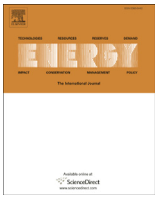
Energy 83 (2015) 65–79

Contents lists available at ScienceDirect

Energy

journal homepage: www.elsevier.com/locate/energy



Energy consumption and greenhouse gas emissions in upgrading and refining of Canada's oil sands products

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ARTICLE INFO

Article history:
Received 10 July 2014
Received in revised form
29 December 2014
Accepted 26 January 2015
Available online 11 March 2015

Keywords:
Life cycle assessment
GHG (greenhouse gas) emissions
Oil sands
Upgrading
Refining
SCO (synthetic crude oil)

ABSTRACT

A model-FUNNEL-GHG-OS (**FUN**damental E**N**gineering Principl**E**s- based Mode**L** for Estimation of **G**reen**H**ouse **G**ases in the **O**il **S**ands) based on fundamental engineering principles was developed to estimate the specific energy consumption and GHGs (greenhouse gas emissions) for upgrading bitumen to produce SCO (synthetic crude oil). The model estimates quantity of SCO produced, the consumption of hydrogen, steam, natural gas and power in two different upgrading operations, namely delayed coking and hydroconversion. Hydroconversion upgrading is more energy and GHG (433.4 $kgCO_2eq/m^3$ of bitumen) intensive than delayed coker upgrading (240.3 $kgCO_2eq/m^3$ of bitumen) but obtains a higher yield of SCO. This research explores bitumen pathways in oil sands – upgrading bitumen to SCO, followed by transporting and refining SCO as compared to transporting and refining dilbit. The energy consumption, GHG emissions and volume of transportation fuels obtained from refining of different oil sands feeds has been investigated. Refining of oil sands products produce 7.9 to 15.72 gCO_2eq per MJ of refined product. Refining of SCO to transportation fuels produces 41% and 49% less emissions than dilbit and bitumen respectively.

1. Introduction

Unconventional oil resources such as oil sands in Canada have gained a lot of attention due to limited conventional oil resources and ever increasing energy demand. The oil sands in Alberta, one of the Provinces in Canada, with 170.2 billion barrels, are the third largest proven oil reserves in world after Saudi Arabia and Venezuela [1]. Production of crude bitumen from Alberta oil sands was almost 1.9 million barrels per day in 2012, 54% of which was upgraded to synthetic crude oil [2].

Bitumen production is projected to increase to 3.8 million barrels per day by 2022 [3]. The growing oil sands industry faces tough decisions as to how to develop this resource further, whether to upgrade bitumen to SCO within the province or to blend it with lighter hydrocarbons to produce dilbit [4]. This decision is further made difficult by the climate policies such as the LCFS (Low Carbon Fuel Standard) [5], the European Fuel Quality Directive [6] and the Alberta SGER (Specified Gas Emitter Regulation) [1] adding strict regulation for reducing GHG (greenhouse gas) emissions. These regulations call for appropriate quantification and assessment of life cycle GHG emissions from these oil resources.

The bitumen recovered and extracted in SAGD (Surface Mining or Steam Assisted Gravity Drainage) is highly dense, viscous and high in sulfur content [7]. All the refineries in North America do not have capability to refine heavy feeds. So to access more markets and ease the transportation, the Canadian crude is upgraded to produce “SCO” (synthetic crude oil). Bitumen is fractionated or chemically treated to yield a higher value product through a process known as upgrading. The aim of upgrading process is to obtain a high quality substitute to crude oil known as SCO or may be limited to reduce the viscosity of product to allow its shipment by pipeline without adding a solvent [8]. Upgrading of the highly viscous and hydrogen deficient bitumen consumes substantial amounts of energy, making it a GHG (greenhouse gas) intensive process. On the other hand, dilbit requires less energy during initial blending [4]. SCO or dilbit is transported to refineries via pipeline. Pipeline transport of heavier feeds such as dilbit requires more energy than SCO [9]. Refining of SCO requires less energy than refining of dilbit and yields different products [10–12]. So it becomes necessary to quantify the emissions in the unit operations of upgrading, transportation and refining so as to compare the bitumen pathways and make informed decisions.

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http://dx.doi.org/10.1016/j.energy.2015.01.085

Nomenclature

GHG	greenhouse gas
SCO	synthetic crude oil
gCO_2eq	grams of carbon-dioxide equivalents
MJ	mega joule
bbl	barrel
GREET	Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation
LHV	lower heating value
SMR	steam methane reforming
NG	natural gas
DHT	diesel hydrotreating
KHT	kerosene hydrotreating
NHT	NAPHTHA hydrotreating
HCD	hydrocracking
FCC	catalytic cracking
SGP	saturated gas plant
UGP	unsaturated gas plant
HYD	hydrogen production

Large scale commercial upgrading technologies comprise either thermal cracking-coking technologies or hydrogen based cracking-hydroconversion technologies [8,12,13]. Of the total bitumen volume upgraded in Alberta, 30% goes through hydroconversion [14]. The quality and characteristics of the product produced depend on the technology chosen. Selection of upgrading technology is primarily based on type of product required and other secondary considerations are capital cost, cost of fuels along with catalysts, coke production, operating complexity and experience, production expandability, constructability and maintainability [14]. The GHG impact of these technologies may not been considered earlier as important factor in selection of the technology but it is gaining importance due to increasing environmental awareness and strict regulations imposed by policy makers.

The two most prominent North American life cycle models in this area are GREET (Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation) [15] maintained by Argonne National Laboratory and GHGenius [16] maintained by Natural Resources Canada. Oil sands pathways can be constructed using these models, but there is no method in these models to estimate the specific energy consumption in the oil sands operations. In the refinery operation, these models do not show the effects of crude quality on energy consumption and GHG emissions. Hence it is not possible to estimate energy consumption and GHG emissions for a particular kind of feed refined in a specific refinery, using these life cycle models. This research is aimed at addressing these gaps in knowledge.

Two earlier studies [11,12] present life cycle GHG emissions from conventional and non-conventional crudes performing a comparative analysis of production of transportation fuels in the U.S. These studies do not calculate project specific energy consumption and GHG emission based on technical parameters. Another work [17] studied the upgrading and refining operation GHG emissions for oil sands based on certain project data. Rahman et al. studied extraction, recovery and refining of five different conventional crude oils which are refined in the North America but did not consider the oil sands-based oil [18,19]. These results have limitations as these cannot be modified to evaluate emissions for a different project. Some studies [10,20,21] have looked into the effects of crude quality and refinery configuration for different feeds. These studies are limited to refinery operation and do not analyze the upgrading and refinery operations on a common platform to study the effects obtaining end products from oil sands feeds.

Charpentier et al. [22] and Bergerson et al. [23] report the range of energy consumption and GHG emissions in oil sands based on confidential data from industry. The results are therefore specific to those projects hence cannot be used for calculation of project specific energy consumption and GHG emissions based on quality of feed and technical parameters of the project. Brandt [7] and Charpentier et al. [24] performed a comparative analysis of GHG emissions in each oil sands operation as reported by earlier studies and life cycle models. Whereas Charpentier et al. [24] called for additional research for better characterization of oil sands technologies and pathways, Brandt [7] recommended modeling GHG emissions of process specific configurations.

Oil sands produce a variety of feeds such as SCO, dilbit and bitumen that are refined to transportation fuels. Each feed depending on its characteristics consumes different amount of energy and emits different GHG emissions. Refining of oil sands feeds end up in different useful end products. So this makes it necessary to study upgrading and refining operations together to compare the net energy consumption and GHG emissions on similar platform. The variety of feeds and technology in oil sands makes each project unique in its energy consumption and GHG emissions. This uniqueness demands the estimation of energy consumption and GHG emissions for each individual project.

This paper presents a detailed data intensive model named FUNNEL-GHG-OS (FUNdamental ENgineering PrinciplEs-based ModeL for Estimation of GreenHouse Gases in the Oil Sands) based on fundamental engineering principles to mathematically estimate project and process specific energy consumption and related life cycle GHG emissions for an upgrading operation in oil sands. FUNNEL-GHG-OS model conducts a comprehensive LCA (life cycle assessment) of transportation fuels from oil sands, within the framework of ISO (International Standard Organization) standards [25]. The system boundary includes all the bitumen pathways possible in oil sands. The oil sands recovery and extraction pathways have been modeled in Refs. [26,27], whereas in this paper the upgrading and refinery pathways for oil sands feeds have been modeled. The impact category analyzed in the LCA is the global warming potential. As the results of LCA depend on the quality of data used in analysis, FUNNEL-GHG-OS performs engineering calculations to provide quality data for LCA.

Two most widely used technologies for upgrading in oil sands — delayed coking and hydroconversion have been analyzed. This research further evaluates the energy consumption and GHG emissions for upgrading bitumen and refining of SCO, dilbit and bitumen feeds on a common platform. A process model [28] built in Aspen HYSYS has been used to study the refining operation. The GHG emissions reported for the unit operations include 1) direct emissions from the combustion of fuel on site and 2) upstream emissions associated with recovery, processing, and transportation of these fuels. The paper does not include the fugitive, venting and flaring, equipment, and land-use emissions. The coke produced in upgrading and refinery operations is assumed to be stockpiled.

2. Methodology

2.1. Functional unit

The functional unit used for life cycle assessment of oil sands-derived fuels is one unit volume of crude feed input to upgraders and refineries. The metric used for presenting the life cycle GHG emissions is kg-CO_2eq per unit volume of crude feed. The emissions also include the effects of other GHGs such as CH_4 and N_2O. However, the results are also presented in g-CO_2eq per MJ (megajoule) of refined product obtained after refining of feeds. The LHV (lower heating value) of fuels (to be consistent with the California GREET model) has been used to define the energy content. Necessary unit conversions are made to present and compare the results with other studies.

2.2. Upgrading

The processing steps of bitumen in upgrading are designed differently for each upgrader depending upon the technology, crude type, required products and other techno-economic factors. Generally, speaking upgrading involves two steps — a vacuum residue conversion step to increase the hydrogen to carbon ratio called primary upgrading, and secondary upgrading which consist of treating the products obtained in primary upgrading to achieve below 0.5% sulfur content in the products [8,29].

The hydrogen to carbon ratio of products may be increased either through carbon rejection (coking) or hydrogen addition (hydro-conversion) processes. This study evaluates the energy consumption and GHG emissions in both of these configurations (coking and hydro-conversion) in upgrading. The coking process produces a solid residue called coke, which is rich in carbon, sulfur and other contaminants. In the hydro-conversion process, the heavy feed is cracked into desirable products in presence of hydrogen, leaving no solid residue. Figs. 1 and 2 show the sub unit operations involved in the two configurations of upgrading analyzed in this study. Specific energy consumption in sub unit operations is mathematically estimated based on basic heat and mass transfer fundamentals. The energy consumed depends on the distillation properties, sulfur content and API of the feed and products. Flow of feed in the upgrading operations is traced based on mass balance and volume percentage of products distilled at each stage. Volume percentage of products distilled depends on distillation curve of the crude.

The energy consumed in sub unit operations is in the form of steam, natural gas, fuel gas and electricity. The default process conditions and sources of energy shown in Table 1, which are used in the development of model, are identified based on the design of the upgrader proposed in Ref. [30]. Fuel energy in atmospheric distillation and vacuum distillation columns is required to heat the crude to its vaporization temperature, and steam is required for stripping the distillation products from the fractionating columns [20]. The energy required in sub unit operations is calculated based on the design conditions and enthalpy of petroleum fractions. The enthalpy of petroleum fractions such as naphtha, diesel, coker diesel, dilbit, atmospheric gas oil, atmospheric residue, vacuum residue, vacuum gas oils and coke vary from 1.38 to 2.94 kJ/kg K [28,29,31]. As identified in Table 1, some of the energy required is obtained by using heat exchangers between feed and products. Steam energy and electricity utilized in each sub unit operation is linearly related to process unit volume feed flow [20] and has been obtained from earlier studies [20,30]. This data used for the development of the model has been detailed in Table 2. The calculations in the model are based on a unit volume of feed input and are assumed to be independent of scale of the plant.

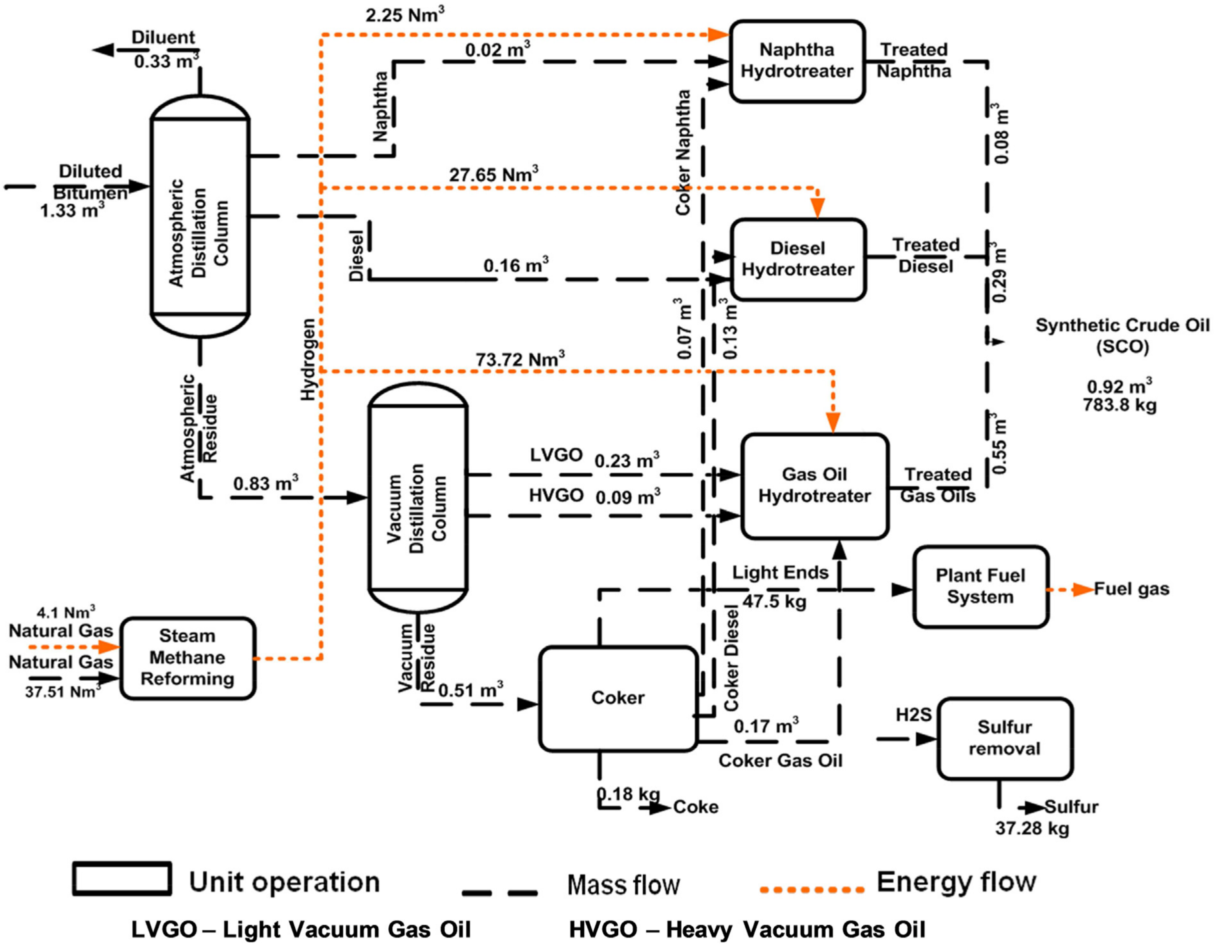

Fig. 1. Sub unit operations in a coking based upgrading operation.

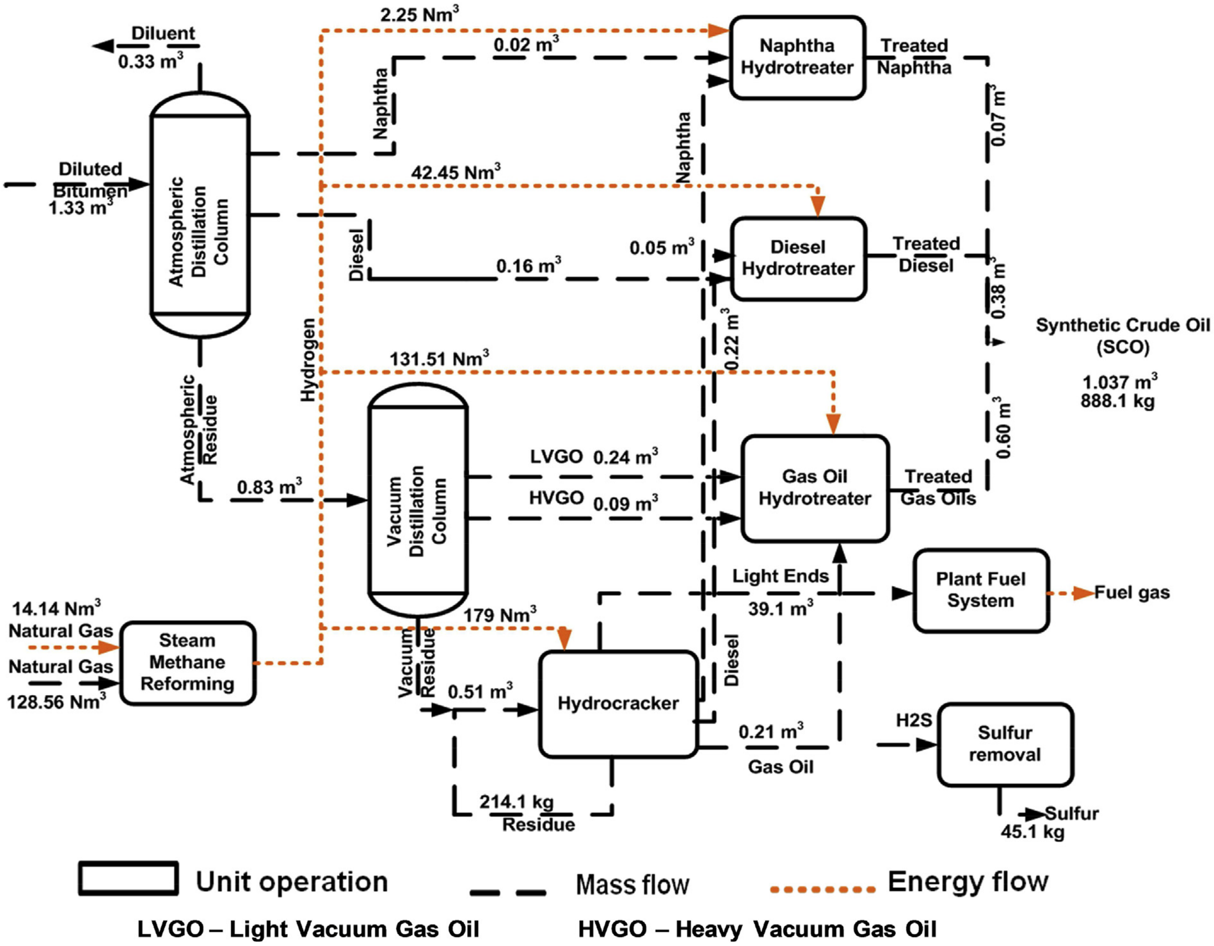

Fig. 2. Sub unit operations in a hydroconversion based upgrading operation.

Another important area of energy consumption is hydrogen production. While, no hydrogen is consumed in delayed cokers, a huge amount of hydrogen is required in ebullated bed hydrocrackers[1] [29]. The naphtha, diesel and gas oil obtained are hydrotreated in secondary upgrading, consuming different amounts of hydrogen. Hydrogen consumption in the sub unit operations is estimated based on [32]. Hydrogen consumption depends on the type of feed and type of product required, hence it is considered as a sensitivity parameter (see Section 3.1.1). Changes in mass and volume of the products occur in secondary upgrading due to removal of sulfur, nitrogen and saturation of aromatic rings. These mass and volume changes are captured in the calculations based on data specified in Ref. [32].

Upgraders employ SMR (steam methane reforming) utilizing natural gas both as feedstock and fuel for meeting their hydrogen requirements [33]. Natural gas requirements are estimated per unit of hydrogen produced based on [34]. Findings from same study are used to estimate the steam and electricity requirements of the hydrogen plant.

Another sub unit operation modeled in this research is the sulfur recovery operation. The feed to sulfur recovery operation is calculated based on the mass balance of sulfur in whole plant. The sulfur inlet to the plant is the sulfur contained in the feed. Some sulfur remains in the product (SCO), or is removed in coke formed in delayed cokers. The remaining sulfur is treated in the sulfur recovery operation in form of hydrogen sulfide gas to form liquid sulfur.

The energy required in upgrading operations for heating the feed and steam production is obtained from natural gas and fuel gas. Light ends from each sub unit operation are combined and treated in the plant fuel system to form the fuel gas. The energy content and emission factor for the produced fuel gas is calculated based on its composition. The composition of fuel gas is plant and time specific depending on the feed to the plant. Similar composition of fuel gas is assumed in both the upgrading configurations. FUNNEL-GHG-OS model explores the use of cogeneration (detailed in supporting information) of electricity in upgrading operation in oil sands. If the electricity produced in cogeneration is in excess of the electricity demand of the plant, the excess electricity is exported to the grid. In the case of no cogeneration, steam is generated on-site in a stand-alone operation using a natural gas-fired industrial boiler. The electricity demand of the plant is fulfilled by importing the electricity from grid.

Emission factors for natural gas equipment used to calculate GHG emissions are imported from GREET [15]. These factors include both combustion and upstream emissions. The natural gas is used as a fuel and as a feedstock in hydrogen production. The natural gas used as feedstock does not undergo combustion, hence only the upstream emissions are applicable to feedstock natural

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[1] Ebullated bed reactor uses an ebullated or expanded bed of catalyst for hydrocracking (hydrogenation and acidic cracking) of residue feed (Gray, 2010). The ebullated bed reactors are favorable for Athabasca or Cold Lake feeds which have high metal content and high Conradson carbon residue (CCR) values. H-Oil and LC-Finning processes use ebullated bed reactor for upgrading of residue feeds.

Table 1
Process conditions considered for modeling energy consumption in upgrading sub unit operations.

Sub unit operation		Feed	Process conditions	Energy source	Comments/references
Atmospheric distillation (ADU)	Naphtha recovery fractionator	Dilbit (diluted bitumen)	160 °F–275 °F	Condensing diluent stream	Initial 160 °F temperature is maintained with tempered water from process units. [30].
			275 °F–450 °F	Steam	
	Diesel recovery fractionator	Light atmospheric gas oil	450 °F–520 °F	Steam	[30]
			520 °F–575 °F	Vacuum residue stream	
			575 °F–720 °F	Natural gas/fuel gas	
Vacuum distillation (VDU)		Atmospheric residue	690 °F–780 °F	Natural gas/fuel gas	[30]
Delayed coker		Vacuum residue	550 °F–925 °F	Natural gas/fuel gas	[29,30]
Hydroconversion		Vacuum residue	550 °F–788 °F	Natural gas/fuel gas	[29]. Initial temperature of feed same as in case of delayed Coker.
Naphtha hydrotreater		Naphtha from	200 °F–560 °F	Feed effluent	[29]. Hydrotreating occurs at temp below 752 °F [29].
		ADU & Coker naphtha	560 °F–608 °F	Natural gas/fuel gas	Initial temperature of feed varies 180 °F –360 °F [30].
Diesel hydrotreater		Diesel from	200 °F–560 °F	Feed effluent	Initial temperature of feed for naphtha and gas oil
		ADU & Coker diesel	560 °F–650 °F	Natural gas/fuel gas	considered similar to diesel.
Gas oil hydrotreater		LVGO + HVGO from	200 °F–560 °F	Feed effluent	
		VDU & Coker gas oil	560 °F–680 °F	Natural gas/fuel gas	

gas. Moreover carbon dioxide is produced as a result of SMR reaction to produce hydrogen. This has been captured based on stoichiometry of the reaction that one mole of carbon dioxide is produced for every four moles of hydrogen. An emissions factor of 880 g of carbon dioxide equivalent per kWh of Alberta's grid electricity used has been used [36]. In the case of cogeneration, where excess electricity is exported to the grid, an emissions factor of 650 g of carbon dioxide equivalent per kWh of displaced grid electricity is used [36]. An emissions factor of 2419.4 gCO_2eq/kg of fuel gas has been estimated based on the composition of gas provided in Ref. [30].

The data in Tables 1 and 2 is default input into the FUNNEL-GHG-OS model. Data specific to other projects may be entered for the estimation of energy consumption and GHG emissions specific to those projects.

2.3. *Refining*

The feed in the form of crude oil, SCO and dilbit is processed in a refinery to obtain gasoline, diesel, jet fuel, and other end products. Refining is a complex process that gives a number of correlated products, detailed and expertise knowledge is required to estimate the energy consumption and GHG emissions. Due to a lack of data available in the public domain, a process model built in Aspen HYSYS [28] was used for the purpose of estimating energy consumption and GHG emissions.

Table 2
Input data used in model development for upgrading operations in oil sands.

	Electricity consumption[a]		Steam consumption	Source
	Value	Units	Value	
Atmospheric distillation	0.9	kWh/bbl	5 lb/bbl Naphtha; 6 lb/bbl kerosene; 4 lb/bbl diesel;	[20,30].
Vacuum distillation	0.3	kWh/bbl	2 lb/bbl AGO; 10 lb/bbl AR; 12 lb//bbl VGO; 15 lb/bbl VR;	
Delayed coker	30	Kwh/t Coke	5 lb/bbl coker naphtha; 5 lb/bbl coker diesel; 5 lb/bbl gas oil;	[20].
Ebullated bed hydroconversion	8	kWh/bbl	50 lb/bbl	[20].
Naphtha hydrotreating	2	kWh/bbl	8 lb/bbl	[20].
Diesel hydrotreating	6	kWh/bbl	10 lb/bbl	[20].
Gas oil hydrotreating	6	kWh/bbl	10 lb/bbl	[20].
Claus sulfur recovery	98	Kwh/t Sulfur	1215 lb/t Sulfur	[20].
Tail gas treatment	463	Kwh/t Sulfur		
Hydrogen production	0.028	Kwh/Nm^3	−0.86 lb/Nm^3 of H$_2$	[20].
Hydrogen requirement				
	Unit	Value Delayed coking	Value Hydroconversion	
Naphtha hydrotreating	scf/bbl	170	170	[32].
Diesel hydrotreating	scf/bbl	581.3	892.4	[30,32].
Gas oil hydrotreating	scf/bbl	912.6	1628	[32].
Hydroconverter	scf/bbl	–	1512	[32].
Hydrogen production				
	Unit	Value		
NG fuel required	m^3/Nm^3 of H$_2$	0.0398		[34].
NG feedstock required	m^3/Nm^3 of H$_2$	0.362		[34].
Efficiency of NG furnace	87%			[35].
NG fired boiler efficiency	85%			[22].
Efficiency of heat exchanger	60%			[26].
Efficiency of gas turbine	32%			[22].
HRSG exhaust recovery	55%			[22].
HRSG direct firing duct burner	95%			[22].

[a] : Grid electricity is used in case of no-cogeneration and electricity produced on-site is used in the case of cogeneration. In case of cogeneration, the electricity is produced using fuel gas from the plant.

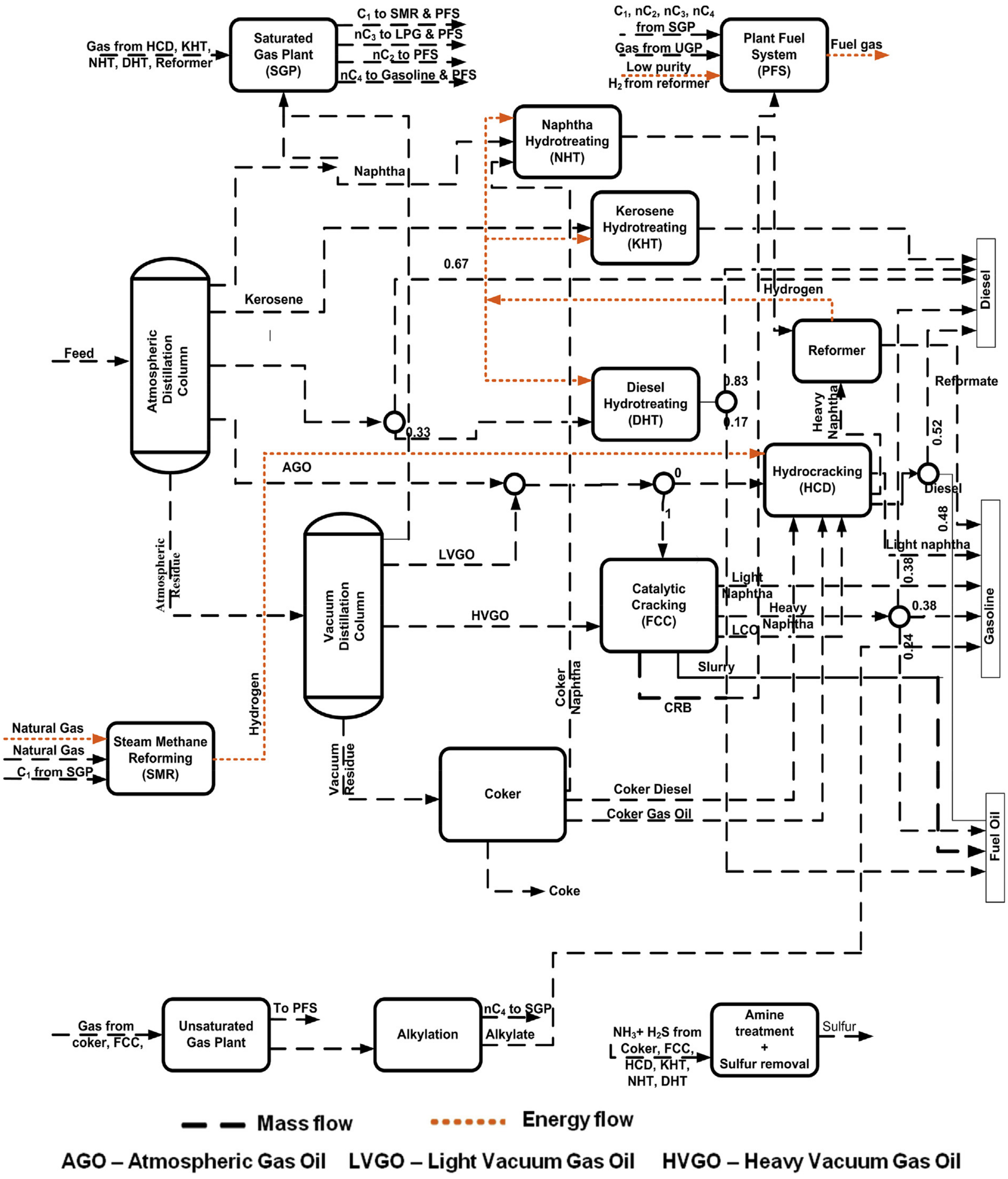

Fig. 3. Process flow in a typical North American refinery configuration capable of refining heavy feeds.

A refinery of typical configuration, as shown in Fig. 3, is modeled. The modeling uses the default configuration, parameters and conditions as used in the built-in sample case in Ref. [28]. The refinery processing units – hydrotreaters, catalytic cracker, hydrocracker, coker, reformer and alkylation unit are simulated using petroleum shift reactors based on the delta base-shift concept [28]. As explained in Ref. [28], each unit is represented by a set of key independent variables (usually feed flowrates and feed qualities) and key dependent variables (usually product flowrates, product qualities, utilities, etc) with their base condition values specified. If the conditions are different from the base point, the dependent variables are calculated from the independent variables using a set of linear equations whose coefficients are the derivatives of the independents with respect to the dependents at the base point. The derivatives are calculated using rigorous first principles models. The utility base values that have been used in simulating the refinery in this research are modified and calculated on basis of unit volume of feed flowrate. This has been done to capture the effect of change in utilities due to change in the feed input.

The distillation curve based on the boiling point of fractions, sulfur content, density and carbon residue of crude feed along with the accompanying light ends are inputs to the refinery model, simulated in this research. Based on the input, the model predicts the utilities and products for each sub unit operation in refinery. The utilities are in the form of fuel, steam and power (electricity energy). The individual utilities in each sub unit operation are summed up to obtain total energy consumption in the refinery operation. The products from refinery as predicted by the model are LPG (liquefied petroleum gas), diesel fuel, jet/kerosene fuel, gasoline and fuel oil. Coke is also obtained as a byproduct from the coker.

The energy consumed in refinery is obtained from fuel gas, natural gas, fuel oil, electricity and coke [11,15]. Natural gas is also required as a feedstock to hydrogen production. Some of the feedstock requirement in hydrogen production is fulfilled by methane produced in the saturated gas plant in refinery. Hydrogen is also produced from reformer in the refinery. The hydrogen from the reformer is low purity and hence after treatment is used in hydrotreating of naphtha, diesel and kerosene. The remaining low purity hydrogen goes to plant fuel system and hence forms a component of fuel gas. The hydrogen required in hydrocracking is of high purity hence is produced from natural gas in steam methane reforming process. Different refineries may have different kinds of hydrogen balances.

3. Results and discussion

3.1. Upgrading

FUNNEL-GHG-OS model described in Section 2.2 has been used to estimate the energy consumption and GHG emissions for upgrading operations. The model has been run using the default data and characteristics of bitumen described in supporting information (see Fig. S4). The volume/mass flowrates of the intermediate products in the upgrader are shown in Figs. 1 and 2.

The total energy required to process a bitumen feed in the upgraders varies depending upon the process utilized. The calculations based on the above methodology estimated 3.34 GJ of energy consumption to upgrade one m^3 of bitumen using delayed cokers and 6.87 GJ in the hydroconversion process. The higher energy consumption in hydroconversion corresponds to the higher hydrogen requirement. Hydrogen production is an energy intensive process [21]. About 70% of the total energy in hydroconversion is required for hydrogen production compared to 42% (see Fig. 4) required in upgrading using delayed cokers. Next to hydrogen production, intensive energy consumption occurs in crude distillation (atmospheric + vacuum) columns. Naphtha, diesel and gas oil hydrotreating contribute in total energy to a smaller scale. These hydrotreating operations consume a lot of energy in the form of hydrogen, which has been accounted in the hydrogen production unit operation. Hence only the remaining fuel energy required to heat the feed to the appropriate temperature is accounted in these operations. As stated in Table 1, majority of heating energy supplied in these operations is a result of heat exchange between the feed and the feed effluent. Hence these hydrotreating operations form a small portion of the energy requirement of the plant.

Table 3 presents the energy consumption of delayed coker and hydroconversion upgraders.

54% and 22% of the energy requirement in delayed coking and hydroconversion respectively is fulfilled by the fuel gas produced in the plant. The remaining energy requirement to upgrade one unit volume of bitumen in delayed coking and hydroconversion process is fulfilled by 47 $m^3$and 157 m^3 of natural gas, respectively. The

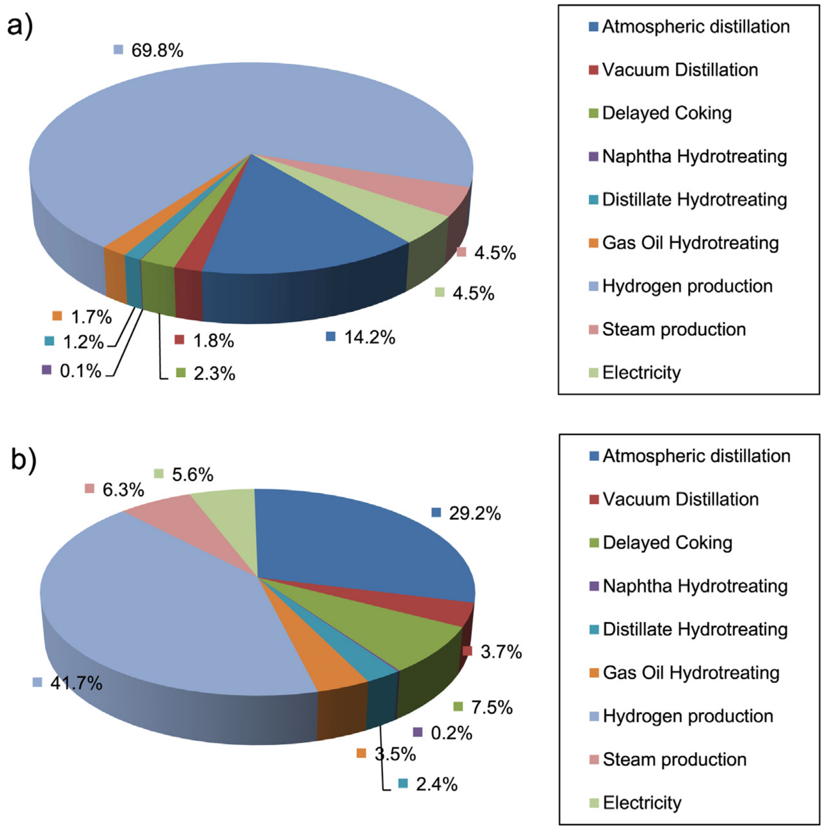

Fig. 4. Distribution of energy consumed in sub unit operations in a) hydroconversion upgrading (6.86 GJ/m^3 of bitumen) b) delayed coker upgrading (3.34 GJ/m^3 of bitumen).

Table 3
Energy consumption and emissions in upgrading operations.

		Units		Delayed coking	Hydroconversion	
SCO produced		m^3/m^3 of bitumen		0.911	1.037	
H_2 requirement		Nm^3/m^3 of bitumen		103.6	355.2	
	Units	**Fuel consumption**		**Units**	**Emissions**	
		Delayed coking	**Hydroconversion**		**Delayed coking**	**Hydroconversion**
Fuel gas	kg/m^3 of bitumen	47.5	39.1	$kgCO_2eq/m^3$ of bitumen	114.8	94.5
No cogeneration						
Natural gas	m^3/m^3 of bitumen	40.4	147.1	$kgCO_2eq/m^3$ of bitumen	79.9	264.2
Steam	lb/m^3 of bitumen	120.7	175.2	$kgCO_2eq/m^3$ of bitumen	[a]	[a]
Electricity	kWh/m^3 of bitumen	51.9[b]	84.9[b]	$kgCO_2eq/m^3$ of bitumen	45.6	74.7
With cogeneration						
Natural gas	m^3/m^3 of bitumen	68.9	197.1	$kgCO_2eq/m^3$ of bitumen	120.7	324.4
Electricity exported	kWh/m^3 of bitumen	−41.4[c]	−83.0[c]	$kgCO_2eq/m^3$ of bitumen	−26.9	−53.9

[a] Emissions from steam production are included in natural gas/fuel gas combustion emissions.
[b] This electricity is imported from the grid.
[c] Negative sign denotes the export of excess electricity to Alberta grid.

electricity demand range from 51.9 kWh/m^3 of bitumen in delayed coker upgraders to 84.9 kWh/m^3 of bitumen in hydroconversion upgraders.

The SCO obtained from delayed coker upgrading differs from the one obtained in hydroconversion in mass, volume and quality. The mass and volume of SCO is traced based on the mass balance in each of sub unit operations whereas estimating the quality of SCO is beyond the scope of this research. As estimated by this model, the volume yield of SCO in hydroconversion is 103.7% compared to 91.1% in delayed coking. As specified in the existing literature, this range can vary from 78% to 94% in delayed coking to 95%–106% in hydroconversion [22,23,32,37]. The higher volume yield corresponds to higher hydrogen consumption in the hydroconversion process [29].

The GHG emissions from upgrading operations are presented in Table 3. Total GHG emissions calculated by the model are 240.3 $kgCO_2eq/m^3$ of bitumen (5.9 gCO_2eq/MJ of bitumen) in delayed coker upgrading and 433.4 $kgCO_2eq/m^3$ of bitumen (10.6 gCO_2eq/MJ of bitumen) in hydroconversion upgrading. Combustion gas along with natural gas feedstock for hydrogen production accounts for 81% and 82.7% of total emissions in delayed coker upgrading and hydroconversion, respectively, with the remaining coming from use of grid electricity. 28.5% of total emissions in delayed coker upgrading and 54.2% in hydroconversion upgrading are from hydrogen production.

With employment of cogeneration in the plant, the natural gas consumption increases in both the upgrading configurations. The natural gas consumed fulfills the steam demand and produces power which is in surplus of electricity demand of the plant. Delayed coker upgraders export 41.4 kWh and hydroconversion upgrader export 83 kWh electricity to the grid for each m^3 of bitumen feed upgraded. As shown in Fig. 5, the net emissions are lowered by 13% in delayed coker upgrading and 16% in hydroconversion upgrading, in lieu of displacing the carbon intensive grid power.

Results described in Table 3 and Fig. 5 are based on a unit of bitumen fed to the upgrading operation. The energy use and GHG emissions can be converted on mass, volume and energy basis of SCO. This is done based mass and volume relationships between bitumen and SCO, estimated by the model. Total GHG emissions on basis of SCO are 263.9 $kgCO_2eq/m^3$ of SCO (7.2 gCO_2eq/MJ of SCO) in delayed coker upgrading and 417.8 $kgCO_2eq/m^3$ of SCO (11.5 gCO_2eq/MJ of SCO).

The model-FUNNEL-GHG-OS developed in this research for upgrading operation in oil sands is validated with results of existing literature. To demonstrate the validity of the model, the GHG emissions for upgrading a particular feed (characteristics shown in Fig. S4) are estimated using the developed model and are compared in Fig. 5 with values reported by existing literature. The values estimated are in 10% range of those reported by Jacobs [12]. The emissions estimated in hydroconversion upgrading are in 2.5% higher than the GHGenius values [16]. GHGenius [16] does not report separate values for different configurations of upgrading. The values calculated in this research using fundamental engineering principles fall in the wide range predicted by GHOST model [22], which is based on a set of confidential data.

3.1.1. Sensitivity analysis

An analysis of the sensitivity of various parameters was conducted to determine their effect on net GHG emissions from the delayed coker and hydroconversion upgrading operations. The following parameters are investigated: sulfur content, hydrogen consumption, steam energy, electric energy and its emission factor, and efficiency of NG (natural gas) heater, steam boiler, heat exchanger. Hydrogen consumption in each of naphtha, distillate, gas oil hydrotreating (and hydroconverter in case of hydroconversion upgrading) has been varied. The effect of the steam requirement and steam conditions are captured in steam energy parameter. The sensitivity corresponds to base case with no cogeneration. As shown in Fig. 6, varying the parameters between ± 30%, the net GHG emissions vary by ± 8% in delayed coker and hydroconversion upgrading operations.

Hydrogen consumption in hydroconverter (in case of hydroconversion upgrading) and gas oil hydrotreating show a prominent effect on net emissions. Hydrogen consumption in naphtha and distillate hydrotreating has a comparatively less effect because of small volume yield of the feed and low hydrogen consumption per barrel of feed. Increasing the total hydrogen consumption of the plant (simultaneously in all hydrogen consuming sub unit operations) by 30%, the net emissions vary by 8.3% in delayed coker and 15.8% in hydroconversion upgrading, making hydrogen consumption the most sensitive parameter.

Increasing sulfur content in the feed requires more hydrogen for its removal. It has been assumed that 3 mol of H_2 are consumed for every mole of sulfur removed [38]. Varying the sulfur content by ± 30%, the emissions vary by 19.4 $kgCO_2eq$. This corresponds to 8.1% variation in delayed coker and 4.5% in hydroconversion upgrading.

Electrical energy is another influential parameter. The electricity requirement and its emission factor have the same effect on net emissions as shown by overlapping lines in Fig. 6. The efficiency of

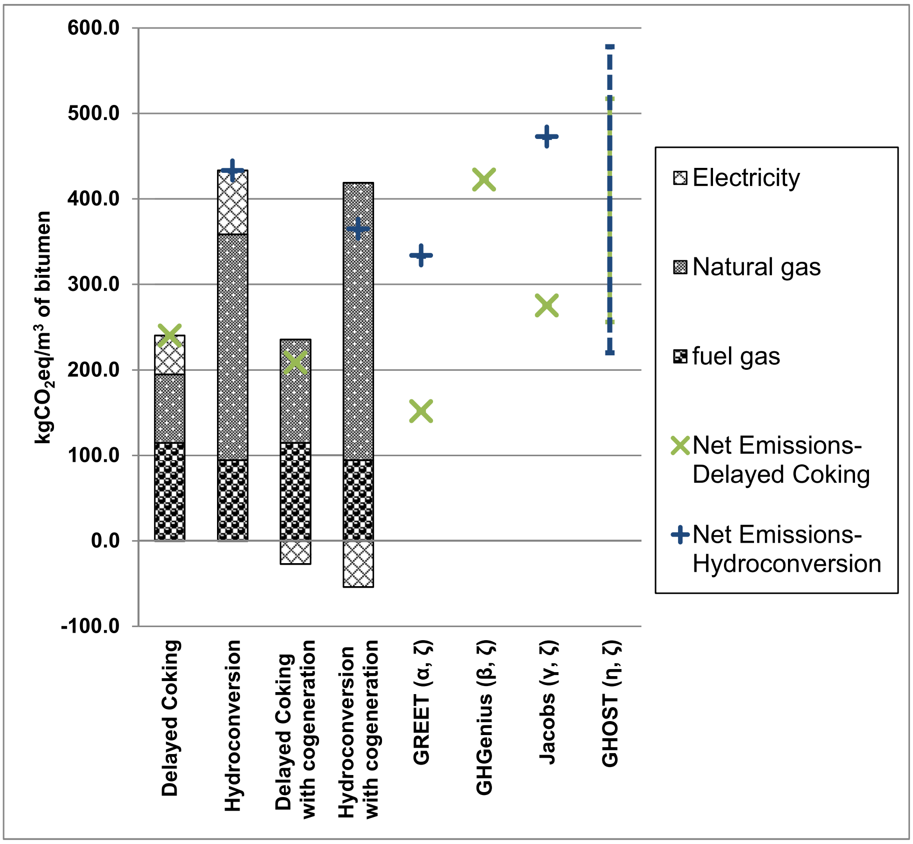

Fig. 5. Emissions in upgrading unit operation in comparison to existing literature and models. (α) Cogeneration has not been considered in the GREET model. (β) GHGenius does not give separate values for delayed coking and hydroconversion. No cogeneration considered in the model. (γ) These values correspond to no cogeneration case in Jacobs report [12]. (η) The range represented includes both the values of with and without cogeneration. Range for emission in delayed coker upgrading (257–517 kgCO2eq/m^3 of bitumen) overlap with emissions in hydroconversion (221–578 kgCO2eq/m^3 of bitumen). (ζ) The values from literature and models have been converted using LHV of bitumen 40.76 GJ/m^3 [16].

NG (natural gas) heater and steam boiler has comparatively less effect on net emissions because of their low variation. Varying the efficiency of heat exchanger by ± 20%, the change in net emissions ranges from −3.5% to 5.3% in delayed coker upgrading and −1.9% to 2.9% in hydroconversion upgrading.

Equipment such as the NG heater, heat exchanger and steam boiler have been used for a long time in industry and their technology has matured hence huge variation in their efficiencies is not possible. So to make the upgrading operations less GHG intensive, reducing the hydrogen and electricity consumption would be a good start. Also producing hydrogen from renewables such as wind can significantly reduce the GHG footprint of upgrading industry [39]. Equally important would be having a low emission factor for the electricity used. Hence shift of electricity generation from carbon intensive coal based electricity to cleaner fuels such as renewables would reduce the carbon footprint of upgrading operations. The sensitivity analysis performed points out the robustness of FUNNEL-GHG-OS model, which can be used to study the impact of project specific parameters on GHG emissions. 30% variation may not be easily noticeable in certain individual parameters, but combined improvements in more than one parameter can be practically achieved and would help to reduce the GHG emissions to the desired level.

3.2. *Refining*

The process model described in Section 2.3 has been used to explore the products obtained, energy consumed and GHG emissions from processing of coker SCO, hydroconversion SCO, dilbit and bitumen. The distillation curves, sulfur content, density and carbon residue of SCO, Dilbit and bitumen used as input to the model are shown in supporting information (Figs. S1–S4 respectively [40]).

On a refining scale of 150 kbpd, the yield of end products obtained per barrel of feed is shown in Table 4. The yield of products from atmospheric and vacuum distillation columns is presented in Fig. S5 in supporting information. The bitumen and dilbit are rich in heavier fractions such as gas oils and residue. SCO from coker and hydroconversion are light feeds rich in naphtha, kerosene and diesel. Dilbit contains a high fraction of naphtha as it is a blend of naphtha and bitumen.

As shown in Fig. 7, SCO from cokers and hydroconversion produces higher volume of products than the heavier feeds-dilbit and bitumen. Dilbit and bitumen produce more volume of fuel oil as compared to SCO. The heavier the feed, the more production of fuel oil. Gasoline, jet fuel and diesel are the useful and desired products. Most refineries minimize the production of fuel oil [12]. Coke is formed as a byproduct in refining bitumen and dilbit. Due to higher carbon residue content (13% in bitumen as compared to 10.5% in dilbit), more coke is formed in case of bitumen. Refining of hydroconversion SCO produces more volume of gasoline and diesel and compared to coker SCO. This is because the hydroconversion SCO is more severely hydrotreated and hydrocracked during its upgrading.

In general, lighter crudes tend to have a larger naphtha fraction than heavier crude (see Fig. S5 in supporting information). Naphtha

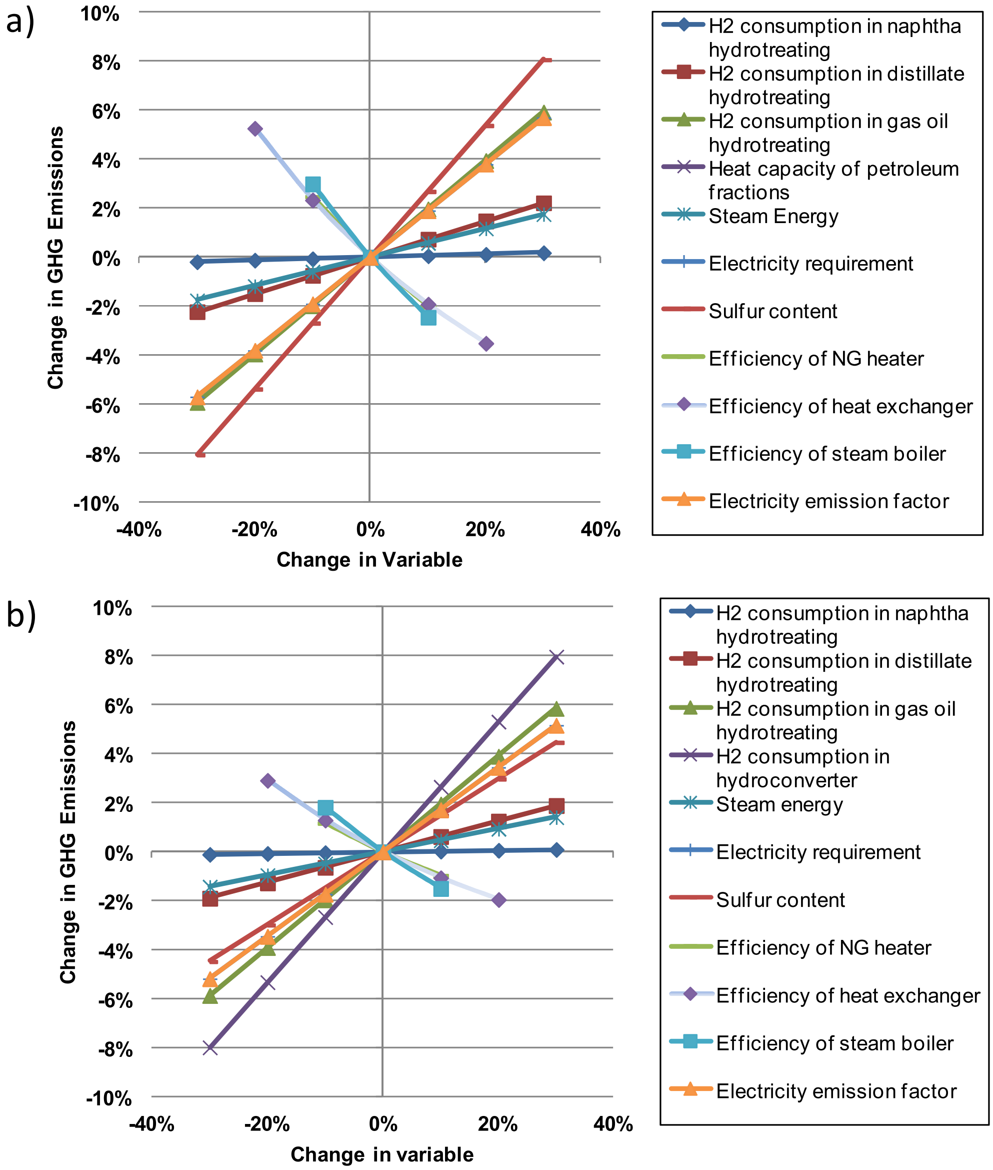

Fig. 6. Sensitivity of GHG emissions on key parameters in a) delayed coker upgrading b) hydroconversion upgrading.

being the easiest fraction to convert to gasoline [20], the volume of gasoline from dilbit should be more than that from bitumen. But Fig. 7 shows the opposite. This is in agreement with the findings of an earlier study [20]. The higher volume of useful products from bitumen than dilbit may be attributed to high mass of input feed in case of bitumen. For the same volume of feeds, the mass of bitumen is 8% more than that of dilbit. The volume of diesel and gasoline obtained on per mass basis of dilbit is more than bitumen, which in agreement with the general thought that higher volume of gasoline and diesel is obtained from lighter crudes with more naphtha fraction.

Table 4
Ends products obtained from refining of different feeds.

Products	Feed				
	Units	Coker – SCO	Hydroconversion – SCO	Dilbit	Bitumen
Fuel gas	bbl/bbl of feed	0.14	0.15	0.22	0.21
LPG	bbl/bbl of feed	0.01	0.01	0.01	0.01
Diesel	bbl/bbl of feed	0.28	0.28	0.18	0.19
Kerosene/ Jet fuel	bbl/bbl of feed	0.17	0.13	0.05	0.02
Gasoline	bbl/bbl of feed	0.48	0.53	0.51	0.54
Fuel Oil	bbl/bbl of feed	0.10	0.11	0.12	0.14
Coke	kg/bbl of feed	0.00	0.00	3.63	4.15

The energy consumption in refining the feeds is shown in Fig. 8. Energy consumed in refining ranges from 557.8 MJ/bbl to 895.1 MJ/bbl of crude, depending on the crude refined. The energy consumption varies depending upon the quality of crude, the end products desired, and the configuration of the refinery [11,12,20]. Bitumen and dilbit being rich in heavier fractions of gas oils and vacuum residue need more energy than SCO to convert the heavy fractions to useful products. The energy consumed in refining coker SCO is less in comparison to hydroconversion SCO as the former is bottomless (no vacuum residue) [12]. Bitumen being the heaviest of all crudes consumes approximately 60% more energy than coker SCO.

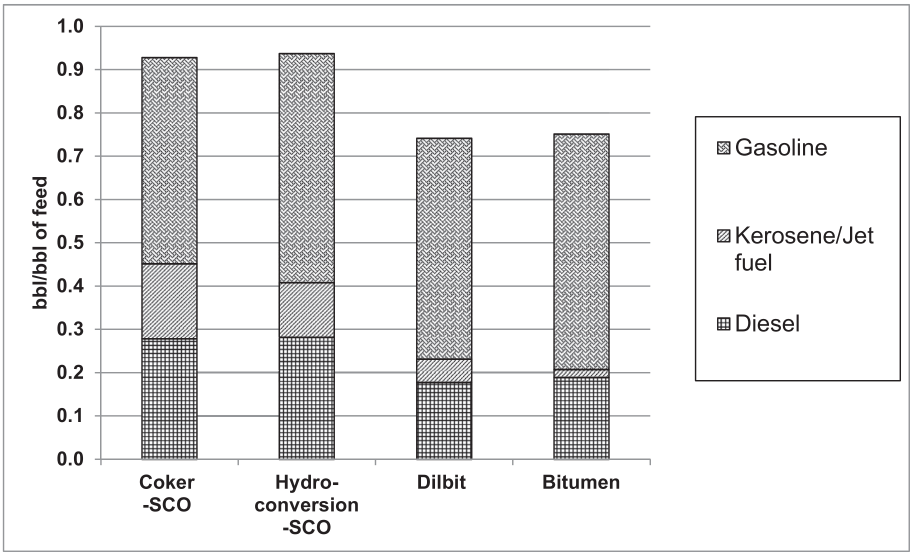

Fig. 7. Yield of useful products obtained from refining of feeds.

To demonstrate the validity of the results obtained in this research, the energy consumed for refining feeds with characteristics shown in Figs. S1–S4 are compared with the values reported in existing literature. Energy consumption modeled for refining of SCO and dilbit fall in the range of those reported by TIAX [11]. The modeled values are 14%–20% smaller than those reported by Jacobs [12]. Prelim [20] reports higher values for dilbit and bitumen than the modeled values. The energy consumption modeled for refining SCO is in good agreement with the range reported by Prelim.

The breakdown of energy consumption for SCO and dilbit is shown in Fig. 9. 22%–30% of the total energy in refining is consumed in the atmospheric and vacuum distillation columns. Reformer, HCD (Hydrocracking) and FCC (catalytic cracking) are other areas of high energy consumption. 9%–18% of total energy is consumed in catalytic cracking. The higher energy consumption in FCC in refining of SCO than dilbit or bitumen is attributed lower total energy consumption in SCO. The energy consumption in the reformer varies from 13% to 16% in case of SCO and 7%–9% in case

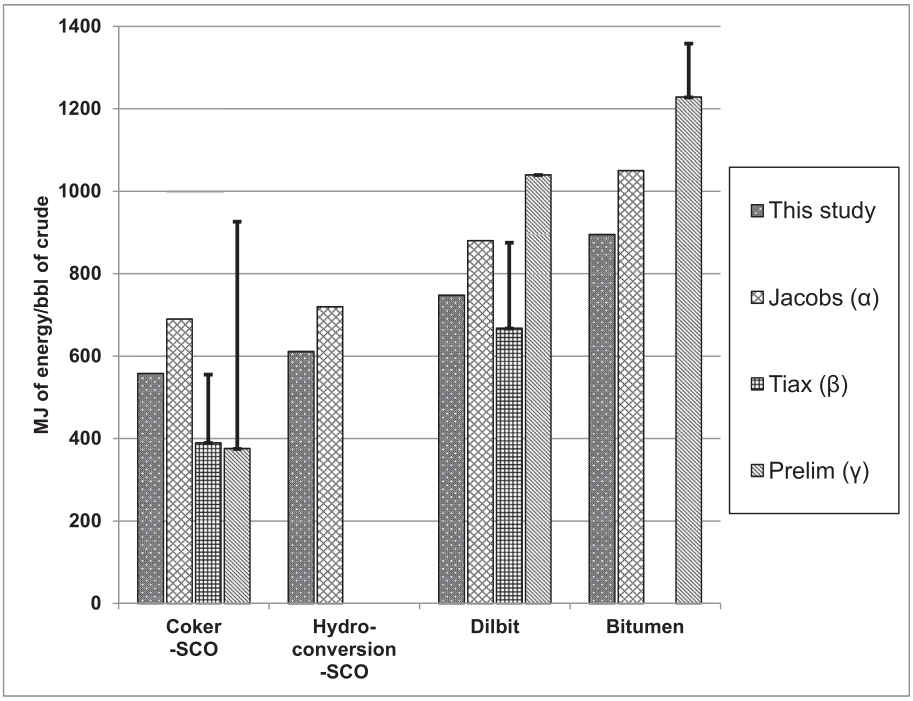

Fig. 8. Energy consumption per barrel of crude modeled in comparison to existing studies. (α) [12]. (β) [11]. TIAX has not separately mentioned the energy consumption for SCO from coker and hydroconversion. The range includes SCOs processed in PADD 2, PADD 3 and California. (γ) [20]. PRELIM does not differentiate between the energy consumption for SCO from coker and hydroconversion. The range includes the energy consumption for varying quality of SCOs processed in different configurations of refinery.

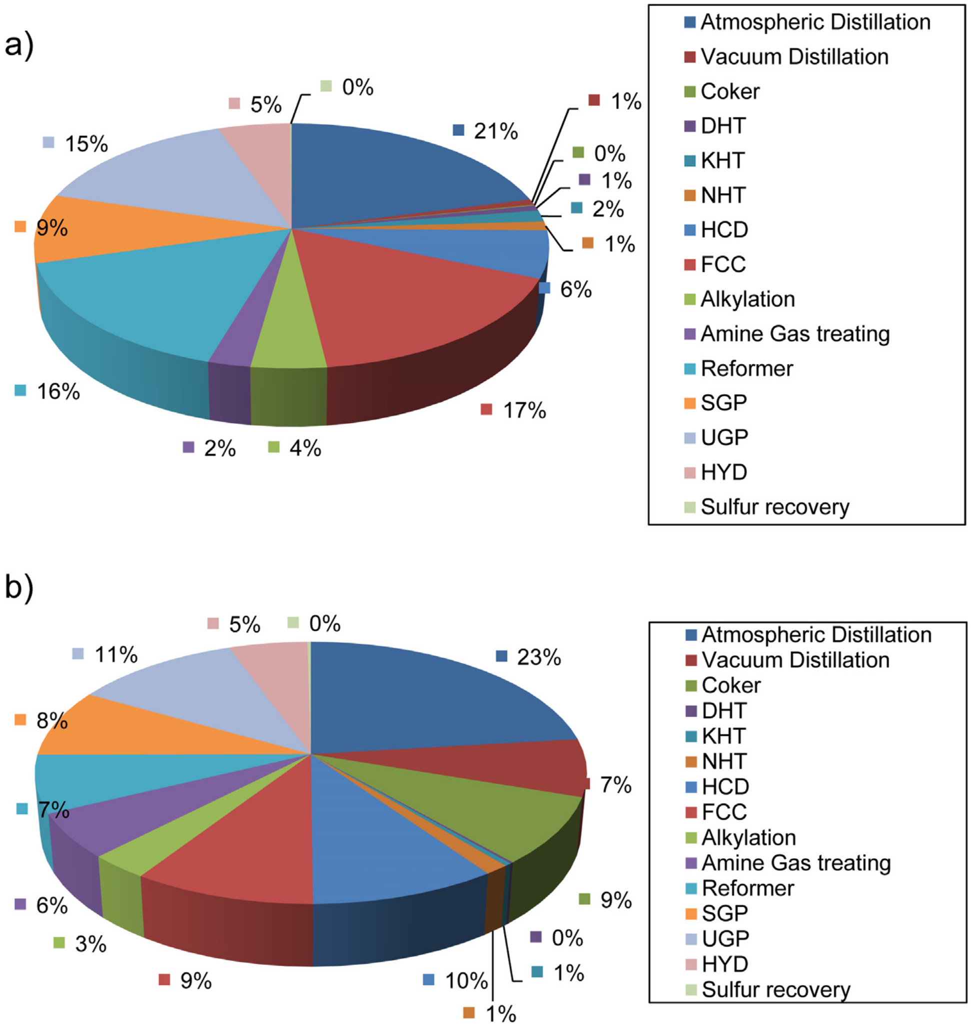

Fig. 9. Breakdown of energy consumption in each of sub unit operation for refining a) coker SCO b) Dilbit.

of dilbit and bitumen. The energy consumed in the reformer is highest in absolute numbers in the case of dilbit because of the high naphtha feed input to reformer. A significant portion of energy (11%–17%) is consumed in the UGP (unsaturated gas plant) and increases as the feed to it increases. But because of more total energy consumption in case of heavy feeds, the percentage of energy consumed is more in case of light feeds. Hydrogen production is an energy intensive process [21]. Energy consumed in hydrogen production is 5%–7% of total refinery energy consumption. The feedstock to this unit operation is methane from SGP (saturated gas plant) and natural gas imported from outside. The gases from hydrotreaters and the reformer are treated and separated in the SGP to produce methane which reduces the external intake of natural gas, making hydrogen production less energy intensive. Steam is produced in sulfur recovery process, making sulfur recovery less energy intensive. In fact net energy in form of steam is produced in Claus sulfur recovery and tail gas treatment [20].

Steam, electricity, coke, fuel gas and natural gas provide the energy required in refining operation. 6%–8% of the total energy required is obtained in the form of electricity. This electricity may be generated on site or imported from the grid. Steam is another major form of energy required. About 14%–17% of total energy required is in the form of steam. It is assumed that all of steam energy is required in form of high pressure steam [20]. Coke deposited on the FCC (fluid catalytic cracking) catalyst is burned off to restore catalyst activity and satisfied some of the energy requirement in the refinery [20]. 10%–19% of total energy can be obtained from coke burn off depending upon the feed. The remaining energy is fulfilled by the fuel gas and natural gas. The type of fuel used for obtained required energy affects the GHG emissions. So, this research explores the use of 100% fuel gas, 100% natural gas or 100% fuel oil to obtain the required energy.

GHG emissions from processing of crude feeds vary from 39 kg/bbl of coker SCO to 63 kg/bbl of bitumen (see Fig. 10). GHG emissions are proportional to the net energy input shown in Fig. 9. Higher energy consumption in heavier feeds such as dilbit and bitumen leads to more emissions. The use of natural gas instead of refinery gas does not affect the net emissions by much, whereas the use of fuel oil instead of refinery gas increases the emissions by 18% for refining bitumen. The GHG emissions modeled per barrel of crude are well in agreement with existing literature. The modeled results fall in the range reported by TIAX [11]. Values reported by Jacobs [12] are 24%–38% higher than the modeled results but also higher than values reported in other literature. This

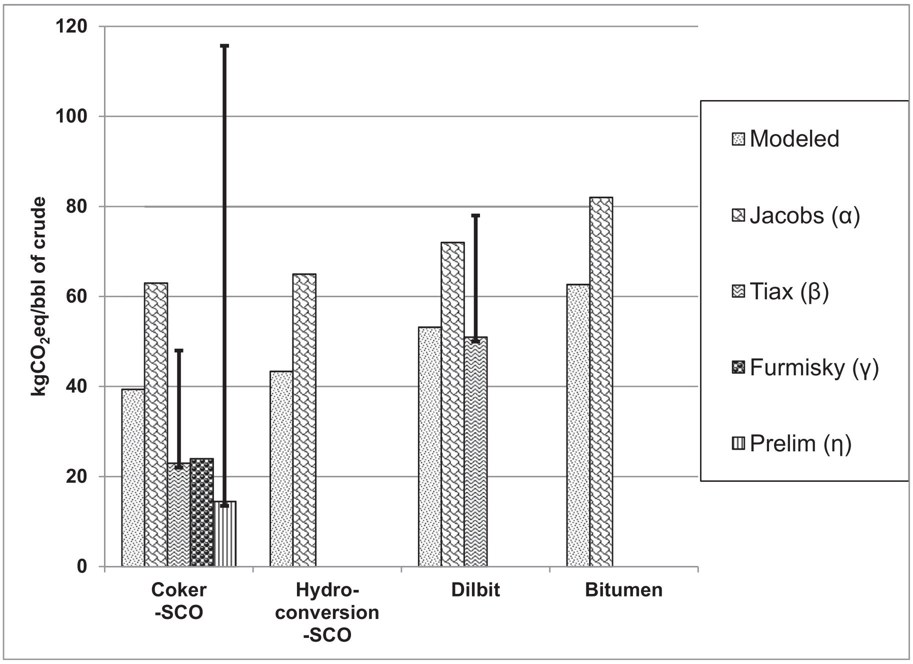

Fig. 10. GHG Emissions per barrel of crude modeled in comparison to existing studies. (α) [12]. (β) [11]. TIAX has not differentiated between the GHG emissions for SCO from coker and hydroconversion. The range includes SCOs processed in PADD 2, PADD 3 and California. (γ) [17]. Did not analyze other crudes. (η) [20].

variation is possible due to consideration of different quality of crude and different configuration of refinery [20,41]. Prelim [20] reports a wide range of GHG emissions for SCO based on the crude type.

Refineries produce a number of correlated products, whose yield depends on the quality of crude and severity of refining. Increased production of one refined product affects the yield of other products, also affecting the overall energy consumption and net GHG emissions in refinery. ISO (International Standard Organization) guideline for lifecycle assessment recommends avoiding allocation wherever possible [21]. Because the purpose of this research is to compare the GHG emissions from refining of different oil sands products, which produces different refined products, it is necessary to have a common base for comparison. As shown in Fig. 11, the common base chosen is total energy content of refined products so that allocation to refined products is avoided. Total energy content in a product of volume yield of the product and its energy content per unit volume. GHG emissions range from 7.9 gCO_2eq/MJ of refined product in case of coker SCO to 15.72 gCO_2eq/MJ of refined product in case of bitumen. Refining of SCO to fuels produces 41% and 49% lower emissions than dilbit and bitumen respectively.

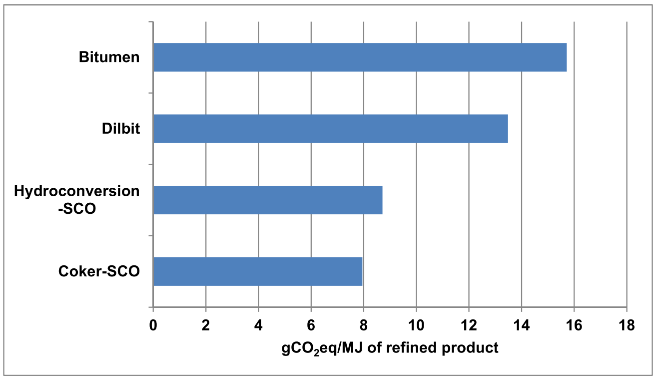

Fig. 11. GHG emissions from refining of oil sand crudes.

While SCO produces lower emissions during refining, the upstream emissions from upgrading of bitumen to SCO needs to be accounted for. Fig. 12 shows the effect of accounting for upgrading emission into the refining emissions. Bitumen goes to refinery as a blend of bitumen and naphtha or diluent. The diluent is separated from the blend in atmospheric distillation column [30]. The burden of these corresponding emissions is attributed to the bitumen feed. Bitumen transportation includes the transportation of bitumen-naphtha blend and back transportation of diluent from refinery to upgrader for 3000 km. In this case, transportation emissions are 5%–21% of total emissions, the later corresponding to the transport of bitumen. The emissions for obtaining end product energy from bitumen through upgrading in hydroconversion process are highest as seen in Fig. 12 [12]. The emissions for obtaining end products from direct refining of bitumen are 19% more than delayed coker case.

4. Conclusion

A detailed data intensive model named FUNNEL-GHG-OS based on first principles has been developed to estimate the project specific emissions in upgrading of bitumen. GHG emissions from upgrading of bitumen in hydroconversion (433.4 $kgCO_2eq/m^3$ of bitumen) are 80% higher than in delayed cokers (240.3 $kgCO_2eq/m^3$ of bitumen). But the volume yield of SCO in the former case is higher by 14%, resulting in 263.9 $kgCO_2eq$ and 417.8 $kgCO_2eq$ emissions per m^3 of SCO respectively. Emissions in upgrading are most sensitive to hydrogen consumption and the sulfur content of the feed. Production of electricity and hydrogen from renewables can significantly reduce the GHG footprint of bitumen upgrading industry to the desired levels. Refining of oil sands crudes consume 557.8 MJ–895.1 MJ per bbl of crude. The yield of refined products

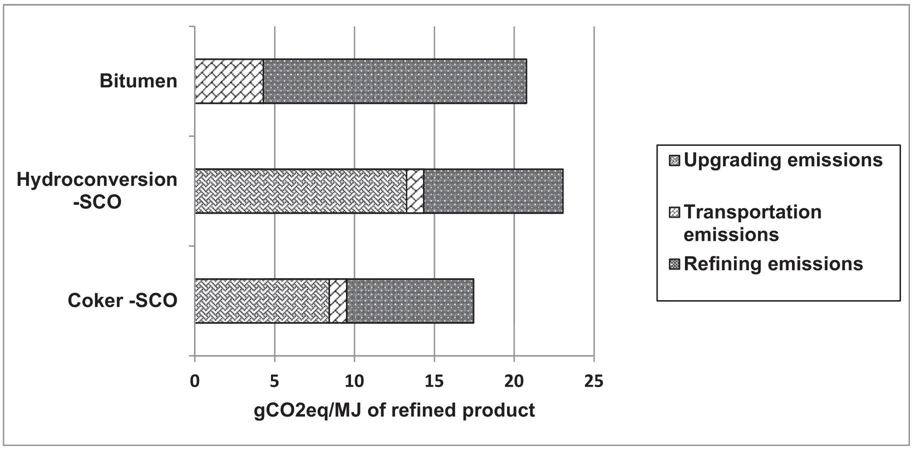

Fig. 12. GHG emissions from upgrading, transportation and refining of oil sand crudes.

from heavier feeds such as bitumen is lower than that from SCO. Refining of SCO to fuels produces 41% and 49% lower emissions than dilbit and bitumen respectively. GHG emissions for obtained refined products through direct refining of bitumen are more than refining it after upgrading in delayed cokers and lower than refining it after hydroconversion upgrading.

Acknowledgments

We thank NSERC/Cenovus/Alberta Innovates Associate Industrial Research Chair in Energy and Environmental Systems Engineering and Cenovus Energy Endowed Chair in Environmental Engineering for providing financial support for this project. We also thank representatives from AI-EES, AI- BIO, Cenovus Energy and Suncor Energy for their inputs in various forms. The authors thank Astrid Blodgett for editorial assistance.

Appendix A. Supplementary data

Supplementary data related to this article can be found at http://dx.doi.org/10.1016/j.energy.2015.01.085.

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