gas requirement (MJ Gas/MJ Crude). Solid lines illustrate deviations that are due to variation in crude properties.
>
> Total gas requirement includes gas associated with heating, steam, and chemical transformation hydrogen via steam methane reforming. Gas requirement from offsite equals total gas requirement minus gas produced onsite; PRISM^{TM} estimates of propane produced are included. Outlier: light sweet synthetic crude oil assay run in configuration where delayed coking and fluid catalytic cracking are present. r^2: coefficient of determination, wr^2: weighted coefficient of determination accounting for gradient of correlation to quantify overestimates and variability together.

Figure 21 shows that PRELIM replicates most of the "natural variability" in total gas requirement and offsite gas requirement resulting from different configurations and types of crude. PRELIM reproduces similar variability of gas requirement for all 22 cases (r^2=0.87 gas requirement). Also, PRELIM replicates the variability in offsite gas requirement for most of the runs (r^2=0.88 offsite gas requirement for 19 out of 22 runs). In addition, Figure 21 illustrates that PRELIM estimates of these gas requirements are consistently high. The deviation in total gas requirement (24% CV(RSMSD) is considered acceptable as it results from the combined effect of several factors and does not end in a large deviation in the overall refinery emission estimates (total gas requirements match ranks at a high intermediate value; wr^2=0.85). Differences in modelling hydrogen requirements (section 5.2.4) only partially explain the deviation in total gas requirements. For example, excluding the models' gas requirement estimates associated with the hydrogen requirements, the deviation in total fuel gas requirement increases (35% CV(RSMSD) indicating the cumulative impact of other factors such as differences in process unit product yields that are a reflection of the range of operating conditions possible (section 5.2.2). Besides that, the significant deviation in offsite gas requirements (46% CV(RSMSD) is considered acceptable for the current version of PRELIM because it does not have an important impact on PRELIM emissions estimates. PRELIM assumes natural gas and refinery fuel gas direct refinery emissions to be very similar. However, deviation in offsite gas requirements has an effect in terms of energy estimates and associated upstream impacts, and should be addressed in future versions of PRELIM (offsite gas requirements match ranks at an intermediate value; wr^2=0.60). Once the deviation in total gas requirements is improved, deviation in offsite gas requirements could be enhanced by reconciliation of differences regarding onsite gas requirement/refinery fuel gas production estimates. Both improvements require detailed analysis and further validation.

PRELIM energy estimates can be beneficial for a more detailed modelling and characterization of the refinery fuel gas. The outlier for offsite gas requirement in Figure 21 demonstrates the effects of PRELIM limitations to account for lighter gases separately. PRISM^{TM} and PRELIM model propane production differently. The “apples to apples comparison” required that PRISM^{TM}'s propane production estimates are included in the calculations of onsite gas production. This is different from the PRELIM estimates that have already propane production as part of the onsite gas or refinery fuel gas production. For some crudes the energy embedded in propane makes a difference in whether PRELIM onsite fuel gas production results in an under or overestimate. It also makes a difference in the magnitude of the deviations in such estimates. Disaggregating the refinery fuel gas characterization could help to improve estimates in energy content of the onsite fuel gas production estimates.

For the purposes of estimating refinery emissions, the proximity between both models in onsite fuel gas production, at this time, is considered acceptable (r^2=0.85 and 27% CV(RSMSD)). There is not “rule of thumb” to estimate the amount of refinery fuel gas in industry, and it varies widely among refineries. Therefore, it is not possible to indicate which model estimates are more accurate. In fact, both can be plausible considering the differences that arise from different operating conditions. The possibility that PRISM r^2 may model less or more severe hydroprocessing as has been discussed (section 5.2.2) also leads to deviations in onsite fuel gas production estimates. Finally, PRISM^{TM} assumes that FCC heavy products are recycled in the delayed coking process. This is not considered in PRELIM which also helps to explain the deviations in onsite fuel gas production calculated in the two models. Nonetheless, the onsite fuel gas estimates impact refinery emissions indirectly through the hydrogen requirement that is associated with the fuel gas hydrogen content. Because onsite fuel gas production/requirement estimates match ranks at between the intermediate and low values (wr^2=0.53), it warrants a more detailed investigation in future versions of PRELIM in order to improve overall refinery emissions estimates.

5.2.4 Hydrogen requirement

An important criterion to evaluate PRELIM performance for modelling effects of crude quality and refinery configuration on refinery GHG emissions is the capability to estimate the hydrogen requirement specific to a crude assay and configuration. Differences in hydrogen requirements will affect refinery energy use and CO_2 emissions estimates through changes in hydrogen demand from the SMR. Comparison of hydrogen requirement estimates from both models mainly compares the effects of two different modelling approaches: the PRELIM approach of global hydrogen balance using hydrogen contents in feedstocks and products, and PRISM^{TM}’s use of a class of hydrogen- consuming chemical reactions to determine the hydrogen requirement to achieve olefins and aromatics saturation (e.g., using a molar ratio of 5 hydrogen atoms to one hydrocarbon molecule for saturation of aromatics or 3.3 for saturation of polyaromatics to monoaromatics)(Castañeda et al., 2011).

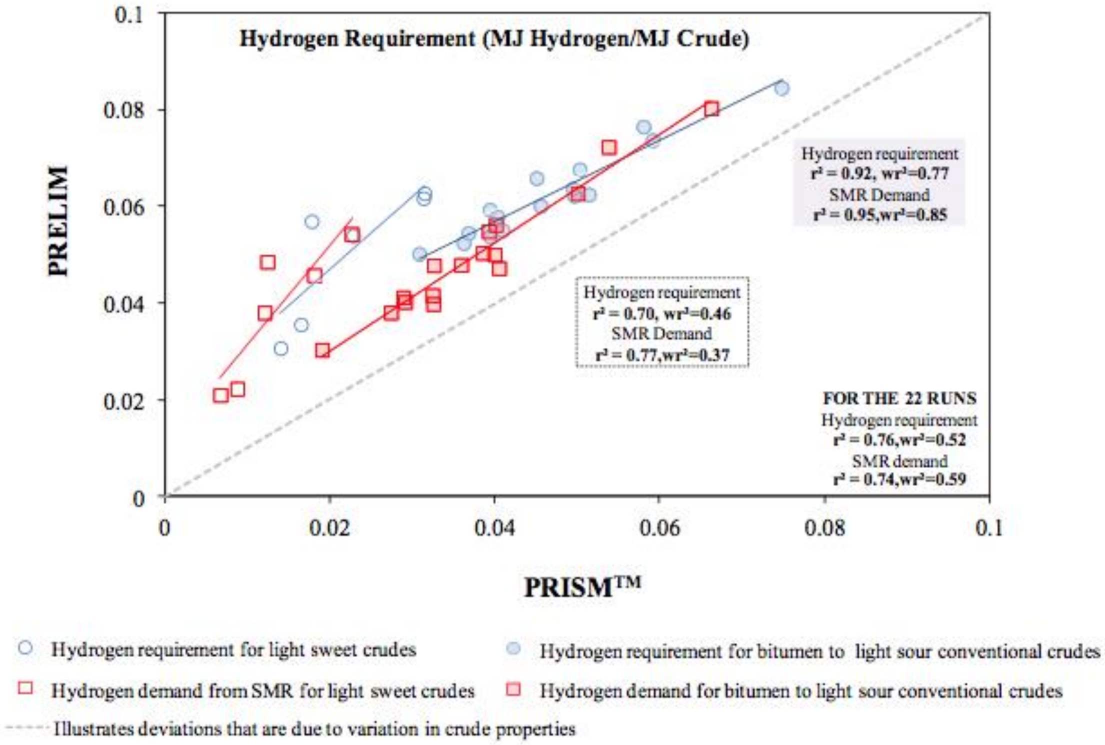


Figure 22: Comparison of fit between PRISM^{TM} and PRELIM refinery hydrogen requirement estimates

> The x-axis shows PRISM^{TM}'s hydrogen requirement (MJ Hydrogen/MJ Crude), and the y-axis shows PRELIM's hydrogen requirement (MJ Hydrogen/MJ Crude). Solid lines illustrate deviations that are due to variation in crude properties.
>
> Hydrogen demand from steam methane reforming (SMR) equals hydrogen requirement minus co-production of hydrogen via naphtha catalytic reforming. r^2: coefficient of determination, wr2: weighted coefficient of determination accounting for gradient of correlation to quantify overestimates and variability together.

The PRELIM approach is as valid as the PRISM^{TM} method to determine crude specific hydrogen requirement. Figure 22 provides three insights: 1) PRELIM consistently overestimates the hydrogen requirement and SMR demand for all runs (51% and 56% CV(RSMSD) respectively). 2) Though PRELIM's calculated hydrogen requirement is consistently high, it has the capability to reproduce PRISM^{TM}'s variability in hydrogen requirement estimates for the range of bitumen to conventional light sour crude assays (r^2=0.92 hydrogen requirement; r^2 =0.95 SMR demand). 3) There are some compromises when using different methods for analyzing the light sweet conventional and light sweet SCO assays' hydrogen requirements (r^2=0.70 hydrogen requirement; r^2 0.77 SMR demand) which limits overall model comparison. Over all runs, PRELIM replicates 76% and 74% of the "natural" variability in hydrogen requirements and SMR demand due to the quality of the crude.

The deviation in variability estimated for the hydrogen estimates and SMR demand for the light crudes can be a consequence of the different level of detail in modelling operating conditions associated with the crude properties in the two models. PRISM^{TM} may determine the level of hydrotreating and/or hydrocracking of a crude based on the structural composition of its fractions while PRELIM assumes all crudes to be treated to result in the same hydrogen specification (PRELIM does not distinguish between the structural compositions of the crude fractions). For example, comparison of the variation in hydrogen requirement estimates for the light crudes in the deep configurations shows that PRISM^{TM} estimates more important variation than PRELIM as a result of including the hydrocracking process unit.

On the other hand, for the interpretation of the high values in the coefficient of variation of the root-mean-square deviation, it is important to recall previous discussion regarding flexibility in product yields and operating conditions that exist for refinery process units and limitations to generalize modelling correlations to all feedstock quality. In particular, for the case of hydrogen requirement, it is important to note that while the equations that PRISM^{TM} uses in its calculations (and therefore, the accuracy of the method used by PRISM^{TM} to determine hydrogen requirement) are unknown, some sets of equations used in the class of hydrogen-consuming chemical reactions method reportedly deviate from experimental data by as much as 29%. Specifically, experimental analysis found that this calculation method mostly underestimates hydrogen consumption, in particular for hydrotreating gas oil fractions (Castañeda et al., 2011). Based on the analysis of hydrogen requirements for hydrotreating processes presented in Castañeda et al. (2011), the performance of the set of equations used by PRISM^{TM} might explain the deviations when analyzing hydrogen requirement for the light crudes, relative to the PRELIM estimates. i.e., There is a set of equations available for calculating hydrogen requirement by the method of class of hydrogen-consuming chemical reactions which perform very well in predicting hydrogen requirement for hydrotreating gas oil fractions (2% deviation) while underpredicting by almost 50% the hydrogen requirement for hydrotreating naphtha fractions.

Also, it is important to consider the interrelationship between modelling parameters. The overestimates on hydrogen requirement and SMR demand are accounted in the variation in gas requirement specific to a configuration and type of crude that is assessed with an acceptable CV(RSMSD) of 24%. Similarly, hydrogen requirement is implicitly affected by the overestimated onsite fuel gas production (refinery fuel gas that has an important amount of hydrogen content) that is also assessed with an acceptable CV(RSMSD) of 27%. Nonetheless, overall model match for these estimates ranks at the limits of intermediate and low value and intermediate value (wr^2=0.52 on hydrogen requirement; wr^2=0.59 on SMR demand). Therefore, this is one of the biggest contributors to the variation at the refinery emissions estimates, and should be the first area of focus for improvements in future version of PRELIM.

5.2.5 Other energy requirements

Overall proximity of PRELIM to PRISM^{TM} estimates for electricity and FCC coke-burned requirements is high. Consistently, PRELIM underestimates electricity and FCC coke-burned energy requirements (21% and 27% CV(RSMSD) respectively) PRELIM also replicates 87% and 99% of the “natural” variability in these estimates for all 22 runs. Overall model match on these outputs ranks at a high intermediate value (wr^2=0.85 on electricity requirement; wr^2=0.80 on FCC coke-burned requirement).

Mostly, differences in the electricity requirement are associated with differences in process unit product yields due to slight modifications in the refinery configurations when modelling PRELIM configurations in PRISM^{TM} and also due to accuracy in process unit yield correlations. For example, in PRISM^{TM} recycling heavy oil derived from the FCC process unit to the delayed coking process unit is modelled, which is expected to impact the yield of intermediate products. PRELIM shows that the electricity requirement is sensitive to this modification.

In the case of the amount of FCC coke estimated to be burned, deviations are mostly due to differences in the assumed energy content of the FCC coke. It is difficult to obtain a high degree of accuracy in determining the coke composition and therefore in its energy content because of the natural variability in composition inherent in this product. Similar to refinery fuel gas, the composition of the coke varies from refinery to refinery. It is a result not only of the process unit feed composition but also of operating conditions such as temperature. The PRELIM modelling approach does not allow for capturing differences in energy requirements due to variations in energy content associated with the FCC coke. Therefore, care should be taken when defining energy requirements for the FCC process unit that may or may not have a surplus of energy in the process unit. Nonetheless, it is the emissions derived from the FCC coke-burned which play an important role in determining overall refinery emissions rather than emissions originating from fuel savings associated with variations in the coke energy content. The co-validation results shows that there is consistency between the models in the estimates of CO_2 emissions from the FCC coke-burned since deviations in FCC coke mass yield are negligible. Further development of modelling related to the FCC process unit can be useful if modelling the hydrotreating requirements for the process unit feed.

Though there are important deviations in energy estimates that should be addressed as PRELIM is improved, the variability in both models is consistent and deviations are for the most part explained. Therefore, PRELIM is considered useful/appropriate in determining reasonable estimates of energy and GHG emissions and even more powerful for comparing the relative magnitude of the energy requirements and emissions rather than absolute values.

5.3 Comparison between the current model and the PRELIM model published in 2012

Minor modifications have been made in PRELIM since 2012 to improve its accuracy, flexibility and the number of crudes that are included in the model. This results in slight variations in the results for similar crude assays run in the new version of the model (PRELIM v.1.0) compared with the publication using the 2012 version of PRELIM (see Abella and Bergerson, 2012). The following are the largest two changes that were made:

1) Change to naphtha hydrotreater calculations:

Utility (steam and electricity) requirements in the naphtha hydrotreater unit were being consistently but slightly overestimated. This then resulted in slight inaccuracies in the hydrogen requirement that could be either over or underestimated. This modification is the reason behind the small differences between the results of emissions of the current version and the 2012 version of the model.

2) Change to hydrogen content of the output stream of the hydrotreaters:

PRELIM uses a default output hydrogen content value for the hydrotreaters to which the hydrogen content of the input stream has to be increased. In the 2012 version of the model, if the input stream to a hydrotreater has a hydrogen content higher than the default output hydrogen content, a negative hydrogen requirement results for that hydrotreater. This can translate to less total hydrogen required than what would have to be met by the SMR unit). We now use mass balance equations to adjust the default output hydrogen content value to a value that brings the otherwise negative hydrogen requirement of the hydrotreater to zero. This change has been applied in the model to make it flexible for investigation of some of the new assays that have been added to the model after 2012. This has not affected the crude assays run in the 2012 version of the model.

To assess the impact of the modifications to the model, the two models were run for the same assays that were presented in the 2012 publication. The main assumptions are copied below from the paper:

- Refining configuration is based on API and sulphur properties of the whole crude for both crude categories Conventional and OS-derived crudes: API (light API > 32, medium 32 > API > 22, heavy API <22) and sulphur content (S) (sweet S < 0.5 wt %, sour S > 0.5 wt %). Sweet light crudes (Sw, L) are run in a hydroskimming refinery; sour light (So, L), sweet medium (Sw, M), and sour medium (So, M) crudes are run in a medium conversion refinery; and heavy crudes (H: conventional, bitumen, dilbits) are run in a full conversion refinery.

- Upgrading process units for the medium conversion refinery include a fluid catalytic cracking (FCC) process unit, and upgrading process units for full/deep conversion refinery include FCC and delayed coking process units.

> Note: 1) These configurations correspond to configurations number 1 (medium conversion: FCC) and 4 (deep conversion: FCC) for medium and deep conversion configurations, respectively. In the current version of the model the configuration selector chooses configurations number 3 (medium conversion: FCC+GO-HC (gas oil hydrocracker)) and 6 (deep conversion: FCC+GO-HC) for the crudes that require medium and deep conversions, respectively. 2) Both the new and the 2012 versions of PRELIM report emissions in kgCO2/bbl of crude whereas the results in the 2012 paper have been reported in gCO2/MJ of crude. The emissions reported in kgCO2/bbl need to be converted (using conversion factors and enthalpy of the crudes) into gCO2/MJ of crude when comparing the results of the model with those reported in the 2012 paper (Abella and Bergerson, 2012).

For the comparison presented here, the percentage difference between the total emissions estimates of the two models was primarily considered. As explained above, the fix in the naphtha hydrotreater calculations was the main source of the differences between the results of the two versions for all of the crudes in the set of the 2012 assays. The differences between the GHG emissions estimates obtained from the two models were mostly insignificant. The differences between the model results for crude assays presented in the 2012 publication are presented in Table 9. Table 10 reports these results in units of kgCO2/bbl of crude in.

Table 9: Comparison of emissions estimates in PRELIM v.1.0 and the PRELIM 2012 version

Assay Name	Notation	Refinery Configuration	PRELIM v.1.0 (gCO_2/MJ crude)	PRELIM 2012 (gCO_2/MJ crude)	Change % (new result with respect to old result)
Mixed Sweet Blend	Conv, Sw, L2	Hydroskimming(0)	2.96	3.22	-8.02
High Sour Edmonton	Conv, So, L2	Medium Conversion: FCC (1)	5.02	4.99	0.62
Midale	Conv, So, M1	Medium Conversion: FCC (1)	5.97	6.08	-1.78
Bow River North	Conv, So, H1	Deep Conversion: FCC(4)	11.19	10.66	4.97
Suncor Synthetic A	SCO, Sw, L2	Hydroskimming(0)	2.78	2.99	-7.03
Husky Synthetic Blend	SCO, Sw, L1	Hydroskimming(0)	2.09	2.20	-5.01
Syncrude Synthetic	SCO, Sw, M1	Medium Conversion: FCC (1)	9.11	9.13	-0.21
Suncor Synthetic H	SCO, So, H1	Deep Conversion: FCC (4)	16.42	15.79	3.95
Albian Heavy Synthetic	Syndilbit 1	Deep Conversion: FCC (4)	12.26	11.81	3.82
Cold Lake	Dilbit 2	Deep Conversion: FCC (4)	11.11	10.47	6.08
Confidential	Bitumen 2	Deep Conversion: FCC (4)	13.77	13.59	1.31
Confidential	Bitumen 1	Deep Conversion: FCC (4)	13.90	13.40	3.74

Table 10: Comparison of emissions estimates in PRELIM v.1.0 and the PRELIM 2012 version (Table 9 results with units of kgCO2/bbl of crude)

Assay Name	Notation	Refinery Configuration	PRELIM v.1.0 (kgCO2/bbl crude)	PRELIM 2012 (kgCO2/bbl crude)	Change % (new result with respect to old result)
Mixed Sweet Blend	Conv, Sw, L2	Hydroskimming(0)	16.24	17.65	-8.02
High Sour Edmonton	Conv, So, L2	Medium Conversion: FCC (1)	27.93	27.76	0.62
Midale	Conv, So, M1	Medium Conversion: FCC (1)	34.18	34.80	-1.78
Bow River North	Conv, So, H1	Deep Conversion: FCC(4)	65.62	62.51	4.97
Suncor Synthetic A	SCO, Sw, L2	Hydroskimming(0)	15.51	16.69	-7.03
Husky Synthetic Blend	SCO, Sw, L1	Hydroskimming(0)	11.67	12.28	-5.01
Syncrude Synthetic	SCO, Sw, M1	Medium Conversion: FCC (1)	51.26	51.37	-0.21
Suncor Synthetic H	SCO, So, H1	Deep Conversion: FCC (4)	97.52	93.81	3.95
Albian Heavy Synthetic	Syndilbit 1	Deep Conversion: FCC (4)	72.60	69.93	3.82
Cold Lake	Dilbit 2	Deep Conversion: FCC (4)	64.45	60.76	6.08
Confidential	Bitumen 2	Deep Conversion: FCC (4)	84.05	82.96	1.31
Confidential	Bitumen 1	Deep Conversion: FCC (4)	86.32	83.20	3.74

The same results are presented with a breakdown of the contributions to the GHG emissions in Table 9 are depicted in Figure 23 (for PRELIM v.1.0) and Figure 24 (PRELIM 2012).

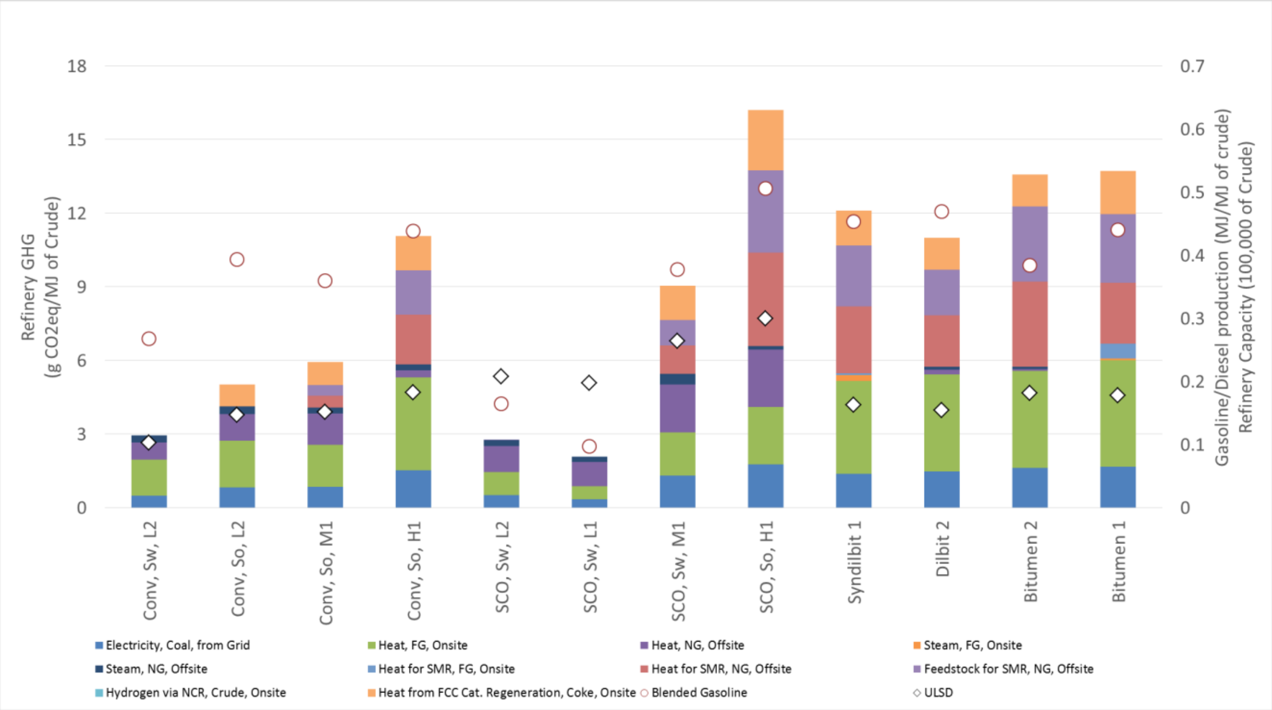


Figure 23: Breakdown of contributions to GHG emissions (results from PRELIM v.1.0)

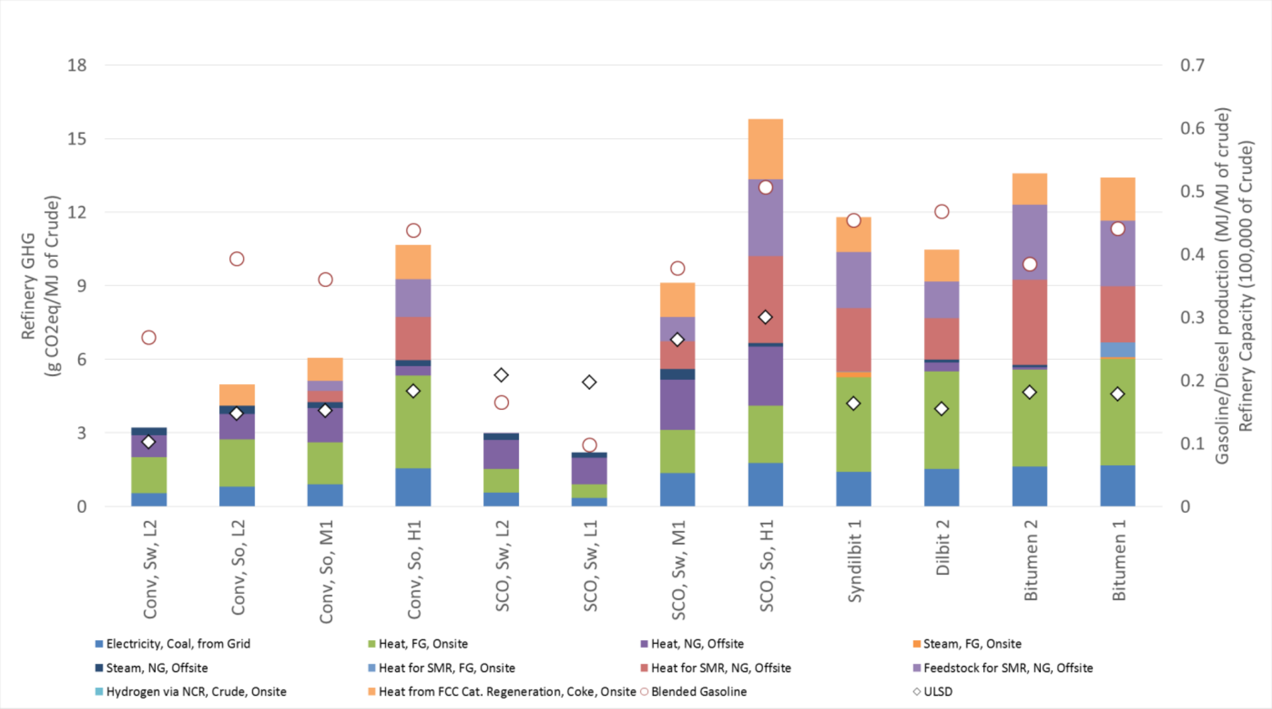


Figure 24: Breakdown of contributions to GHG emissions (results of PRELIM 2012)

5.4 Comparison of PRELIM GHG predictions with estimates in the literature

Straightforward comparison of PRELIM results with the literature is not possible, in particular due to the use of different allocation methods, system boundaries, assumptions about process energy requirements, etc.

A National Energy Technology Laboratory (NETL) study (NETL, 2009) reports refinery emissions of approximately 13 gCO2e/MJ gasoline for Venezuelan upgraded bitumen and Canadian oil sands. These estimates are lower than what PRELIM reports (approx. 21 gCO2e/MJ of gasoline). However, this study reports similar emissions for other conventional and nonconventional crudes which may mean that the model used did not differentiate between crudes based on detailed assay information. For example, this report states assumptions including the fact that the emissions from some of the most carbon intensive imported crude oils such as Venezuelan Heavy were not included due to modelling uncertainties. In addition, linear relationships to relate GHG emissions from refining operations based on API gravity and sulphur content of the whole crudes was assumed.

A Jacobs study (Jacobs Consultancy, 2009) reports total refinery GHG emissions of approximately 83 and 72 kg CO2e/bbl of crude for a bitumen with an API of 9, and a dilbit with an API of 20, respectively, which is consistent with the results of PRELIM (total GHG emissions of approx. 86 and 65 for a bitumen and a dilbit with similar APIs). Also, an IHS energy study (IHS Energy, 2014), reports refinery emissions of 81 and 71 kgCO2e/bbl of crude for bitumen and dilbits.

Compared to the results of a report prepared by Life Cycle Associates, LLC study (Life Cycle Associates, LLC, 2009), that reports refinery GHG emissions of approximately 10 gCO2e/MJ of gasoline for bitumen, PRELIM reports higher GHG emissions (approx. 21 gCO2e/MJ of gasoline). Inclusion of the indirect upstream emissions as well as the specific assumptions that exist for different processes (unit processes, power plants, allocation methods, etc.) in PRELIM may explain the difference in these estimates between these studies (see Abella and Bergerson, 2012).

The comparison made between the results of PRELIM and other sources for bitumen and dilbit is summarized in Table 11.

Table 11: Comparison of GHG emissions predicted by PRELIM and GHG emissions reported in the literature for Bitumen and Dilbit

Crude	Bitumen		Dilbit	
GHG emissions	kg/bbl of crude	gCO2e/MJ of gasoline	kg/bbl of crude	gCO2e/MJ of gasoline
PRELIM*	86	21	65	15
IHS Energy	81	-	71	-
Jacobs	83	-	72	-
NETL	-	13	-	-
Life Cycle Associates	-	10	-	-

*PRELIM estimates GHG emissions in the range of 66-72 kgCO2e/bbl and 86-91 kgCO2e/bbl for the dilbit and bitumen assays that are currently available in the model.

5.5 Assessment of transformation methods and quality of assay data

This section summarizes the evaluation of the transformation methods of the publicly available assay data as well as the quality of the PRELIM crude assay data that results from these transformations (see section 4.3). Basically, this is a comparison between H/CAMS data and Crudemonitor data processed via PRELIM. First, the deviations between the H/CAMS and PRELIM assay parameters values for each crude in each crude assay parameter are discussed including the opportunities for improvement. The quality of the data is analyzed based on how differences between PRELIM assay information and the information reported for H/CAMS affect precision and interpretation of PRELIM GHG estimates. You can learn more about the deviation between the H/CAMS and PRELIM assay parameters values for each crude in Abella (2012; Table 12, Appendix C).

5.5.1 Assessment of transformation methods

In general, there is a good agreement between H/CAMS and PRELIM for most assay parameters (78% of parameter values have a deviation equal or below 12%), and the most significant differences can be explained by PRELIM approach of using average data. The comparison of the two different datasets demonstrates several points:

> The approximations and correlations used to determine crude fraction hydrogen content and Kw factor are appropriate. Deviations are around 3% or lower for all of the fractions of the majority of assays. The deviations in hydrogen content are up to 8% for the synthetic crude oil assay, and they are an exception over all the nine assays.
>
> Temporal variation explains differences in crude distillation assay data. For example, after reviewing the synthetic crude oil assay information, it is found that the differences in the percent mass yield at a particular temperature can be up to 8% for the samples analyzed from 2004 to 2009 (used to determine the average distillation curve in current PRELIM assay inventory). Such difference in the percent mass yield can represent large deviations in the crude fraction mass yields. The case of the synthetic crude oil assay illustrates that the approach of using average data has an important effect for the distillation curve data (an effect not found in other parameters), and then in the determination and interpretation of refinery GHG emissions specific to a crude.
>
> The approximation to estimate MCR is suitable. For most assays, the deviations in the values for this parameter are consistent with what is found when analyzing the approximation using the 50 confidential assays tested. The largest deviations in the values of this parameter result from disagreement between the sources of data. For the light sweet synthetic crude assay, CCQMP reports neither a vacuum residue fraction nor an MCR in this fraction while H/CAMS does report them. Temporal variation does not explain the large deviations in sulphur, nitrogen, and API estimates (nitrogen is present in the PRELIM assay inventory only for information purposes; PRELIM calculations neglect its effect on hydrogen requirements based on evaluation of its impact on GHG emissions estimates). Table 12 in Appendix C of Abella (2012) shows that for some cases the deviations in these crude assay parameters are beyond 20%. CCQMP data show that the deviation (calculated in percentage as 100 times the standard deviation of parameter values divided by average of those parameters) for those parameters are mostly below 10% for different crudes in different fractions (fractions wider than

the fractions used in PRELIM). Deviations higher than 10% (as is the case for PRELIM assay compared to H/CAMS assays) happen occasionally in CCQMP data for sulphur content and are up to 15%.

The regression method used to determine sulphur and API (also nitrogen) of the crude fractions could have been affected by the number of observations but also due to the use of less detailed data to develop a more detailed assay. The large deviation in the fractions' sulphur content values happens for the assays derived from CCQMP data rather than for the assays obtained from confidential sources. It suggests that a more detailed assay (i.e., assay information for less wide fractions) can improve the accuracy of the regression method employed.

Alternative methods to the polynomial regression can be explored in order to obtain better API estimates for the distillation residue fractions. The use of conversion of distillation curves on mass basis (simulated distillation methods) to distillation curves on volume basis could be an option to be investigated and to obtain the required accuracy in the volume yields of each crude fraction. Sulphur content has a minor or negligible effect in PRELIM response; therefore, higher accuracy in this parameter at this stage of model development is not needed.

5.5.2 Overall Quality of PRELIM Assay Data and Interpretation

As a whole, the quality of the assay data is considered meaningful for the purposes of estimating the refinery GHG emissions estimates. The deviation in overall refinery GHG emissions (for all 99 runs) is 5% CV(RSMSD). Figure 25 shows that in general, using the different assay data (H/CAMS and PRELIM), proximity in PRELIM GHG estimates for the overall refinery emissions is high. In most of the cases, using PRELIM assay data leads to underestimation of the overall refinery GHG emissions (only 1 out of the 9 assays showed overestimation for 3 out of 11 refinery cases tested); however, the deviation is not higher than 12% (light synthetic crude oil assay: 11% CV(RSMSD) when measured against estimates using H/CAMS assay data). Because the comparison of assay data involves crudes of different quality, it is expected that a similar performance will result when the larger assay inventory is explored. While there are deviations resulting from a comparison of the two datasets, such deviations do not play a large role in the overall refinery emissions estimates. This suggests that the transformation methods proposed and implemented in PRELIM are robust to include in PRELIM assay inventory.

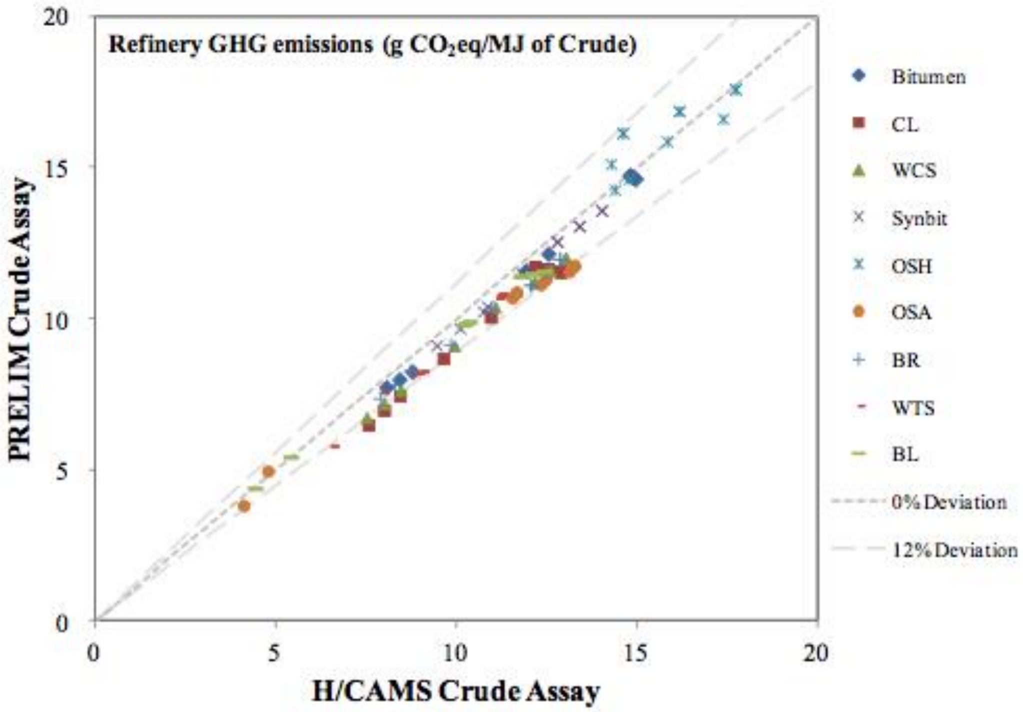


Figure 25: Comparison of fit between PRELIM overall refinery GHG emissions estimates using H/CAMS and PRELIM crude assay data.

> The x-axis shows the PRELIM's GHG estimates (g CO_{2eq}/MJ) using H/CAMS assay values, and the y-axis shows PRELIM's GHG estimates (g CO_{2eq}/MJ) using PRELIM crude assay inventory. Diagonal dotted lines illustrate deviations that are due to variation in crude properties.

It is advisable to consider that current PRELIM crude assay inventory uses average data which can affect the assessment of crude assay quality. In Figure 25, the deviation in PRELIM GHG estimates for the synthetic crude oil assay result from individually small deviations in hydrogen content of each fraction with relatively large deviations in fraction volume yield. (i.e., deviations in crude fraction hydrogen content are up to 8% and deviations in crude fraction volume yield are up to 41%). The deviations in hydrogen content of the crude fractions are in the expected margin of error for hydrogen content estimates using analytical methods (Choudhary et al., 2008). However, deviations in crude oil distillation curve information warrant attention and have to be explained by temporal variation. The significance of using average data is mostly related to analyzing crude-specific GHG emissions for a refinery product. Figure 26 shows that using the different assay data (H/CAMS and PRELIM), the deviation in the gasoline and diesel GHG emissions estimates for all crudes is mostly below 10% (for 67% of the estimates; all 11 cases and 6 out of 9 assays). However, when analyzing GHG emissions specific to the case of the light synthetic crude oil assay a large deviation exists (29% CV(RSMSD) for gasoline and 75% CV(RSMSD) for diesel GHG estimates). The deviation results from the combined effect of the deviations in hydrogen content of the fractions and in the distillation curve, and it can be interpreted as the effect of temporal variation on the crude assay information. Outliers in Figure 26 specific to two diluted bitumen assays are not considered relevant because they correspond to a "hypothetical" case when the crudes are run in a medium refinery configuration (hypothetically as they are not currently being processed in this type of refinery); however, the deviation demonstrates the effects of average crude distillation curve data as well. The deviations for those diluted bitumen assays are mainly related to deviations in their distillation curves. GHG emissions estimates for a particular crude using PRELIM assay data will differ somehow from estimates using assay data from a single sample; therefore, it is important to consider that PRELIM assay data will represent an average quality of these crudes.

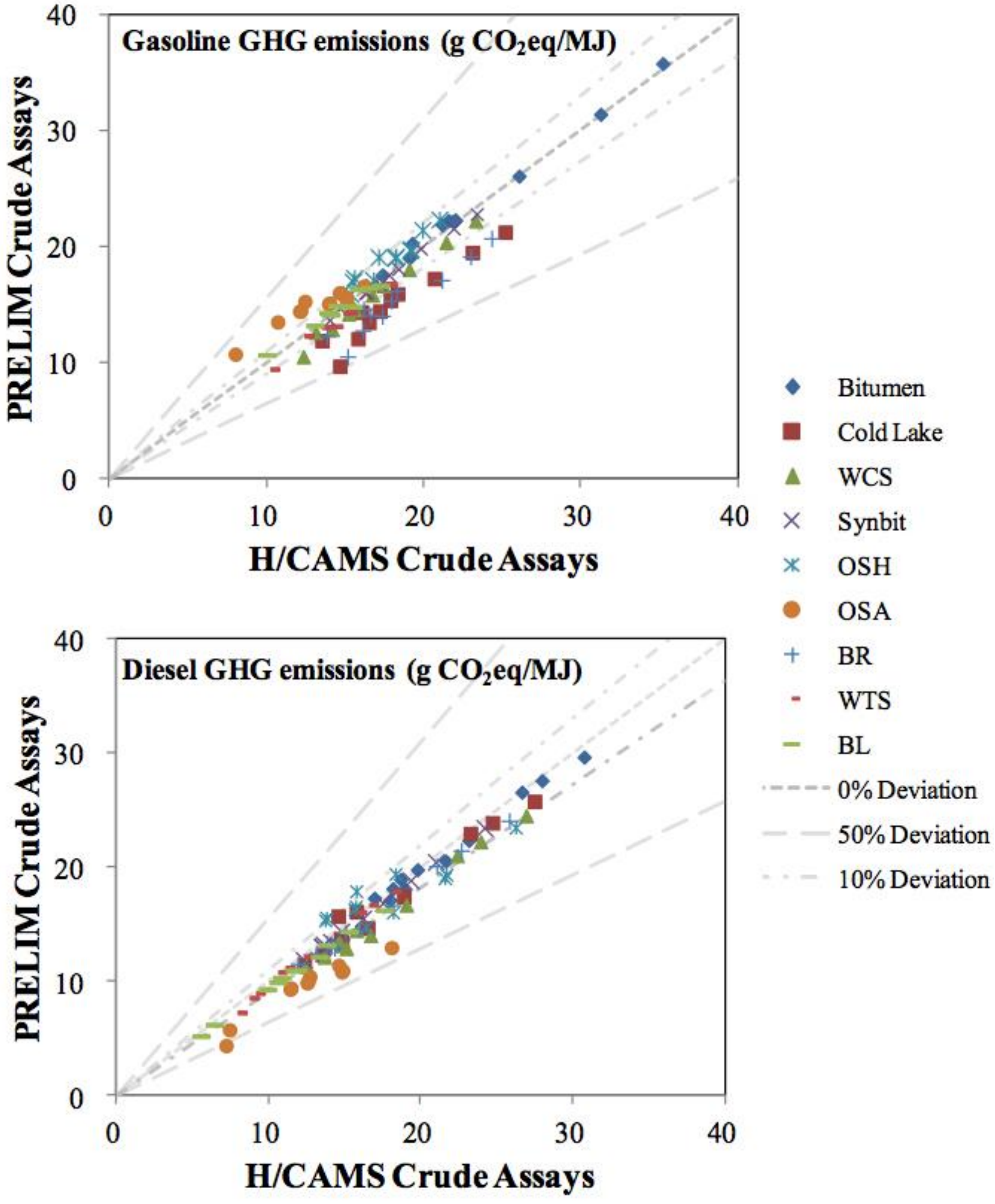


Figure 26: Comparison of fit between PRELIM (a) gasoline and (b) diesel GHG emissions estimates using H/CAMS and PRELIM crude assay data

> The x-axis shows the PRELIM's GHG estimates (g CO_{2eq}/MJ) using H/CAMS assay values, and the y-axis shows PRELIM's GHG estimates (g CO_{2eq}/MJ) using PRELIM crude assay inventory. Diagonal dotted lines illustrate deviations that are due to variation in crude properties.

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