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Evaluation of energy and greenhouse gas emissions of bitumen-derived transportation fuels from toe-to-heel air injection extraction technology

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ABSTRACT

The currently used in situ oil sands recovery methods are energy and greenhouse gas emissions intensive. New methods such as toe-to-heel air injection extraction (THAI) are proposed to mitigate these challenges. This study aims to evaluate the energy and greenhouse gas emissions performances of bitumen-derived transportation fuels from THAI. A bottom-up process model was developed based on first engineering principles to assess the material, energy use, and greenhouse gas emissions of each unit operation. Three transportation fuel production pathways were examined: refining without upgrading and upgrading through either delayed coking or hydroconversion before refining. The extraction, upgrading, refining, transportation, and combustion life cycle stages of the pathways were considered. Sensitivity and uncertainty analyses of input parameters were conducted. The results show that the transportation fuels' well-to-combustion emissions range is $113.5_{-14.5}^{+14.5}$ g CO₂eq./MJ for the three pathways. The combustion and extraction stages have the most impact and contribute more than 63% and 21%, respectively, of the overall emissions of the pathways. The air-to-oil ratio was found to be most influential parameter affecting global results. The well-to-combustion emissions of THAI-based transportation fuels are in the range of current bitumen recovery methods. Any improvements in the air-to-oil ratio could significantly reduce the global emissions of these pathways.

1. Introduction

Petroleum fuel production, at around 100 millions barrels per day (mbpd), makes up one-third of global energy use and this use is expected to increase by 19% by 2030 [1]. Efforts to meet this demand have led to the exploitation of unconventional crude resources such as the oil sands in Alberta, a western province in Canada with the largest hydrocarbon base in North America [2]. This is because of the large amounts of oil sands in Alberta (165.4 billion barrels of proven reserves), most of which are deep underground in large bitumen deposits [3]. Bitumen can be recovered from the oil sands and converted into useful petroleum fuels using in situ steam assisted gravity drainage (SAGD) or surface mining followed by upgrading and refining,

respectively [3]. The recovery and conversion processes are energy and greenhouse gas (GHG) emissions intensive [4–6].

With increasing concerns about climate change impacts, global, national, and local governments are developing GHG emissions reduction initiatives. The California Low Carbon Fuel Standard (LCFS) [7], the European Fuel Quality Directive [8], the pan-Canadian carbon pollution price [9], and the Clean Fuel Standard (CFS) [10] are a few examples. These initiatives and regulations call for appropriate assessment and quantification of the life cycle GHG emissions of various transportation fuels; this can be done through life cycle assessment (LCA).

LCA is a widely used tool that uses systems thinking to evaluate the impact of a product or technology. It considers all material and energy

Abbreviations: ADU, atmospheric distillation unit; AGO, atmospheric gas oil; AOR, air-to-oil ratio; API, American Petroleum Institute; AR, atmospheric residue; Bbl, barrel; Bpd, barrels per day; Cp, centipoise; CSS, cyclic steam stimulation; DCU, delayed coking upgrader; DHT, diesel hydrotreating unit; EF, emission factor; FCC, fluid catalytic cracking; FWKO, free water knockout vessel; gCO₂eq, grams of carbon dioxide equivalent; GHG, greenhouse gas; GHT, gasoil hydrotreating unit; GJ, gigajoule; GWP, global warming potential; HC, hydrocracking; HCU, hydroconversion upgrader; HVGO, heavy vacuum gas oil; ISC, in situ combustion; ISO, International Organization for Standardization; KHT, kerosene hydrotreating unit; LCA, life cycle assessment; LHV, lower heating value; LPG, liquefied petroleum gas; LVGO, light vacuum gas oil; MJ, megajoule; NG, natural gas; NHT, naphtha hydrotreating unit; PFS, plant fuel system; SAGD, steam-assisted gravity drainage; SCO, synthetic crude oil; SGP, saturated gas plant; SMR, steam methane reforming; T&D, transportation and distribution of transportation fuels; THAI, toe-to-heel air injection; UGP, unsaturated gas plant; VDU, vacuum distillation unit; VR, vacuum residue

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streams into the system during all life cycle stages from the extraction of the resources to final use, disposal, and recycling [11,12]. Performing an LCA can help provide insights into the environmental footprint during different life cycle stages of a product or a system. These insights could help both industry and government representatives determine whether a system or a product complies with environmental policies and regulations. An LCA could also facilitate climate policy developments and formulations. LCA has four main stages as defined by the International Organization for Standard (ISO) guidelines: goal and scope definition, life cycle inventory, life cycle impact assessment, and interpretation [11,12]. In the goal and scope definition, the study purpose along with the system boundary, functional unit, assumptions, limitations, and allocation methods are identified. The second stage lists all material and energy inputs of each life cycle stage. The impact assessment links the inventory results to environmental issues such as climate change. In the interpretation stage, the main contributors to the overall results are identified and options for reducing environmental footprints are proposed [13].

Given the need to reduce GHG emissions, measures to lower GHG emissions and energy consumption associated with bitumen extraction processes are sought.

About 80% of the bitumen deposits in Alberta can be recovered through in situ methods such as cyclic steam stimulation (CSS) and SAGD [14]. Currently, about 1.6 million barrels per day (mbpd) (57% of total production) of bitumen are produced from in situ recovery in Alberta and this figure is projected to reach 2.22 mbpd by 2030 [15]. Commercialized in situ recovery methods such as CSS and SAGD use large amounts of natural gas to produce steam in the recovery of bitumen [3]. The large energy requirements result in GHG emissions of 45–190 kg CO₂eq. to extract one barrel of bitumen [4,16]. The produced bitumen is viscous; thus it requires diluent to meet pipeline transportation specifications and upgrading to meet refinery specifications [4,17]. In addition, the level of upgrading (partial or full¹) influences how much of the resource (i.e., hydrogen for hydrotreating and hydrocracking) is used in the refinery [18,19]. Therefore, several new bitumen recovery technologies that could improve the environmental performance of petroleum fuels through their entire life cycle stages are being considered.

In order to reduce the environmental footprint of oil sands-derived fuels, bitumen in situ recovery methods such as solvent-based recovery (SBR) [20–22], in situ combustion (ISC) [23], toe-to-heel air injection (THAI) [24], and many others have been proposed [25–28]. In SBR, a light vapor solvent is injected into the reservoir to heat bitumen, reduce its viscosity, and precipitate its heavy components to partially upgrade its physical and chemical properties [21]. In ISC, pressurized or enriched air is injected into the reservoir to initiate combustion. The combustion heat reduces bitumen viscosity and burns its heavy components while improving bitumen quality [29]. However, these extraction technologies have high solvent consumption and associated costs for solvent recycling and purification, which negatively affect the economics of SBR processes [22,30]. ISC has a low sweep efficiency² due to uneven propagation along the combustion front in the vertical producer well, which leads to low extraction rates [31,32]. In order to improve ISC, THAI is proposed.

An overview of THAI is shown in Fig. 1. A horizontal producer well is used in the ISC configuration; this improves both reservoir combustion and sweep efficiency [31]. Although THAI technology is not yet commercialized, there are three ongoing research and development (R&D) projects, one each in Canada, China, and India [33]. The THAI

recovery technique is expected to have a high oil recovery factor (up to 85%), significantly reduce bitumen viscosity, and increase bitumen API [34]. In addition, the aromatics, resins, and asphaltene contents of bitumen are also expected to be lower with the THAI recovery technique [35].

Although THAI is considered to require less water, less cost, and have a higher oil recovery factor than CSS and SAGD [32,36], there is no study that assesses the life cycle energy and GHG emission footprints of the THAI process for the extraction, upgrading, and refining of bitumen from the oil sands. Earlier studies focus largely on understanding and improving the performance of THAI operations. Greaves and colleagues developed a numerical simulation using 3-D cell experimental results to accurately predict the degree of bitumen upgrading and the peak temperature of combustion inside the reservoir from the THAI process [37]. Ado et al. developed a detailed dynamic simulation model to predict oil production rate, oil recovery, the amount of oxygen in the produced gas, and the optimum air-to-oil ratio³ for stable combustion in the extraction stage of the THAI process [38]. Boone and colleagues estimated the GHG emissions of THAI based on its pilot performance for the extraction stage only [30]. The impacts of partially upgraded bitumen on downstream processes such as the transportation, upgrading, and refining stages in terms of energy consumption and GHG emissions, including the associated uncertainties, were not addressed. There is a need to estimate the life cycle energy consumption and GHG footprints of THAI process-based transportation fuel production.

The overall objective of the study is to conduct a comprehensive LCA of the THAI process based on engineering principles. The specific objectives are to:

- Develop a process model to quantify the energy consumption requirements at each stage of fuel production from bitumen for the THAI process including extraction, transportation, upgrading, and refining.
- Compare the energy and GHG emissions performance of three alternative fuel production pathways based on THAI process: direct refining, delayed coking, and hydroconversion upgrading.
- Conduct sensitivity and uncertainty analyses to understand the impact of various input parameters on the life cycle energy consumption and GHG emissions of petroleum fuels derived through the recovery of bitumen by THAI.

2. Method

A bottom-up model was developed to estimate energy use and GHG emissions. The model framework is based on International Organization for Standardization (ISO) recommendations [11,12]. All the inputs and outputs of the system in the form of material and energy are considered.

2.1. Goal and scope definition

The GHG emissions of transportation fuel production through the THAI extraction process were assessed with the aim of answering the following research questions: What are the environmental impacts of bitumen extraction through the THAI process? What are the energy- and GHG emissions-intensive units in each life cycle stage of this technology? How are overall life cycle GHG emissions sensitive to parameters? What are the uncertainties in the input data and results? Which THAI-based fuel production pathway has lower energy consumption and GHG emissions? How does THAI compare with SAGD in terms of well-to-combustion (WTC) GHG emissions?

The functional unit used in this study is 1 MJ of transportation fuels (gasoline, diesel, jet fuel). The energy and material inputs are aligned

¹ Partial upgrading is done mainly to improve the API of bitumen to reduce or eliminate the need to add diluent. In full upgrading, in addition to API improvement, bitumen impurities such as sulfur, metal, and asphaltene are greatly reduced.

² Volume of the reservoir that is contacted by the injected fluid.

³ The amount of air at standard conditions that is required to extract one barrel of bitumen.

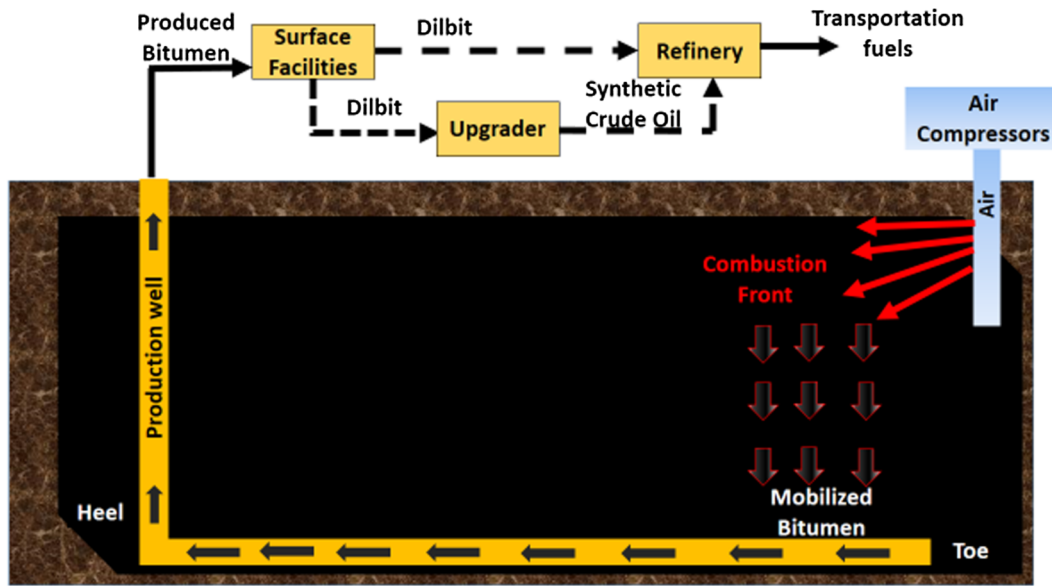


Fig. 1. High-level diagram of the THAI process.

with the functional unit. The model does not include construction, land use change, or site reclamation; they are out of the scope of the study due to the lack of data. It should be noted that in mining operations, the impacts of land use change are significant because all vegetation and top soil are removed to recover the bitumen from shallow reserves, while in situ methods, such as SAGD and THAI, bitumen is extracted from deep wells underground; therefore, the land use impact is up to 90% lower than surface mining [3].

This study only considers crude transportation via pipeline, bitumen upgrading in delayed coking and hydroconversion upgraders, and deep conversion refining of bitumen. Partial upgrading methods, other refinery configurations, and rail transportation of the crude are not considered.

2.2. System boundary

Fig. 2 depicts the WTC life cycle stages of transportation fuel production from oil sands. After the bitumen is extracted from the reservoir, it is processed in surface facilities to remove produced gases, water, and other impurities. The separated bitumen is then mixed with lighter hydrocarbons, known as diluent, to decrease its viscosity and density so that it can be transported by pipeline. The mixture of diluent and bitumen, known as dilbit, can be sent to an upgrader to produce a higher quality crude (synthetic crude oil [SCO]) or blended with lighter crude before being refined. The transportation fuels produced in the refinery are later combusted in vehicle engines [6,16]. In this study, we

considered three pathways for the production of transportation fuels from THAI. In pathway I, four stages over the life cycle – bitumen extraction, crude transportation, refining, and fuel combustion – are considered. In pathways II and III, five stages over the life cycle – bitumen extraction, upgrading, crude transportation, refining, and fuel combustion – are considered. In pathway II, a delayed coker is used and in pathway III, a hydroconversion upgrader is used (see Fig. 2). In all three pathways, all life cycle stages from bitumen extraction to transportation fuel combustion are considered.

2.3. Process description and data acquisition

This section describes each life cycle stage in the defined system boundary.

2.3.1. Extraction and surface facility

The detailed process schematic for the extraction stage is shown in Fig. 3. Initially, there is a long preheating period of several months in the reservoir where pressurized, high temperature steam is circulated through the injector well [39]. Compressed air is then injected into the formation to serve as the oxygen for the combustion in the reservoir [30]. The combustion is either initiated spontaneously or from an electrical igniter [40]. Because of the high heat of combustion, the pressure inside the reservoir increases to 4000 kPa [39,41]. The emulsion produced in the production well is comprised of bitumen, water, and the combustion gases. The emulsion is brought to the surface

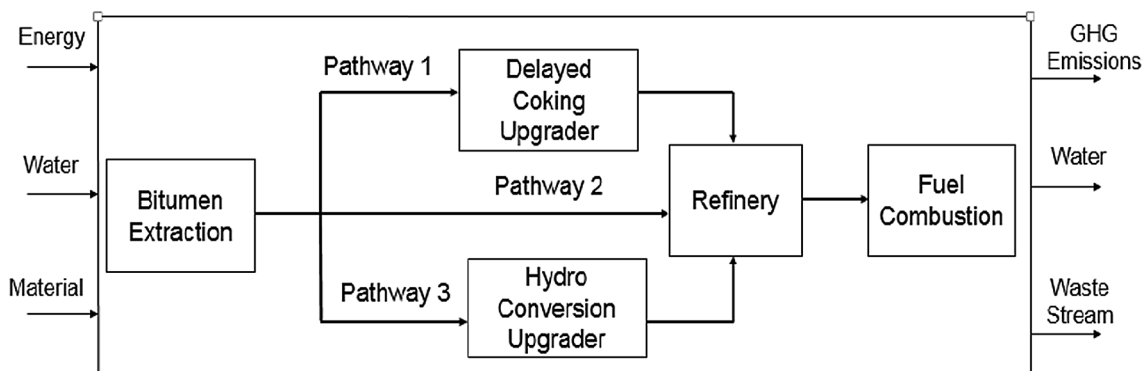


Fig. 2. Cradle-to-grave schematic of transportation fuel production from bitumen.

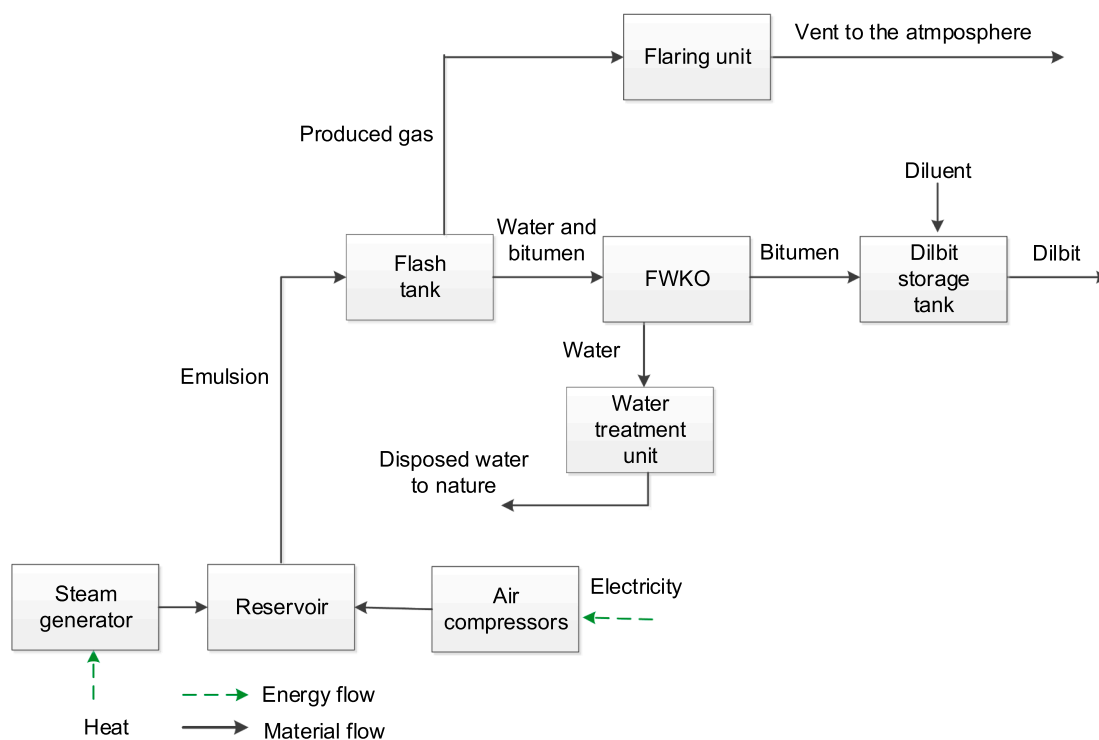


Fig. 3. Unit operations involved in extraction units for bitumen extraction in the THAI process.

through a flash tank where gaseous components are separated from the liquid. The liquid is sent to the free water knock out vessel (FWKO), which uses gravity to separate the water from the emulsion [42]. The separated water from the FWKO unit is then sent to the water treatment unit before being disposed of [39]. Bitumen from the FWKO is treated and blended with diluent in a storage tank [43]. The produced gases from the reservoir are sent to the flaring unit, where they are combusted by electrical igniters in tall stacks [40].

2.3.2. Upgrading

There are different upgrading technologies for processing dilbit [44]. Fig. 4 presents a schematic of delayed coker and hydroconversion upgraders, the most common upgrading technologies in Canada [45,46]. The dilbit is fed to the atmospheric distillation unit (ADU), where diluent, naphtha, diesel, and the atmospheric residue (AR) are separated. The AR is sent to the vacuum distillation unit (VDU), where gasoil and the vacuum residue (VR) are separated. The VR is then sent to the conversion unit, either a coker or hydroconversion unit, to reduce its sulfur, nitrogen, and aromatic content [16]. In delayed coking, the VR is thermally cracked into lighter fractions while producing coke, a solid residue rich in carbon, nitrogen, and sulfur [47]. In the hydroconversion unit, the VR is converted into lighter products in the presence of catalysts and pressurized hydrogen [48]. Liquid products of the conversion unit are mixed with matching liquid streams produced in the ADU and the VDU and are directed to the corresponding hydro-treater units where hydrogen is added to the streams to further reduce the impurities [49]. Hydrotreater liquid products are combined and form SCO. The purged gases in the plant are routed to the amine treater unit where aqueous alkylamine solutions are used to remove the H_2S and CO_2 from the feed. The H_2S stream is then converted to elemental sulfur in the Claus sulfur recovery unit. However, this unit is not capable of converting all the H_2S . The unconverted hydrogen sulfide is sent to the tail gas treatment unit to be converted to elemental sulfur [48]. The treated gas in the amine treatment unit is routed to the plant fuel system (PFS).

The hydrogen requirements of the upgraders are met through the steam methane reforming (SMR) process, wherein steam and methane

are reacted at high temperature and pressure conditions to produce hydrogen [50].

2.3.3. Refinery

Fig. 5 shows the configuration of the deep conversion refinery considered in this study. Refineries use various chemical and physical processes to maximize product yield and produce diesel, jet fuel, fuel oil, gasoline, liquefied petroleum gas (LPG), fuel gas, and coke. A deep conversion refinery has three more processes than an upgrader: cracking, reforming, and alkylation. In the cracking units (fluid catalytic cracking [FCC] and hydrocracking), large hydrocarbons are broken down into smaller molecules in the presence of catalysts, hydrogen, and steam. The reforming unit involves a catalytic process that rearranges, restructures, and breaks down the low octane naphtha into higher octane reformates in the presence of a catalyst to produce gasoline. Alkylation converts *iso*-butane, propene, and butene into high-octane gasoline products using catalysts [51–53].

2.3.4. Fuel delivery, distribution, and combustion in vehicles

Transportation fuels are delivered from refineries to bulk terminals by barge, ocean tanker, rail, and pipeline. Trucks are then used to distribute the fuels from bulk terminals to vehicle fueling stations.

2.4. Model development

2.4.1. Extraction stage

The pump work for emulsion extraction was calculated using Equation S.1 in the supplementary information (SI) section. In order to calculate the energy use and associated GHG emissions during the preheating period, the amount of steam used for preheating was divided by the amount of bitumen produced during the lifetime of the well. The compressor work was calculated using Equations S.2–S.5 (found in the SI). Air is compressed in several stages. At each stage, the outlet is cooled and compressed again. Since the injection pressure is high, it is assumed that the maximum compression ratio in each stage is 5. A higher compression ratio results in an excessive outlet air temperature, which increases energy consumption and decreases efficiency [54].

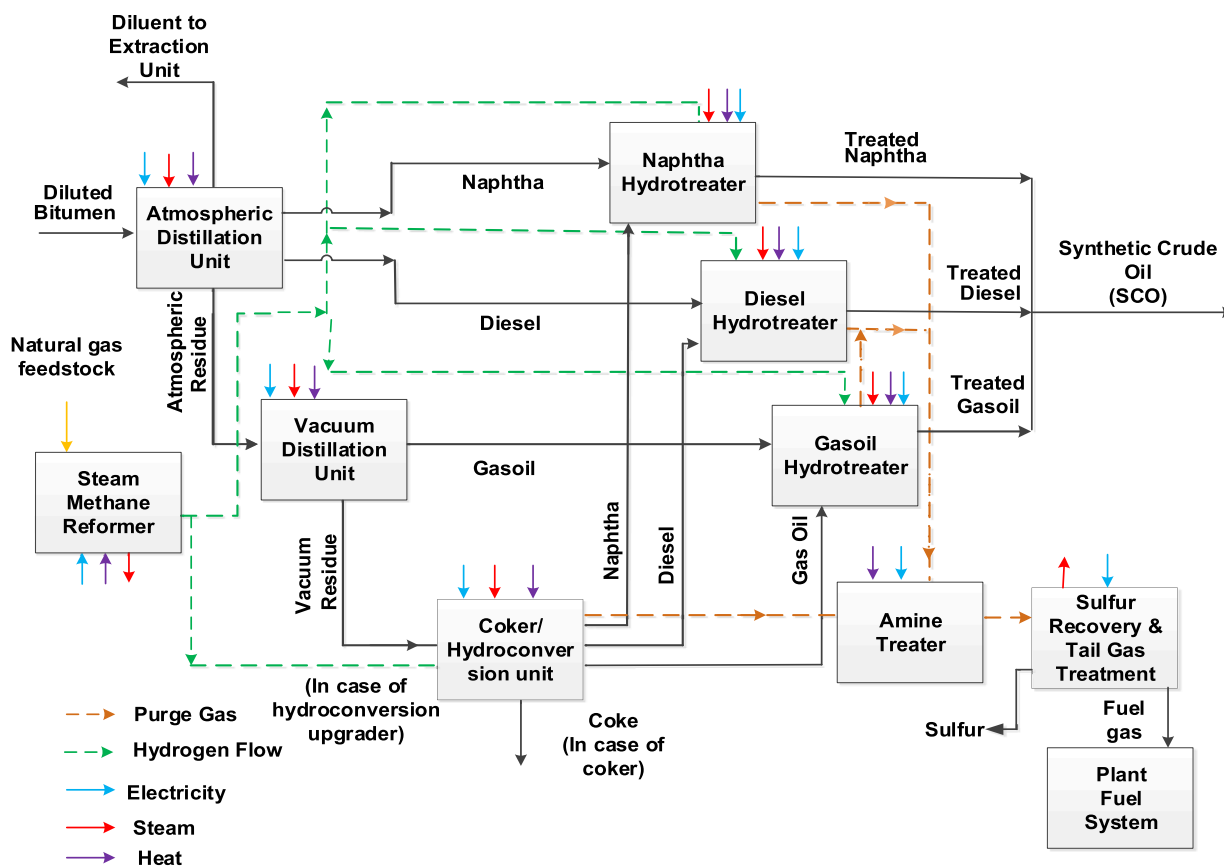


Fig. 4. Process flow diagram of the upgraders for processing THAI-based bitumen.

Associated GHG emissions from reservoir combustion [4] and flaring the produced gas are calculated with Eqs. (1–2); compositions of produced gas are presented in Table S4 in the SI; and the assumption is that the volume of produced gas is equal to the amount of injected air in the reservoir [4,5].

$$GHG_{\text{reservoir combustion}} = AOR \times \%CO_2 \times \rho_{CO_2} \quad (1)$$

$$GHG_{\text{flaring}} = AOR \times \sum_{i=1}^4 (\%C_i \times CEF_i) \quad (2)$$

where the GHG emissions of reservoir combustion and hydrocarbon flaring are in kg CO₂eq/m³ of bitumen, AOR is the air-to-oil ratio (m³/m³), %CO₂ is the volume percent of CO₂ in the produced gas, ρ_{CO₂} is the carbon-dioxide density at standard conditions (1.87 kg/m³ [6]), %C_i is the mole percent of hydrocarbon i in the produced gas, and CEF_i is the combustion emission factor of hydrocarbon i (kg CO₂eq/m³).

Further details on the calculation of energy and GHG emissions for the extraction stage are provided in sections S.1–S.7 in the SI.

It is assumed that natural gas is used to heat the reboiler. The combustion emissions, as well as the upstream emissions associated with recovery, production, and distribution, are considered in the GHG emissions assessment.

It is assumed that Alberta's electricity grid is used to supply electricity in the extraction stage; all the GHG emissions associated with its production and transmission are considered in the model.

The default values used in the model for the simulation of the extraction stage are presented in Table S.4 in the SI.

2.4.2. Upgraders

Rigorous upgrader models were developed in Aspen HYSYS Version 9 to obtain mass balance and utility consumption from each unit operation [55]. A typical upgrading capacity of 150 kbpd was considered

[56]. The Peng-Robinson equation of state was the fluid package selected in Aspen HYSYS. An ebullated-bed reactor was used to simulate the hydrocracking unit. The operating conditions of the conversion and hydrotreater units were taken from the literature [47,57,58]. The correlations suggested by Edgar [59,87] (as shown in Eqs. (3–5)) and the properties of the hydrotreated liquid products [49] (as shown in Table S.6 in the SI) were used to estimate the hydrogen requirements in the hydrotreater units. The hydrogen consumption in the hydroconversion unit is assumed to be 1.5% of the weight of the VR, as suggested by several authors [48–50]. Energy and feedstock requirements for H₂ production in the SMR unit were taken from the literature [60]. The utility consumption in the amine treater, sulfur recovery and tail gas treatment units were calculated based on values suggested by Pacheco et al. [18].

$$HDS = 97.5 \times (scf/bbl) \times wt\% \text{ sulfur removed} \quad (3)$$

$$HDN = 325 \times (scf/bbl) \times wt\% \text{ nitrogen removed} \quad (4)$$

$$HDA = 27 \times (scf/bbl) \times wt\% \text{ aromatic saturated} \quad (5)$$

where HDS, HDN, and HDA are hydrodesulphurization, hydrodenitrogenation, and hydrodearomatization.

Steam produced in the Claus sulfur recovery unit is used to fulfil a portion of the plant's steam demand. Natural gas is assumed to be the main source of heat and steam production. It is also assumed that the combustion of the produced gas in the plant fuel system (PFS) unit supplies a portion of the plant's heat demand, and its energy content and GHG emissions factor were calculated based on its composition. Using coke for heat and steam production is GHG emissions intensive [61]. Currently, coke is mostly stockpiled in Canada because of low natural gas prices and strict environmental regulations [18,62]. Thus, coke is assumed to be a by-product and is stockpiled. Finally, it is assumed that the electricity demands of the upgraders are satisfied by the

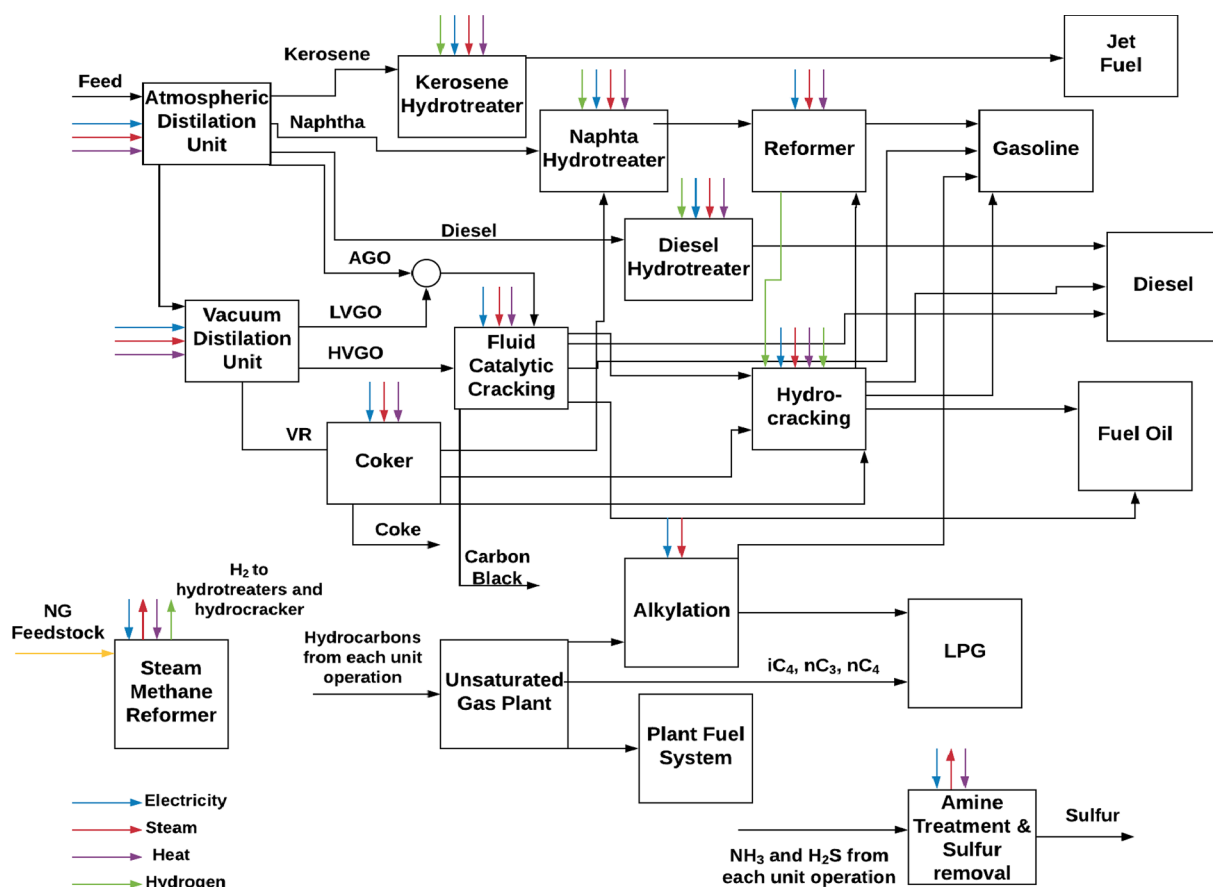


Fig. 5. Deep conversion refinery configuration for processing of THAI-based bitumen.

Alberta grid. The values presented in Table S.5 in the SI are used to develop the LCA model for the upgrading stage.

The same methods, assumptions, and values were used for H₂ production, the source of heat, the calculation of energy consumption in the amine treater, the Claus sulfur recovery unit, and the tail gas treatment unit in the refinery section.

2.4.3. Refinery stage

The built-in deep conversion refinery model in Aspen HYSYS was used to simulate the refinery process for dilbit and SCO produced in upgraders at a refining capacity of 150 kbpd [55]. Aspen HYSYS obtained the yields from the separation units (ADU and VDU) and the associated energy consumption based on the crude's distillation curve and physical and chemical properties, such as the API and the sulfur content [63,64]. The crude assays for SCO and dilbit are presented in Tables S.2 and S.3 (in the SI). Other processing units in the refinery are simulated with petroleum shift reactors. These reactors are empirical models that calculate the product yields and utility consumption of each unit operation based on feed flow rate, feed properties, and a set of linear equations [65].

It is assumed that the refineries are located in the USA, as 94% of the non-upgraded bitumen produced in Alberta and 56% of the upgraded bitumen is exported to US refineries [66]. Refinery electricity emissions factors were calculated by taking the weighted average of each state's electricity emission factor and the corresponding refinery capacity of each state [16]. However, we also conducted a sensitivity analysis of bitumen processing in Alberta's refinery and hence used the associated electricity emission factors.

Since refinery processes result in several products, and products do not undergo the same processes, proper allocation of the refinery products is required [67]. The energy consumption and associated GHG

emissions were allocated at the sub-process level in this study, as suggested by ISO 14040 and ISO 14044 [11,12]. The energy consumption and associated GHG emissions in each unit operation were distributed among the product streams based on the product's mass. The quantity and type of energy use were traced through the refinery from the ADU to the refinery products. Fuel oil, coke, LPG, and produced gas are considered by-products. The energy consumption and associated GHG emissions were distributed to gasoline, diesel, and jet fuel in proportion to their mass yields and per MJ of product (MJ of gasoline/diesel/jet fuel). The lower heating values (LHVs) of transportation fuels were taken from GREET [68]. The values presented in Table S.7 are used to develop the LCA model for the refinery stage.

2.4.4. Crude transportation and transportation and distribution of transportation fuels stages

Adapting Nimana et al.'s [17] pipeline model for the transportation of 750,000 bpd of bitumen or SCO, we estimated the energy consumption and associated GHG emissions at the crude transportation stage. In order to account for the diluent amount, the shipped volume was increased to 855,288 bpd in the dilbit case and diluent was calculated using Eq. (S.10) in the SI. It is assumed that 100% of the diluent is recycled and sent back to the extraction site after being processed in the upgrader or refinery [69]. The detailed calculations and formulas are presented in Eqs. (S.10–S.18) in the SI. The emissions factor of the electricity used for transportation to the upgrader is taken from Alberta's grid mix, and for transportation to the refinery, the distance weighted average for the electricity emissions factor across the Alberta-Gulf Coast pipeline path was used [17]. It is assumed that the bitumen extraction site, upgrader units, and refineries are located in Fort McMurray, Fort Saskatchewan, and the Gulf Coast, respectively [6,17].

The GHG emissions attributed to the transportation fuels'

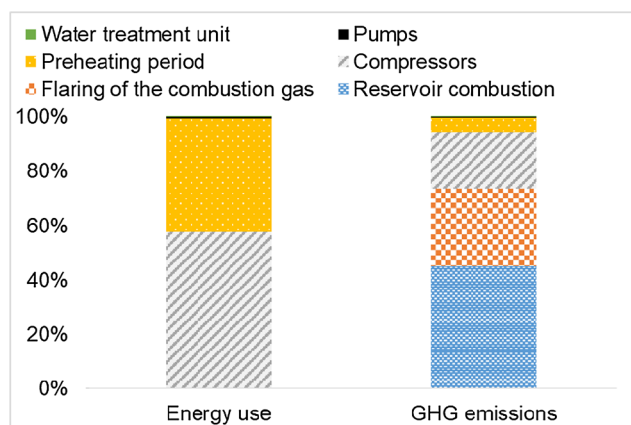


Fig. 6. Shares of energy use and GHG emissions in different unit operations in crude extraction in the THAI process.

transportation and distribution (T&D) to bulk terminals and fueling stations were imported from Argonne's GREET model [68]. The values presented in Table S.8 in the SI are used to assess the energy use and GHG emissions during the crude transportation and transportation and distribution of transportation fuels.

2.4.5. Combustion of transportation fuels

GREET model values were used to estimate the GHG emissions in the transportation fuels' combustion stage [68]. GHG emissions at each life cycle stage are aggregated and normalized to the functional unit in order to estimate the total emissions per MJ refinery output, as shown in Eqs. (S.26 and S.27) in the SI. The GHG emissions were allocated to gasoline, diesel, and jet fuel based on their mass yields in the refinery.

2.5. Sensitivity and uncertainty analyses

The Morris global sensitivity analysis method was used to screen and determine the sensitive input parameters [70]. The method is based on a partial derivative calculation in randomized locations of the whole range of inputs and is more robust than a local sensitivity analysis that only analyzes the variations in a limited range of input variables. Table S.11 in the SI lists the range of input variables considered for the sensitivity analysis.

Uncertainty analysis was used to determine the most probable ranges of GHG emissions in each transportation fuel production pathway. Uncertainty analysis was performed only on the sensitive inputs, using a Monte Carlo simulation [71]. First, the range of input variables and their distributions were identified. Then, random inputs were generated and used to calculate the results [72].

Due to the lack of data for input variables, triangular and PERT distributions, which require minimum, mode, and maximum values, were considered in this study for performing the Monte Carlo simulation [72,74]. Triangular distribution is used when limited data is available on the input variable and the mode is known. PERT puts more weight on the mode and less on the minimum and maximum. However, large amounts of historical data or expert opinion are required in order to use it [73].

The mode considered for the AOR is based on the performance of the Kerrobert pilot plant in Canada [33]. The AOR range is wide because reservoir properties differ around the world [33,40,75]; thus, the PERT distribution is used in order to put more weight on the technology's performance in Canadian reservoirs.

PERT is also used to put more weight on the Aspen HYSYS values determined for hydrotreaters (HTs), hydrocracking units (HCs), and reformer H_2 consumption/production. The range of H_2 consumption in the refinery HT units given in the literature is wide because of differences in the feedstock (heavy, light, medium, sweet, sour, etc.) [5].

Since the objective of this study is to analyze the THAI bitumen and produced SCO, considering the wide range from the literature is not appropriate. Therefore, a range of $\pm 25\%$ of the base case value is considered in sensitivity and uncertainty analyses. Specifications of transportation fuels and desired refinery product yield determine the H_2 consumption in the HC unit. H_2 production in the reformer unit is affected by the reaction pressure, desired octane number of the gasoline, and the level of reduction in the aromatics and benzene required to meet environmental regulations [52,76–78]. Values reported in the literature for H_2 in the reformer and the HC unit were used to conduct sensitivity and uncertainty analyses. Given the limited availability of data, a triangular distribution was used for the other parameters.

The modes are the default values in the model (shown in Tables S.4, S.5, S.7 and S.8). The range of input variables and their corresponding distributions are listed in Table S.12 in the SI.

3. Results and discussion

This section provides the key findings of the study. First, the detailed analysis and associated results of the important life cycle stages that significantly contribute to the overall GHG emissions of the transportation fuel are presented. This is followed by the overall life cycle GHG emissions results.

4. Extraction and surface facilities

The overall energy consumption of the THAI extraction process is 273.2 MJ per barrel of bitumen. As shown in Fig. 5, the compressors are the main energy-intensive units and consume 57% of the overall energy, followed by the natural gas boiler, at 42%. The water treatment unit and pumps consume only 1% of the energy.

The GHG emissions associated with each unit operation in the extraction stage are also presented in Fig. 6. The combustion in the reservoir is the main contributor to the overall GHG emissions in this stage. Next to reservoir combustion are the flaring of the produced gases and the compressors. The GHG emissions associated with the combustion in the reservoir were estimated to be in the range of 14.5–16.8 $gCO_2eq./MJ$ of transportation fuels. A high amount of energy is required to mobilize the bitumen from the reservoir. In the THAI operation, the energy to move the bitumen can be met through the combustion in the reservoir. The AOR in this case is relatively high. To produce one m^3 of oil requires about 1500 m^3 of air; considerable GHG emissions are released through the reaction between air and light hydrocarbons in the reservoir. The GHG emissions associated with the flaring of produced gases and compressors were estimated to be 8.4–7.3 $gCO_2eq./MJ$ and 5.5–6.3 $gCO_2eq./MJ$ of transportation fuels. These values are a function of the AOR. An increase in the AOR increases the amount of produced gas from the reservoir and the compressor power. Preheating the reservoir contributes only 5% to the overall GHG emissions; this figure is low mainly because of the short preheating period. The pumps and water treatment unit have a negligible impact on the GHG emissions.

4.1. Upgrading

The base case energy consumption values for the delayed coking upgrader (DCU) and the hydroconversion upgrader (HCU) are 0.73 and 0.9 GJ/bbl of bitumen, respectively. The fuel required for heat and steam generation, along with the natural gas used as feedstock for hydrogen production, is the largest source of energy consumption. Electricity contributes only 2% and 2.8% of the overall energy consumption in the DCU and the HCU, respectively. A significant portion of the heat requirement in both upgraders is met using the gas produced in the plant (48% in the DCU and 34% in the HCU). The hydroconversion upgrader consumes more energy because it requires more hydrogen, which results in higher fuel, feedstock, and electricity consumption.

Table 1
Upgrader yields and utility consumption.

Upgrader yields			
	Unit	Delayed coking	Hydroconversion
SCO	m ³ /m ³ bitumen	0.96	1.09
SCO	kg/kg bitumen	0.84	0.96
Coke	kg/bbl bitumen	13.62	–
H ₂ S	kg/bbl bitumen	2.88	4.42
Utility consumption			
	Delayed coking	Hydroconversion	Units
Fuel gas	5.12	4.07	kg/bbl bitumen
NG ^a	12.1	16.7	m ³ /bbl bitumen
Steam ^{a,b}	8.59	11.06	kg/bbl bitumen
Electricity	4.24	7.33	kwh/bbl bitumen
H ₂ ^a	1.93	2.55	kg/bbl bitumen

^a Emissions from hydrogen and steam production are included in natural gas, fuel gas, and electricity emissions.

^b 2.79 MJ/kg is considered for the LHV of the steam [47].

Furthermore, the hydrocracking unit consumes more electricity than the delayed coker unit does. This is because of the high compression energy required by hydrogen for the optimal hydrotreating reaction and the pump energy required for increased product yield [49,69]. The utility consumption in each upgrader unit operation is presented in Table 1.

The SCO produced in the DCU is different from that obtained from the HCU in quality, mass, and volume yield. The simulation results show the DCU and the HCU mass yields of 84% and 96%, respectively. The increased yield in the hydroconversion unit is due to the improved conversion of the vacuum residue to lighter hydrocarbons, leaving little or no by-product coke. That said, 8.8 wt% of the bitumen is converted to coke in the DCU. Furthermore, higher hydrogen consumption and lower gas production in the HCU results in a higher mass yield than in the delayed coker. Detailed information on upgrader yields can be found in Table 1.

GHG emissions from the upgraders range from 8.11 to 8.39 gCO₂eq./MJ in the DCU and from 9.06 to 9.37 gCO₂eq./MJ in the HCU for the three products. There are two main reasons for the relatively higher GHG emissions from the HCU. First, the HCU uses the hydrogen- and emission-intensive hydrocracker to convert the vacuum residue (VR), and the coker unit does not consume hydrogen. Second, the higher yield of vacuum residue in hydrocracker compared to the coker means more products are treated in hydrotreaters [49,79].

Fig. 7 presents the GHG emissions percentage contributions of different unit operations involved in both upgraders. Hydrogen production appears to be the main contributor, with 43.70% and 47.20% from the DCU and the HCU. This is mainly because of the large steam requirement and of natural gas both as fuel and as feedstock in the SMR process [60]. The ADU is the second largest contributor to GHG emissions with shares of 32.50% and 26.2%, from the DCU and the HCU, respectively. The consumption of natural gas and fuel gas are the key

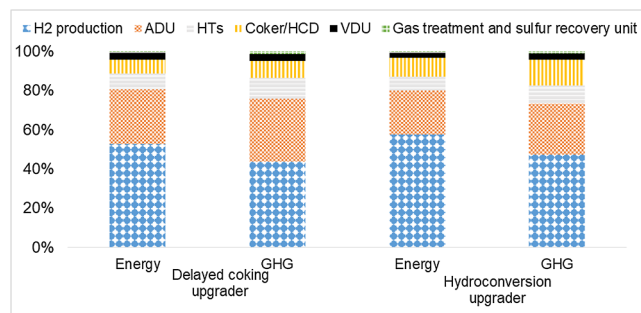


Fig. 7. GHG emissions contribution from different unit operations in delayed coking (DCU) and hydroconversion (HCU) upgraders.

Table 2
Refinery yields and utility consumption.

Refinery yields				
	Unit	Bitumen	DC SCO	HC SCO
Gasoline	bbl/bbl crude	0.58	0.43	0.43
Diesel	bbl/bbl crude	0.23	0.33	0.31
Jet fuel	bbl/bbl crude	0.20	0.26	0.26
Fuel oil	bbl/bbl crude	0.08	0.05	0.04
LPG	bbl/bbl crude	0.02	0.01	0.01
Fuel gas	kg/bbl crude	6.81	3.29	2.67
H ₂ S	kg/bbl crude	2.20	0.07	0.04
Coke	kg/bbl crude	13.06	0.00	0.02
Utility consumption				
NG	m ³ /bbl crude	13.13	7.40	7.87
Steam ^a	kg/bbl crude	28.90	15.10	15.60
Electricity	kwh/bbl bitumen	12.60	8.54	8.04
H ₂ ^b	kg/bbl bitumen	0.97	–0.26	–0.40

^a 2.79 MJ/kg is considered for the LHV of the steam [47].

^b The produced H₂ in the reformer unit exceeds the H₂ consumption in the hydrotreaters and the hydrocracker unit for both SCOs.

sources of GHG emissions, with more than 90% contribution. Electricity forms only 7% and 9% of the emissions from the DCU and the HCU, respectively.

4.2. Refinery

The deep conversion refinery model described in section 2.3.3 was used to determine product yield, energy use, and associated GHG emissions for bitumen both directly sent for and undergoing upgrading. Bitumen is rich in heavier fractions such as vacuum residue and gasoil, and SCO is a lighter crude rich in naphtha, kerosene, and diesel (see Table S.3 in the SI). Refining SCO yields more diesel and jet fuel than bitumen does, while more gasoline is produced in the bitumen pathway. Moreover, 8.80 wt% of bitumen is converted into coke during the refining process, as stated in section 3.2. On the other hand, SCO produces little or no coke (bottomless) in the refinery. More fuel oil is produced in the bitumen refinery than the SCO refinery because bitumen has more heavier fractions than SCO does [6]. Because of the pre-processing of bitumen into SCO, H₂S production is considerably lower for SCO in the refinery. Additional information on refinery yields is provided in Table 2.

The energy consumed to refine bitumen is 0.65 GJ/bbl and is 0.35 and 0.36 GJ/bbl for DC and HC SCO. Fig. 8 gives the breakdown of energy use shares for refining bitumen, delayed coker SCO, and hydroconversion SCO. Refining bitumen requires up to 87.5% more heat and 56.0% more electricity than SCO does. There are two main reasons for this. First, bitumen is much richer in heavy ends that require more heat for vaporization and separation in distillation units. Second,

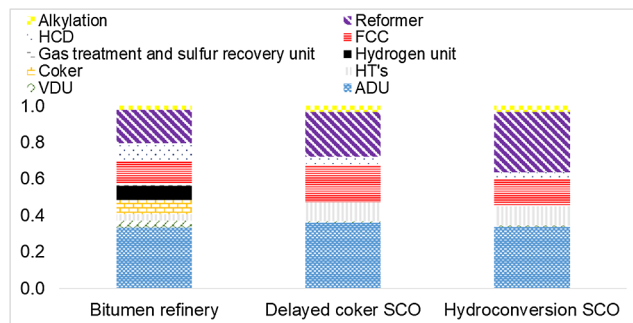


Fig. 8. Share of energy use in the refining of bitumen, delayed coker SCO, and hydroconversion SCO.

because of the low H/C ratio and the high sulfur, metal, and nitrogen content of bitumen compared to SCO, more H₂ and a more severe treatment are required to convert the bitumen into final products and meet desired specifications. The produced gases in different unit operations are directed to the PFS unit and used to satisfy a portion of the heat requirement in the refinery. These gases supply 54.2%, 46.8%, and 45.1% of the heat demand for bitumen refining, DC SCO, and HC SCO, respectively.

As shown in Fig. 8, the ADU is the major contributor to the overall heat consumption, followed by the reformer and the FCC unit. Heat consumption in the reformer is relatively high and almost equal to that of the ADU in the hydroconversion SCO refinery. This is because of the large fraction of naphtha distillate in the HC SCO that undergoes an energy-intensive reforming process [80] (see Table S.3 in the SI). The FCC and alkylation units are the most electricity-intensive units. The energy consumption of the coker unit for refining the DC and the HC SCO is not significant, unlike in bitumen refining. This is because the coker and hydroconversion SCO have little or no vacuum residue, while bitumen has 30 wt% (see Table S.3 in the SI). As illustrated in Table 2, the H₂ produced in the reformer unit exceeds the H₂ requirements of the DC SCO and HC SCO refinery. Hence, zero energy consumption is assigned to the H₂ production unit for the SCO refinery. However, this unit makes up 8.20% of the overall heat and 2.60% of the electricity use in refining the bitumen. It is assumed that the excess H₂ is exported to the nearby chemical and petrochemical facilities and an emissions credit equal to what is emitted to produce this amount of H₂ is assigned to it.

The GHG emissions associated with refining bitumen and SCO are presented in Fig. 9. Refining SCO emits fewer GHGs than bitumen because of the lower processing energy requirements. However, SCO undergoes the emission-intensive upgrading process. Hence, the life cycle assessment approach is used to compare the environmental performance of these products. The allocated refinery emissions for jet fuel are considerably lower than for other products. This is because only three unit operations are used in the production of jet fuel (ADU, VDU, and kerosene hydrotreating unit [KHT]). Diesel produced from bitumen is the most emissions intensive because of the high H₂ requirement in the DHT and the HCD units. The GHG emissions associated with producing transportation fuels are slightly lower in processing HC SCO than DC SCO. This is because of the higher H/C ratio and lower sulfur content of HC SCO compared to DC SCO, which is a result of severe hydrotreating and hydrocracking during the upgrading stage.

4.3. Crude transportation

The model predicts crude transportation GHG emissions of 0.46 gCO₂eq./MJ in pathway 1, 0.38 gCO₂eq./MJ in pathway 2, and 0.32 gCO₂eq./MJ in pathway 3 under the base case assumptions.

The reason GHG emissions are highest in pathway 1 is that diluent is transported for 3000 km along with the bitumen and returns back to the

production facility, while in the SCO pathways, the diluent is transported for only 500 km to the upgrader unit and recycled back to the extraction site. Furthermore, SCOs are lighter and less viscous than dilbit and so require lower pumping energy.

GHG emissions from the transportation of bitumen to the hydroconversion upgrader are lower than to the coker upgrader because a lower volume flow of dilbit is transported to the HCU to produce the same amount SCO by the DCU (Table 1). This is because the HCU produces more SCO by processing the same volume of dilbit in the DCU. As discussed earlier, unlike the DCU, more hydrogen is required by the HCU to convert vacuum residue that would have been discarded as coke.

4.4. The WTC comparative assessment results

Table 3 presents the global WTC GHG emissions of THAI-based transportation fuels. Gasoline, diesel, and jet fuel are the main output products considered. For each product, three alternative energy conversion pathways were analyzed. In each pathway, the combustion stage has the highest share of global GHG emissions, more than 63%. Following combustion is extraction with a contribution of 22%. The refinery and upgrading stages make up 4.8–13.0% of the WTC GHG emissions. The GHG emissions from the transportation of crude and transportation fuel are minimal in all cases.

4.5. Uncertainty analysis

The results discussed thus far are based on default inputs and a number of modelling and parameter assumptions. However, each input has uncertainty associated with its base values and hence a range that needs to be considered when assessing the variation in the results. Sensitivity analysis was performed to identify the key parameters and areas in which GHG emissions can be reduced. Uncertainty analysis was carried out on the sensitive inputs to obtain the most likely ranges of GHG emissions. This section describes the WTC sensitivity and uncertainty analysis.

The tornado plots in Fig. 10 are used to identify the inputs with the largest influence on the output uncertainty. The AOR appears to be the most influential parameter affecting global results in all pathways, as seen in its wide range and its effect on compressor work, reservoir combustion, and the amount of produced fuel gas. The amount of CO₂ in the produced gas is the second most influential parameter.

Tornado plots for diesel and jet fuel production are presented in Figs. S.10–S.15 in the SI. The uncertainty results are shown in Fig. 11 using the 5th and 95th percentiles (P5, P95).

The uncertainty results show WTC GHG emissions for gasoline production in the range of 104.10–121.98, 109.56–127.80, and 108.90–127.85 gCO₂eq./MJ gasoline in pathways 1–3, respectively. Diesel WTC emissions were found to be 110.40–128.02, 109.51–127.34, and 108.04–124.07 gCO₂eq./MJ diesel in these pathways. The production of jet fuel results in WTC GHG emissions of 99.34–106.63, 105.04–122.56, and 104.06–122.56 in pathways 1–3, respectively. The WTC GHG emissions mean for jet fuel is lower than for gasoline or diesel because there are fewer unit operations in the jet fuel refinery, as discussed in 2.3.3.

Since all the error bars overlap, it is difficult to say which pathway is the better option. The bars overlap because of the conservative approach used to define the input distributions and range of variables. The results can be improved with more accurate data from industry. However, the emissions means for gasoline and jet fuel production in pathway 1 are lower than in the other two pathways, largely because neither goes through the GHG emissions-intensive upgrading stage. Furthermore, the gasoline yield is higher from bitumen than SCO. The diesel production WTC GHG emissions mean in pathway 3 is lower than in pathways 1 and 2, mainly because HCU yields more diesel than the DCU and the refining HC SCO yields more diesel than bitumen does.

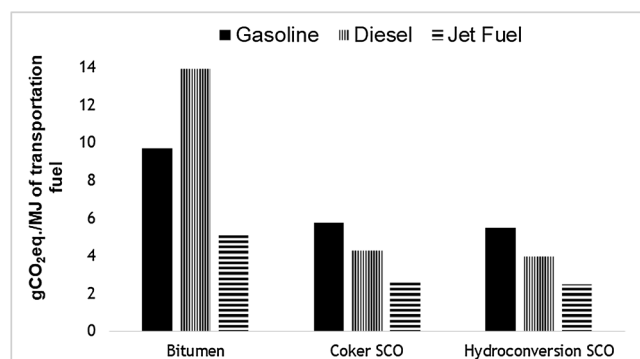


Fig. 9. GHG emissions associated with refining bitumen and SCO.

Table 3
Breakdown of WTC emissions in the production of transportation fuels through different pathways (gCO₂eq./MJ).

Life cycle stages	Gasoline			Diesel			Jet fuel		
	P1	P2	P3	P1	P2	P3	P1	P2	P3
Extraction	29.0	29.5	26.4	28.4	28.9	25.8	28.0	28.5	25.5
Upgrading	0.0	8.4	9.4	0.0	8.2	9.2	0.0	8.1	9.1
Crude- transportation	0.5	0.4	0.3	0.5	0.4	0.3	0.5	0.4	0.3
Refinery	9.6	5.8	5.6	13.9	4.3	4.0	5.1	2.6	2.5
T&D	0.5	0.5	0.5	0.4	0.4	0.4	0.4	0.4	0.4
Combustion	72.7	72.7	72.7	74.9	74.9	74.9	72.8	72.8	72.8
Total	112.3	117.3	114.9	118.2	117.2	114.7	106.8	112.8	110.6

P1: Pathway 1, P2: Pathway 2, P3: Pathway 3.

4.6. Comparison of life cycle GHG emission of THAI with SAGD and surface mining

A comparison of this study’s results and the surface mining and SAGD WTC emissions found in the literature was carried in order to determine which technology has lower GHG emissions. The studies report the range of GHG emissions in surface mining and SAGD to be 86.2–115.6 and 98.1–131.8 gCO₂eq./MJ [81–86]. Our model results for transportation fuel production pathways are within the range of all

reported values for SAGD except TIAX’s [79]. TIAX uses a simple approach to estimate pre-refinery emissions and assumes a medium conversion refinery that is less GHG emission intensive than the deep conversion one.

Although THAI has an emission-intensive extraction stage, the higher quality of the produced bitumen results in lower emissions in the upgrading and refining stages, and so its WTC impact is comparable with SAGD-based transportation fuel.

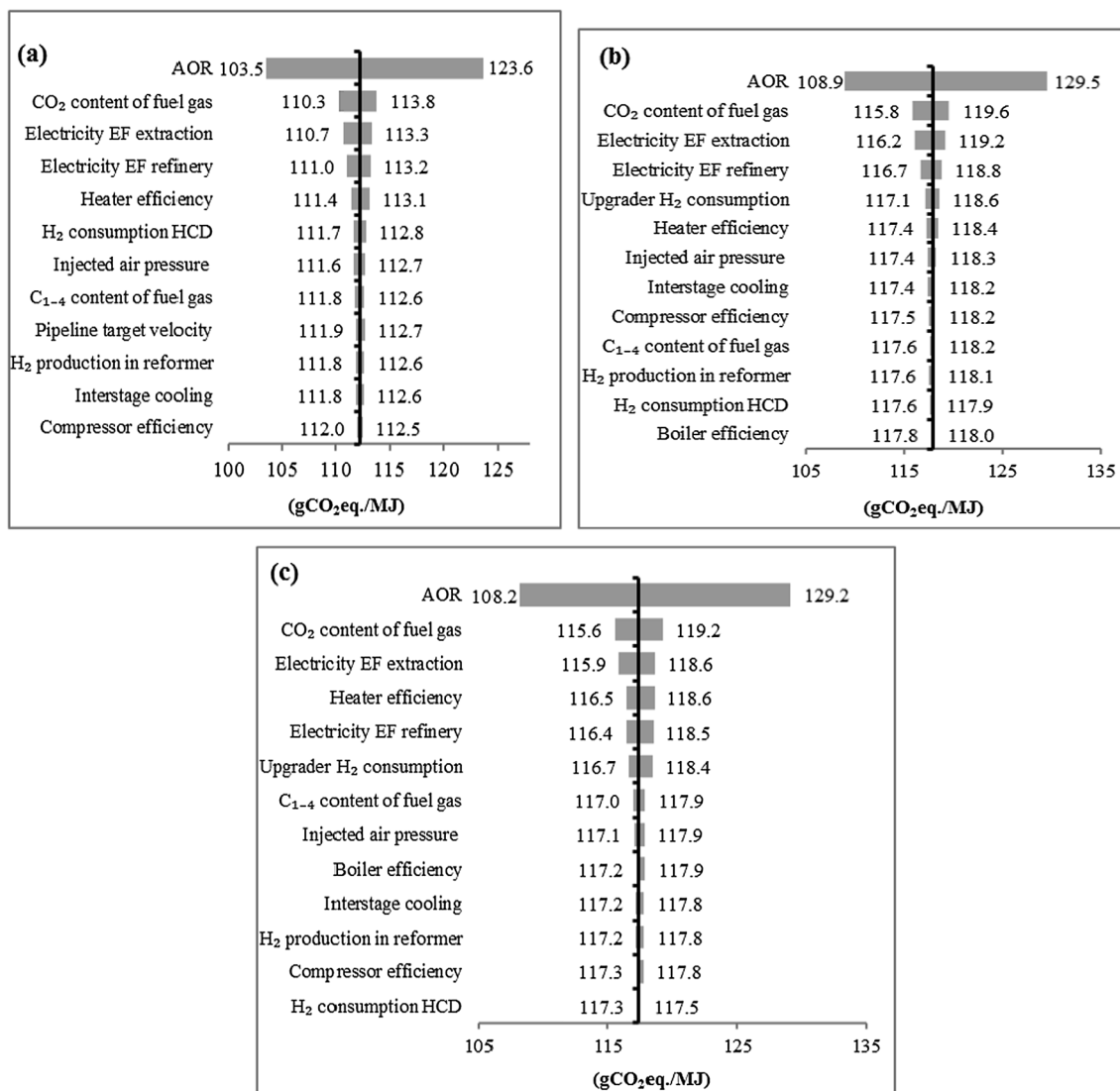


Fig. 10. Tornado plots for the WTC emissions in the production of gasoline in different pathways. (a): Pathway 1; (b): Pathway 2; (c): Pathway 3.

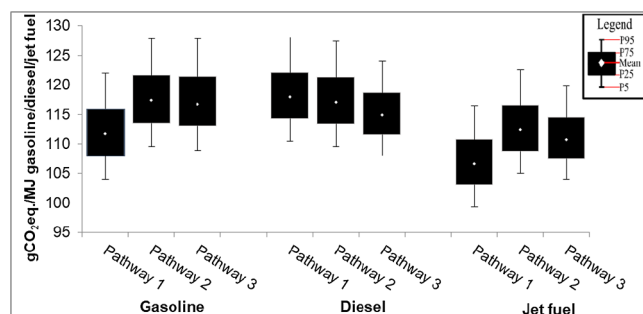


Fig. 11. Uncertainty in WTC GHG emissions in the production of transportation fuels from THAI.

5. Conclusion

This study developed a bottom-up WTC model to evaluate the energy consumption and associated GHG emissions of transportation fuels produced through the THAI extraction method. Different pathways for transportation fuel production were considered to determine the least emission-intensive pathway.

The results indicate that the WTC GHG emissions are in the range of 104–128, 108–128, and 99–123 g CO₂eq./MJ for the production of gasoline, diesel, and jet fuel, respectively. The combustion emissions dominate the well-to-combustion emissions at 63–67%. The extraction stage is the second most emission-intensive stage and constitutes 21–25% of well-to-combustion emissions. The well-to-combustion emission results show that the air-to-oil ratio is the most significant variable affecting the environmental performance of the toe-to-heel-air injection extraction process. Any improvement in the air-to-oil ratio could significantly lower the environmental impact of the recovery method. We compared this study's results with steam assisted gravity drainage well-to-combustion emissions results in the literature and found that the well-to-combustion emissions of SAGD and THAI are within the same range. The uncertainty results provide the most likely ranges of the GHG emissions for each product and alternative pathway considered but also highlight the need to further refine key input parameters to have a better interpretation. The results of this study provide a framework for oil sands producers and policy makers to make more informed decisions for GHG emission reduction strategies for THAI-based bitumen products.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at <https://doi.org/10.1016/j.fuel.2019.115930>.

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