Life Cycle Assessment (LCA) of Oil Sands-Derived Transportation Fuels Produced from the Vapor Solvent-Based Extraction Process

By

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Abstract

Oil sand is a mixture of sand, clay, water, bitumen and other minerals. Production of transportation fuels like gasoline, diesel, jet fuel, etc. from the oil sands reserved in deep underground reservoirs require external stimulant to lower the viscosity of bitumen. The established thermal extraction techniques like steam assisted gravity drainage (SAGD), cyclic steam stimulation (CSS) are energy- and greenhouse gas (GHG) intensive. Among several new technologies to reduce the GHG of transportation fuels produced from oil sands, the solvent extraction process (SEP) is a promising energy-saving technology that uses superheated solvent for bitumen extraction. However, with limited understanding of this technology, more detailed investigation is required to understand its impact on energy consumption and GHG emissions throughout the life cycle of bitumen produced from oil sands. To estimate life cycle (LC) energy consumption and GHG emissions from oil sands-derived transportation fuels, several life cycle assessments (LCAs) have been conducted by different researchers. Most of these studies use deterministic point estimates with insufficient uncertainty analysis. Because of lack of transparency and differences in emissions results reported by previous oil sands projects, it has become important to accurately quantify and provide realistic ranges of project-specific life cycle energy consumption and GHG emissions.

In this study we developed a bottom-up data-intensive model to evaluate the WTW energy consumption and GHG emissions of the oil sands obtained from the SEP. The model was designed based on a production capacity of 25,000 barrels per day (bpd). Three pathways were developed to examine all the operations required to produce transportation fuels from bitumen (extraction and surface processing, upgrading, transportation, refining, and transmission and distribution) along with identifying the key energy and emissions sensitive parameters. In pathway I bitumen is upgraded through delayed coker upgrading before refining, in pathway II bitumen is directly refined without upgrading, and in pathway III bitumen is upgraded through hydroconversion process and then refined. The upgrading and refining processes were simulated. A comprehensive LCA for transportation fuels (gasoline, diesel, and jet fuel) was conducted in which the developed pathways for solvent extracted bitumen were explored. Refinery sub-process level (mass-basis) allocation was used to allocate GHG emissions among the products. Further, conservative statistical distributions for the sensitive inputs were developed from the literature and simulated through Monte Carlo simulations.

GHG emissions from vapor solvent extraction and recovery range from 24.8-29.1 kg CO_2 eq./bbl of bitumen, which represents a wide range of variability in input parameters. The SEP is an electricity-sensitive extraction process (it consumes 48.7% of the total energy required), unlike steam assisted gravity drainage (SAGD), and the solvent-to-oil ratio ($SOR_{solvent}$) is the key parameter affecting GHG emissions. Hydroconversion upgrading is more energy- and GHG-intensive than delayed coker upgrading but yields more synthetic crude oil (SCO). The SCO produced from the upgraders has fewer heavy fractions and a major fraction of the SCO (42-51%) distillates as fuel gas in deep conversion refineries. Since the produced bitumen has inherently low asphaltene and a high API (American Petroleum Institute) gravity, bitumen can be refined without upgrading, the credit of which is attributed to the extraction process. LC GHG emissions range from 92.4-120.0 g-CO_2 eq./MJ of gasoline and 103.6-248.9 g-CO_2 eq./MJ of diesel, respectively, depending on the pathway and uncertainty in well-to-refinery (WTR) GHG emissions (excluding transportation emissions) range from 101.3-143.3, 132.2-169.9, and 82.7-109.3 kg CO_2 eq./bbl of bitumen in pathways I, II and III, respectively.

The results from this study will assist government and industry in strategic decision making on environmental comparisons with traditional bitumen extracting processes and on potential implementation in the oil sands energy industry.

Preface

This thesis is an original work by Mohammad Ikthair Hossain Soiket under the supervision of Dr. Amit Kumar. Chapter 2 of this thesis is a version of paper prepared for submission to a peer-reviewed journal for publication as Soiket, M.I.H., Oni, A.O., and Kumar, A., “The development of a process simulation model for energy consumption and greenhouse gas emissions of a vapor solvent-based oil sands extraction and recovery process”. Chapter 3 of this thesis is a version of paper prepared for submission to a peer-reviewed journal for publication as Soiket, M.I.H., Oni, A.O., and Kumar, A., “Estimation of energy consumption and greenhouse gas emissions of upgrading and refining bitumen produced by solvent extraction process”. Since this thesis is a paper-based thesis, the readers are expected to find some repetitions in text. I was responsible for the concept formulation, data collection, model development and validation, and manuscript composition. A.O. Oni contributed by assisting in model development, reviewing the results, and formatting the manuscripts. A. Kumar was the supervisory author and was involved with concept formation, evaluation, assessment of results, and manuscript composition.

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Above all, I thank you God for making me capable of what I am today. I thank God for the countless opportunities that he has provided me and for always guiding me towards the right direction of my life.

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Abbreviations

ADU	Atmospheric distillation unit
AGO	Atmospheric gas oil
AGR	Acid gas removal
API	American Petroleum Institute
bbl	Barrel
BC	Black carbon
bpd	Barrels per day
cp	Centipoise
CSS	Cyclic steam stimulation
cSt	Centistokes
DCU	Delayed coker unit
DEA	Diethanolamine
DHT	Diesel hydrotreater
ESEIEH	Enhanced Solvent Extraction Incorporating Electromagnetic Heating
FCC	Fluid catalytic converter
FWKO	Free water knock-out
GHG	Greenhouse gas
GOHT	Gas oil hydrotreater
GP	Gas permeation
GWP	Global warming potential
HCU	Hydroconversion unit
HEN	Heat exchanger network
HVGO	Heavy vacuum gas oil
IGF	Induced gas flotation
ISO	International Organization for Standardization
iSOR	Instantaneous solvent-to-oil ratio
KHT	Kerosene hydrotreater
LCA	Life cycle assessment
LCI	Life cycle inventory
LCIA	Life cycle impact assessment
LHV	Lower heating value

LPG	Liquefied petroleum gas
LVGO	Light vacuum gas oil
MER	Maximum energy recovery
NHT	Naphtha hydrotreater
PADD	Petroleum Administration for Defense District
PFS	Plant fuel system
ppm	Parts per million
SAGD	Steam assisted gravity drainage
SBEP	Solvent-based extraction process
SCO	Synthetic crude oil
SEP	Solvent extraction process
SGP	Saturated gas plant
SMR	Steam methane reforming
SOR	Solvent-to-oil ratio
TEG	Triethylene glycol
TTW	Tank-to-wheel
UGP	Unsaturated gas plant
VDU	Vacuum distillation unit
VFF	Venting, flaring, and fugitive
VOCs	Volatile organic compounds
WTT+C	Well-to-tank + Combustion
WTW	Well-to-wheel

Chapter 1

Introduction

1.1 Background

According to the World Energy Outlook, oil consumption will be 103.5 million barrel (mb)/day in 2040, up from 92.5 mb/day in 2015 [1]. With limited conventional crude oil resources, it is difficult to meet this increasing global energy demand. Unconventional oil resources such as the oil sands in western Canada could be a possible solution. The amount of technically recoverable unconventional oil reserves are estimated to be over 2.1 trillion barrels [2]. The oil sands can be found in several locations such as Venezuela, Russia, and the United States. The Athabasca deposit in Alberta has the largest and most developed reserves [3]. In 2012, Alberta produced 1.9 mb/day of raw bitumen, and this figure is expected to increase to 3.8 mb/day by 2022 [4].

Oil sands are a mixture of bitumen, sand, clay, and water. Bitumen is separated from oil sands to produce oil. Bitumen, unlike conventional oil, is so viscous that it acts like cold molasses at room temperature [3]. At 10^oC, bitumen is as hard as a hockey puck and cannot flow or be pumped under natural conditions [4]. Thus heat is required to extract bitumen. Of the 142,000 km^2 oil sands reserve land, only 3% is surface minable [3]. The common established in situ methods to extract bitumen are steam assisted gravity drainage (SAGD) and cyclic steam stimulation (CSS) [4].

Because bitumen is highly viscous (viscosity > 10^5 mPa.s), it is very difficult to refine at natural conditions. Also, few of the refineries in North America have the capability to refine bitumen [5]. For these reasons, bitumen is upgraded to ease transport and refine in refineries. In the upgraders, bitumen viscosity and density are reduced by chemical separation to remove undesirable components [6]. The lighter components produced from the upgraders are blended together to form synthetic crude oil (SCO), a superior quality crude with high API (American Petroleum Institute) and low viscosity. The produced SCO is then sent to the refinery to be converted into transportation fuels like gasoline, diesel, jet fuel, etc. In addition, bitumen properties can be improved by mixing it with naphtha or natural gas condensate. Bitumen mixed with naphtha is called dilbit [4] and can be transported by pipeline. Dilbit can be refined in a refinery. Sometimes bitumen is also mixed with SCO (the mixture is called “synbit”) to meet pipeline specifications. Once synbit is transported to the refinery, it is refined to produce transportation fuels.

In 2014, bitumen production accounted for 81 % of Alberta’s total oil production [7]. Overall raw bitumen production was increased by 10.5 % in 2013. Significant greenhouse gases (GHGs) are emitted through the production and combustion of transportation fuels from bitumen and conventional crudes. According to the Environmental Protection Agency (EPA), 27% of the GHG emissions in the United States in 2015 were from burning fossil fuels for cars, trucks, ships, trains, and planes, and over 90% of these fossil fuels were petroleum-based [8]. In 2014, 165 metric tonnes (Mt) of GHGs (more than 28 % of the GHG emissions in 2015) were produced from Canada’s transportation sector, and it is projected that emissions from the transportation sector will increase to 201 Mt CO_2 eq. by 2020 [9]. Emissions from the production of transportation fuels from bitumen are even higher than those from conventional crudes [10]. It is important to address GHG emissions from oil sands-derived liquid fuels for sustainable oil sands market growth and to meet global energy demand.

As mentioned earlier, heat is required to extraction bitumen from the in situ reservoirs. The thermal extraction methods SAGD and CSS use steam as a source of heat [11, 12]. Considerable energy is required to produce the steam, which makes the thermal extraction methods more energy- and emissions-intensive [13] compared to conventional crude extraction methods. The produced bitumen needs to be upgraded in order to refine it. Upgrading is also an energy- and emissions-intensive process [14]. Because of this, there is always an environmental concern/GHG emissions debate from the oil sands vs. GHG emissions from conventional crudes. This debate has become acute due to the enforcement of strict environmental regulations such as the Low Carbon Fuel Standard (LCFS) and the European Fuel Quality Directive that demanded a 10% reduction in life cycle GHG emissions from transportation fuels [15, 16]. Also, the Alberta government has initiated a Climate Leadership Plan that restricts GHG emissions from oil sands to 100 mega tonnes of CO_2 eq./year [17]. So, in order to comply with these restrictions and to expand oil sands market growth, it is necessary to reduce not only extraction emissions but also the life cycle emissions from oil sands-derived transportation fuels.

To overcome the challenges of reducing GHGs, several new techniques/methods have been implemented by different companies at different scales. In these new methods, steam, solvent, or electrical or electromagnetic heating are used to extract bitumen from the reservoirs. Electromagnetic heating methods like Enhanced Solvent Extraction Incorporating Electromagnetic Heating (ESEIEH) and ET-DSP [18, 19] show promising oil recovery rates and better bitumen properties, but considerable investigation on controlling the heating process is still needed to commercialize these techniques. Some other researchers implemented in situ combustion techniques like the toe-to-heel air injection method (THAI) [20] and combustion assisted gravity drainage (CAGD) [21], in which a portion of oil sands is burned to supply heat. These methods have a high risk because it is very difficult to control the combustion reaction and there is a high possibility of burning the entire reservoir. Potential solvent-based extraction methods are VAPEX (vapor solvent extraction) [18] and N-solv [19]. Solvent extraction methods suffer from poor oil recovery rates that can be improved by superheating the injected solvent [22]. Research conducted by Nenniger and Dunn [23] showed that by superheating the vapor solvent, oil recovery can be increased to several orders of magnitude. The vapor solvent extraction method also results in bitumen with a high API gravity and low asphaltene content [24], which might be possible to refine without upgrading.

In order to determine the total GHG reduction from the solvent extraction process (SEP) and to draw meaningful conclusions, it is important to develop the life cycle energy consumption and emissions of transportation fuels from vapor solvent-extracted bitumen. A life cycle assessment (LCA) is a powerful tool that can be used to determine the direct and indirect environmental impacts from a fuel throughout its entire life cycle [4]. An LCA is comprised of four major components [25]: goal and scope definition, life cycle inventory analysis, life cycle impact assessment, and life cycle interpretation. The goal and scope define the functional unit, assumptions and limitations, system boundary, and allocation methods while setting the context of the study. The next component, the life cycle inventory analysis, quantifies the input and output for each sub-unit operation. The life cycle impact assessment classifies and allocates various inputs based on relative weighting factor. Finally, the interpretation stage verifies and communicates results effectively. So, with an LCA it is possible to estimate life cycle energy consumption and GHG emissions by developing well-to-wheel (WTW) transportation fuel production pathways from solvent-extracted bitumen.

1.2 Literature review and research gap

The available literature examines the WTW emissions from transportation fuels and incorporates both upstream and combustion emissions. The established models can be divided into two types based on the approach followed to calculate life cycle energy consumption and GHG emissions. The first type, such as Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation (GREET) [26] and GHGenius [10], use a top-down approach in which high level aggregate data are used to calculate industry average emissions. The second type, such as TIAX [27], Jacobs [28], Petroleum Refinery Life Cycle Inventory Model (PRELIM) [29], **FUN**damental **EN**gineering **P**rincipl**E**s-based **M**ode**L** for **E**stimation of **G**reen-**H**ouse **G**ases in the **O**il **S**ands (FUNNEL-GHG-OS) [14, 30], and GHOST [31], use a bottom-up approach in which energy consumption and GHG emissions in each sub-unit operation are calculated using fundamental engineering principles. In both types (top-down and bottom-up), the life cycle energy consumption and GHG emissions from bitumen-derived transportation fuels are estimated based on thermal extraction methods like SAGD and CSS. Until now, there is no model available in the literature that estimates life cycle energy consumption and GHG emissions from bitumen-derived transportation fuels based on solvent extraction methods. Moreover, the top-down models present results in an aggregated manner, which makes it difficult to predict the life cycle energy consumption and GHG emissions for specific crudes. The GHG emissions are reported as average GHG emissions, which does not consider the impact of crude quality, and the results are not path-specific. The bottom-up models only examine the sub-unit operations, which are energy- and GHG emissions-intensive, because of lack of data and process complexity [25]. This leads to high modeling errors. Overall, the bottom-up approach is better than the top-down approach because bottom-up models calculate energy consumption and emissions for specific crudes and provide results as detailed as possible.

Another key problem is that all the models provide deterministic point estimates for the WTW life cycle energy consumption and GHG emissions without uncertainty analyses. Some oil sands operators report their annual GHG emissions without sensitivity analyses [32-34]. So the results presented in the models and reports are different because of differences in system boundaries and assumptions. Thus it is necessary to conduct project-specific LCAs to accurately calculate the life cycle energy consumption and GHG emissions from transportation fuels produced from solvent-extracted bitumen. Instead of point estimates, a conservative range of results can be generated by conducting uncertainty analyses on the critical parameters. This will improve model reliability and assist in identifying potential areas of energy and GHG emissions reduction. Different pathways can also be developed to compare and identify the least energy- and GHG emissions-intensive production path.

1.3 Research motivation

The following statements best summarize the factors that motivated this research:

- The current literature reports well-to-wheel (WTW) emissions for thermal extraction processes. It is important to develop project-specific WTW pathways for the vapor solvent extraction process to accurately estimate the life cycle energy consumption and associated GHG emissions of the SEP.
- To determine the overall advantages and disadvantages of the SEP over SAGD and CSS, it is not sufficient to compare extraction methods alone. Project-specific pathways identical to thermal extraction processes should be developed for the SEP to determine the added benefits and drawbacks of the SEP over SAGD and CSS throughout the entire life span of bitumen.
- Since the energy and GHG intensity of transportation fuels production from bitumen is dependent on the production pathway, it is important to quantify the energy consumption and GHG emissions in each pathway to compare the pathways and to answer questions like: “Is it possible to refine partially upgraded bitumen produced from the SEP without upgrading?”
- The new oil sands extraction technologies are still in the development stage. Therefore, it is necessary to understand the solvent extraction process to identify the most energy- and GHG emissions intensive technical parameters before the technology is implemented for commercial scale production.
- Most current LCA models report WTW GHG emissions as deterministic point estimates. These models do not consider variation or changes in operating conditions so they are not reliable. In order to represent the variations or changes in operating conditions fairly, especially those highly sensitive to energy consumption and GHG emissions, uncertainty ranges are required.

- To formulate new environmental policies, it is necessary to quantify GHG emissions from oil sands-derived liquid fuel production and use based on comprehensive science based assessment.

1.4 Research objectives

The overall objective of this research is to develop a WTW GHG emission model for solvent based extraction of bitumen and transportation fuel production from it. The specific objectives are summarized below:

- Develop a simulation model to estimate energy consumption and GHG emissions in each major unit operation (vapor solvent extraction, upgrading, transportation, and refining) in the life cycle of transportation fuels like gasoline, diesel and jet fuel.
- Calculate and compare the overall life cycle GHG emissions in various oil sands pathways including upgrading bitumen to SCO followed by refining with transporting bitumen and refining bitumen without upgrading.
- Identify sensitive technical parameters and develop probability distributions of the parameters using publically available data.
- Determine uncertainty in WTW emissions for gasoline, diesel, and jet fuel produced from solvent-based extraction of bitumen

1.5 Scope and limitations of the thesis

This research evaluates the GHG emissions from oil sands-derived liquid fuel production and combustion for solvent-based extraction methods. To calculate total GHG emissions, only the main greenhouse gases like CO_2, CH_4, and N_2O are taken into consideration. Due to the lack of data, infrastructure emissions from extraction, upgrading, transportation, and refinery units are not included in this research. For refinery mass and energy balance, a generic in-built Aspen HYSYS refinery model is used. The scope and limitations of this study are discussed further in chapters 2 and 3.

1.6 Organization of the thesis

This thesis is paper-based and is written in such a way that each chapter can be read independently. Because of this, assumptions, data, and results are repeated between chapters. There are five chapters and three appendices in this thesis as presented below:

Chapter 2, the development of a process simulation model for energy consumption and greenhouse gas emissions of a vapor solvent-based oil sands extraction and recovery process: This chapter describes the development of the data-intensive process simulation model based on the vapor solvent extraction process. This chapter includes the assumptions, the system boundary and working principles of the SEP, the results obtained from oil sands extraction and recovery operations, and the uncertainty ranges in emissions due to variations in technical parameters.

Chapter 3, estimation of energy consumption and greenhouse gas emissions of upgrading and refining bitumen produced by solvent extraction process: This chapter presents the total energy consumption and GHG emissions in upgrading and refining solvent extracted-bitumen through three bitumen pathways. In two pathways, delayed coker and hydroconversion upgrading, models are developed for the conversion of bitumen to SCO. The later part of this chapter investigates refining oil sands products such as bitumen and SCO using a refinery process model. Uncertainty in emissions due to upgrading and refining operations is also included in this chapter.

Chapter 4, A life cycle assessment of oil sands-derived liquid fuel production based on the solvent extraction process (SEP): This chapter combines the results of the extraction, upgrading, and refinery operations detailed in chapter 2 and 3 into the WTW life cycle emissions of transportation fuels produced from solvent-extracted bitumen. The energy consumption and GHG emissions from the transportation of feedstock from the extraction or upgrading unit into the refinery are also reported in this chapter.

Chapter 5, Conclusions and Recommendations for Future Work: This last chapter concludes the key findings of the research. The last subsection discusses the recommendations for future work.

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Chapter 2

The development of a process simulation model for energy consumption and greenhouse gas emissions of a vapor solvent-based oil sands extraction and recovery process[1]

1. Introduction

With increasing growth in global energy demand in recent decades, rapid depletion of limited conventional oil resources is a concern. The quest to meet demand has shifted toward unconventional oil sources such as heavy oil and bitumen. Bitumen is a highly viscous oil with an American Petroleum Institute (API) gravity of less than 10 and a viscosity higher than 10^5 millipascal seconds (mPas) at standard conditions (15°C) [1]. Bitumen is too heavy to flow or be pumped [2] and thus needs to be heated or diluted. For this reason, it is more energy intensive to extract and process bitumen into final products than conventional oil resources [3].

Currently bitumen is extracted from the oil sands either by surface mining or thermal extraction (beneath the ground) [4]. Surface mining involves excavating deposits within a 0.4-1.4 stripping ratio (the ratio of the overburden thickness to oil sands ore thickness) with a typical ore thickness of 90 m [5]. However, only 12% of Alberta's deposits lie at a depth of 75 m or less, where surface mining is possible, and the rest lies at a depth of 75-750 m [6], where thermal processes are used.

The most commonly used in situ thermal extraction processes are cyclic steam simulation (CSS) and steam assisted gravity drainage (SAGD) [7]. In CSS, a single well is used for steam injection and oil production [5], while SAGD uses two horizontal wells, one is located slightly above than the other [5]. Steam is injected through the injection (upper) well, which heats the bitumen through condensation. The diluted bitumen, along with the condensed water, flows to the production (lower) well by gravity and is pumped to the surface for further processing [4].

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[1] The results of this chapter is prepared for submission as Soiket, M.I.H., Oni, A.O., Kumar, A., "The development of a process simulation model for energy consumption and greenhouse gas emissions of a vapor solvent-based oil sands extraction and recovery process" in a peer-reviewed journal.

Thermal extraction processes such as SAGD, CSS, and in situ combustion inject fluids like steam or air into the reservoir, which acts as a heating source, to change the properties of the bitumen [6] to make it flow. These processes are complicated and require large tailing ponds to dispose the injected fluid [6].

Another challenge for these thermal processes is the confinement chamber [8], where considerable heat is lost. Moreover, blow backing steam from the new reservoirs into the old depleted chambers might increase the steam-to-oil ratio (SOR_{steam}) and might eventually sterilize a considerable amount of bitumen [8] Thermal in situ processes are highly water- and energy-intensive and emit considerable GHGs [9]. The emissions from the CSS and SAGD processes range from 80-120 kg/barrel (bbl) and 65-115 kg/bbl of bitumen, respectively [9].

Environmental regulations such as the Paris Agreement [10], Kyoto Protocol [11], the Pan-Canadian Agreement on Climate Change [12], the California Environmental Protection Agency [13], and the European Commission's Climate Action [14] demand significant reduction in life cycle GHG emissions from transportation fuels. Through the Climate Leadership Plan in Alberta, the government legislated the maximum emissions from oil sands to be 100 mega tonnes of CO_2 eq./year [15]. The legislation also demands a 45% reduction in current methane gas emissions from oil and gas operations and implemented a carbon price of $20/tonne starting in 2017 [15]. These regulations demand the development of new technologies to increase recovery and reduce the carbon footprint of oil sands-derived fuel.

Life cycle assessment (LCA) is a tool to trace the environmental footprint of a product from cradle to grave. It allows quantification and assessment of GHG emissions. LCA models should be developed to understand the full impact of new technologies [14] and to make environmental comparisons with current thermal extraction processes.

The use of a vapor solvent instead of steam promises to be much more effective [16-18], but the solvent-alone process suffers from poor rates of recovery [17, 18] because molecular diffusion is less effective than thermal diffusion [19]. However, solvent-based processes have less heat loss and less environmental impact, and there is a possibility for downhole upgrading [19]. Solvents are more effective in removing methane than hot water, and methane is an effective heat and mass transfer poison for solvents [19]. Thus solvents provide better controlling opportunities and limit blowback into the old depleted reservoirs [8]. The poor extraction rate with solvents can be overcome by injecting heated vapor solvent at modest extraction temperatures (40^{o}-50^{o}C) [8]. The solvent penetration rate in diluted bitumen is higher in magnitude than in raw bitumen [20].

The hot vapor solvent extraction is a new process that was invented based on the concept of solvent diffusion into diluted bitumen [21]. This process has a wellbore configuration similar to SAGD. In this process, solvents like propane, butane or pentene [26] is injected through the injection well. The solvent remains a vapor and condenses on the extraction surface [21]. Solvent selection in this process is very important because bitumen will be diluted using the solvent's latent heat of condensation [8]. The most preferred solvent is propane [21] because it is less expensive than bitumen and can deliver heat at temperatures like 40^{o}C [22]. Condensed solvent diffuses with diluted bitumen and is pumped to the surface. Solvent is then separated from the bitumen and purified. The purified solvent will be heated, compressed, and re-injected into the reservoir [21] to start the next cycle.

Researchers have developed LCA models [23-28] to calculate overall energy consumption and GHG emissions predominantly for the SAGD process. However, research on vapor solvent-based extraction processes is limited. The BEST (Bitumen Extraction Solvent Technology) pilot plant demonstrated a similar extraction technology [29] at field scale and reported that at the present rate of technology adaption, the solvent extraction process will produce 85% fewer GHGs than SAGD. Rezaei et al. [30] examined the production rate of vapor solvent extraction (VAPEX) by superheating the injected solvent. It was found that by superheating the solvent, it is possible to increase the oil production rate and reduce the $SOR_{solvent}$. Another study conducted earlier [31] investigated the mass transfer of solvent inside bitumen during solvent extraction. This study found a higher oil recovery rate in the vapor solvent extraction process than in VAPEX because of increased convective mixing and increased rate of interface advancement. But until now, no research has been conducted to estimate energy consumption and to track the GHG footprint from the solvent extraction process. LCA models developed by the Argonne National Laboratory (GREET) [28], Natural Resources Canada [27], Jacobs Consultancy [25], and TIAX LLC [26] are limited to surface mining and SAGD. Those models are inadequate to depict the solvent extraction process, and it is not possible to estimate energy consumption and emissions from solvent extraction with these models. So it is important to develop a specific energy consumption and GHG emissions model for the recovery and extraction of solvent-based oil sands production. This research is an effort to address this gap.

The objective of this research is to develop a data-intensive solvent-based oil sands extraction model to estimate extraction energy consumption and life cycle GHG emissions of the extraction and recovery process. The specific objectives are to:

- Develop a solvent extraction process (SEP) model defining well configuration, reservoir conditions, and associated surface facilities to separate and purify the solvent from the emulsion.
- Evaluate and compare the overall energy consumption and GHG emissions of SEP with SAGD.
- Determine the SEP emissions uncertainty by performing a Monte Carlo simulation using a range of realistic data as input.

2. Methods

2.1 Plant layout overview and system boundary

Two well configuration similar to SAGD [32] was considered for the extraction process. Figure 1 shows all the unit operations for recovery and surface processing of bitumen. The production capacity of the plant is considered to be 25,000 bpd and the system boundary has been defined as follows: the boundary starting point is the production of bitumen from the production well and the termination point is the transportation of dilbit to the next unit. Separated water is stored and then disposed of. Vapor solvent is injected via the injection well into the reservoir. The solvent reduces the viscosity of bitumen through heating and diffusion. The bitumen-solvent emulsion drains to the bottom production well by gravity. The emulsion is pumped to the surface and there the solvent is separated from the bitumen. The separated solvent is purified and heated again to be converted into hot vapor solvent. The bitumen is then mixed with diluent and transferred to the next unit for further processing. The blue lines in Figure 1 indicate two options: bitumen can either be mixed with diluent as dilbit or be directly transferred to an upgrader or a refinery. Due to solvent hold-up in the extraction and recovery process, additional solvent will come from the make-up solvent unit. Solvent in the make-up solvent unit and diluent in the diluent storage tank come from a supplier outside the boundary.

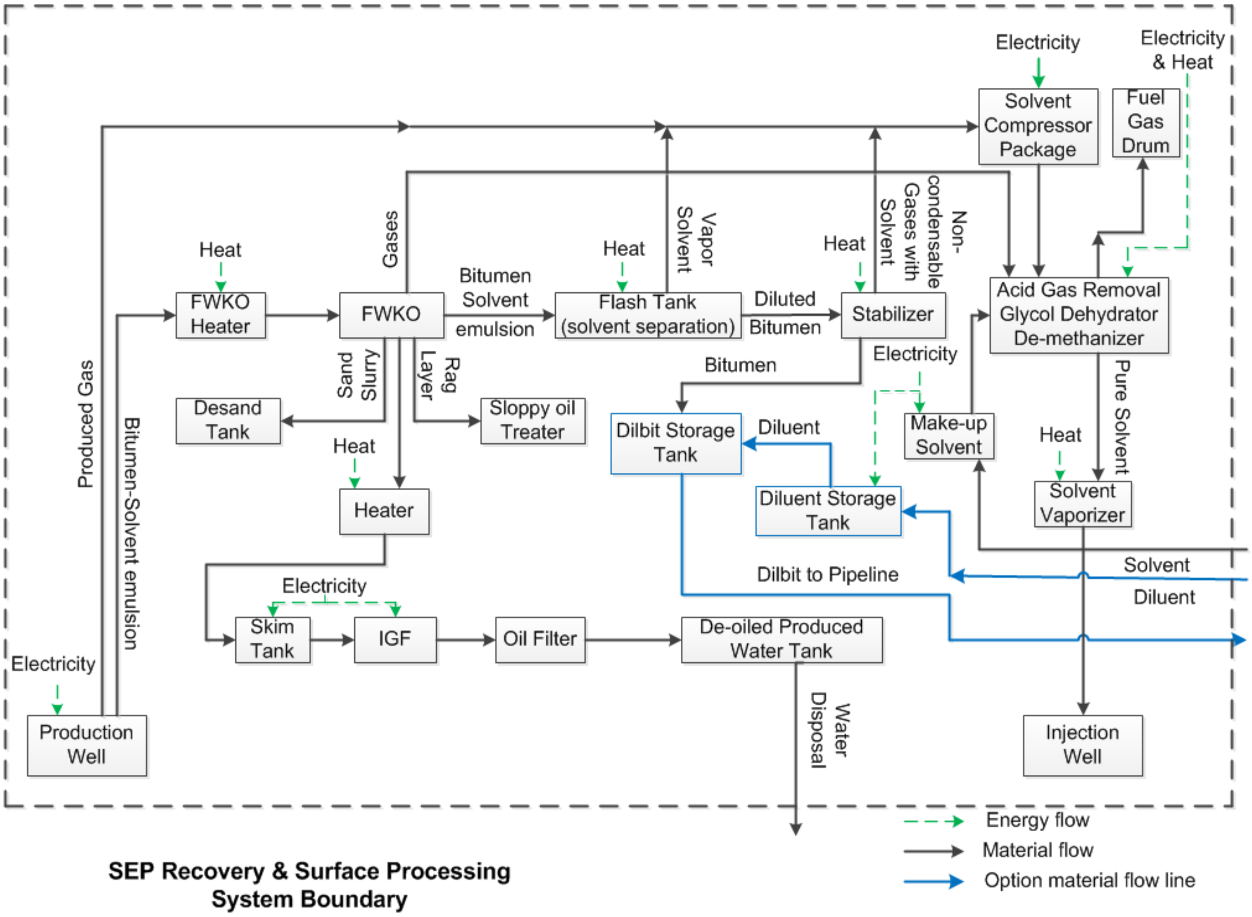


Figure 1 - Unit operations and system boundary of the solvent extraction and recovery process. Heat is provided by natural gas (either by producing steam or burning).

The functional unit for an LCA of oil sands-derived fuels is considered in terms of kg of CO_2-equivalent gas emitted per bbl of bitumen extracted (kg CO_2 eq./bbl). The lower heating value (LHV) of bitumen and fuels is considered to calculate energy consumption and GHG emissions. The simulation model uses default parameters with the provision to input user data. The emissions calculated for sub-unit operations include (i) combustion emissions due to burning produced fuel gas on site and (ii) upstream and combustion emissions associated with transferring and burning natural gas in order to provide required heating for extraction and surface processing. In this model it is assumed that all the electricity will be supplied from the Alberta grid. The paper also includes fugitive emissions from leakage and the irregular release of gases as well as venting and flaring emissions but does not include emissions due to land use. Land-use emissions for in-situ production are less than 0.4 CO_2/MJ of product [33].

2.2 Mass and energy analysis

The following basic assumptions were made in developing the model equations:

1. The system is in a steady state flow condition
2. Change in mol% is equivalent to change in vol%
3. The temperature and pressure at the reference state are T_o = 25 °C and P_o = 101 kPa, respectively.

The simulation model developed in this study is based on mass and energy balance equations. The simplified fundamental mass and energy equations are, respectively [30]:

$$\sum \dot{m}_i = \sum \dot{m}_e \tag{1}$$

$$\sum \dot{E}_i + \dot{Q}_{cv} = \sum \dot{E}_e + \dot{W}_{cv} \tag{2}$$

The efficiency of the equipment is defined as the ratio of total output energy to the input energy supplied.

$$\eta = \frac{E_e}{E_i} \tag{3}$$

here $\dot{m}_e, \dot{E}_e$ and $\dot{m}_i, \dot{E}_i$ are output and input mass flow rate and energy, respectively. $\dot{Q}_{cv}$ and $\dot{W}_{cv}$ are the input heat flow rate and external work rate respectively for a control volume.

Using the equations above, we calculated the energy loss in each unit operation. To calculate the amount of heat generated from the produced gas and the additional amount of natural gas required to meet the total heat (steam and heat) requirement, we used the following equations:

$$\textit{Heat generated by produced gas (kJ/bbl)} = \sum_{i=1}^{n} \frac{(LHV)_i * m_i}{\eta_f} \tag{4}$$

$$\textit{Natural gas required (kg/bbl)} = \frac{Heating\ required\ from\ natural\ gas\ (\frac{kJ}{bbl})}{\eta_b * natural\ gas\ LHV\ (\frac{kJ}{kg})} \tag{5}$$

where *i* refers to individual gas component, *LHV* = lower heating value (kJ/kg), m_i = mass flow rate of produced gas (kg/bbl) and η_f and η_b are the furnace and boiler efficiency, respectively. Equation (5) was used to calculate both heat and steam production from natural gas as $\eta_f = \eta_b$ = 80% [31]. Steam quality was assumed to be 100% in this study [32].

Equations (6) and (7) were used to calculate the electricity consumed in the pump and compressor, respectively.

$$\text{Pump work (W)} = \frac{m(kg/s).g(m/s^2).h(m)}{\eta_p} \tag{6}$$

$$\text{Compressor work (W)} = \frac{Q(m^3/s).\Delta P(Pa)}{\eta_c} \tag{7}$$

Here, *m* is the total mass of the bitumen-solvent emulsion, *h* is the height of the reservoir from bottom to surface, *Q* is the total gas feed in the compressor, *ΔP* is the compressor pressure difference between input and output, and η_p (90%) [33] and η_c (75%) [34] are the pump and compressor efficiency, respectively.

2.2 Estimation of life cycle emissions

Energy consumption is calculated using fundamental engineering principles. The emissions from the process were evaluated using the emission factors from literature [28]. For natural gas, GHG emission factors include both upstream [5] and combustion emissions. For produced gas, only combustion GHG emissions are taken into consideration as those gases are produced on site. All the electricity required in the plant is assumed to be supplied from the Alberta grid, which is one of the largest hydrocarbon base in North America and where most of the oil sands in Canada are located. Electricity production in Canada is moving towards natural gas-based production due to the phasing out of coal, but there are still some operational coal-fired power plants. So upstream emissions for electricity production were calculated based on a mixture of coal and natural gas supply (70% coal and 30% natural gas), which is in good agreement with literature [28, 38]. Combustion emissions related to electricity production were also taken from the NIR [38]. In this research, it was assumed that GHG emissions consist of only CO_2, CH_4, and N_2O gases. Venting emissions were calculated using the global warming potential (GWP) of these gases, collected from the Intergovernmental Panel on Climate Change (IPCC) Fifth

Assessment Report [39]. Flaring and fugitive emissions were also estimated from the GHG emissions data provided by the NIR for oil sands mining, extraction, and upgrading [38]. All the emissions factor values are provided in the Supporting Information (Appendix A) section of this paper.

2.4 Bitumen production from the SEP process – an overview of unit operations

2.4.1. Injection

This unit involves the injection of vapor solvent through the injection well. The distance between the injection and production wells is considered to be 5 m [5]. Propane is purified by surface processing units (99 mol%) and injected as a vapor solvent at 70°C at a pressure of 1800 kPa [21]. The reservoir temperature and pressure are assumed to be 8°C [21] and 200 psi [22], respectively. All of the non-condensable gases are maintained at 1 mol% in the injected solvent. Solvent purification is an energy-intensive process [40] and, considering the reservoir conditions, injected solvent can bear approximately 6-7 mol% of non-condensable gases without causing solvent poisoning [21]. The reservoir wells are 300 m in length with a pay zone (the zone where much of the oil is found) of 15 m [41]. The injection well is 148 m below the surface [41]. All the assumptions considered for reservoir conditions are presented in Table 1.

Table 1 - Key assumptions in reservoir conditions

Parameter	Values	Comments	Sources
Reservoir temperature	8°C	-	[20]
Reservoir pressure	200 psi	Shallow reservoir	[21]
Reservoir length	300 m	-	[40]
Depth of injection well	148 m	-	[40]
Pay zone	15 m	-	[40]
Porosity	35 (%)	-	[40]
Permeability	5 Darcy	-	[40]

2.4.2. Bitumen extraction

The heated vapor solvent is injected through the injection well at a higher pressure than the reservoir pressure. The injected solvent provides heat to dilute bitumen. The initial hot solvent accumulates at the top of the injection well but after releasing heat, the solvent falls because of the increase in density, and new injected solvent fills the empty space at the top, creating a solvent chamber at the bitumen interface. It is assumed that the chamber pressure is 1500 kPa

[21]. The solvent-bitumen interface temperature is considered to be 45°C (the bubble point of solvent) [42]. The solvent heats the bitumen to the bubble point. The condensed solvent diffuses with the diluted bitumen. The diffusivity of the solvent in the diluted bitumen is significantly higher than solvent diffusing in raw bitumen [8] and thus recovers a large portion of bitumen and leaves behind a significant amount of asphaltene in the reservoir [43]. Solvent-to-oil ratio ($SOR_{solvent}$) of the extraction process is assumed to be 4 [41]. All the key extraction assumptions are presented in Table 2.

Table 2 - Key assumptions for bitumen extraction

Parameter	Values	Comments	Sources
Solvent-to-oil ratio (SOR)	4	-	[40]
Solvent bubble point	45°C	-	[41]
Solvent chamber pressure	1700 kPa	-	[20]
Solvent hold-up in the reservoir	20 (%)	-	[40]
Solvent composition	99 (mol%) propane and 1 (mol%) non-condensable gas	-	[20]
Produced gases	1-12 m^3/m^3 of bitumen	-	[43]
Produced water	1.75 (wt%) of bitumen	-	[44]
Solvent chamber pressure	1500 kPa	-	[20]

Through heating and diffusion, bitumen viscosity is lowered, and the solvent-bitumen emulsion goes into the production well by gravity drainage. Because of the solvent's high diffusivity and high asphaltene precipitation, the produced bitumen coming up from the production well is partially upgraded (14° API), unlike SAGD bitumen [43]. The bitumen-solvent emulsion drains at the solvent chamber pressure and is extracted to the top at 650 kPa by mechanical lift. The extraction pressure is selected based on the propane saturation curve [44]. The emulsion needs to be extracted at a moderate pressure in order to maintain its stability. The properties of bitumen before and after extraction are provided in Table 3.

Table 3 - Key assumptions in bitumen properties

	Initial		Final	
Parameter	Values	Comments/Sources	Values	Comments/Sources

Table 3 - Key assumptions in bitumen properties

API gravity	8°	[5]	14°	[42]
Viscosity (cp)	7x10^6	[37]	10	[14]
Density (kg/m^3)	1020	[41]	958.1	As the produced bitumen will have very low asphaltene content, it will behave like crude oil [46]
Asphaltene (wt%)	12.7	[44]	3	[42]
Metals (ppm):				
Ni	137.5	[1]	30	[42]
V	68.5	[1]	77	[42]
Fe	77	[1]	5	[42]
Bitumen lower heating value (LHV) (GJ/bbl)			6.48	[43]
Emulsion pressure at production well top (kPa)			650	Assumed to maintain the stability of the emulsion [45]

2.4.3. Solvent separation

The first step after extraction is to separate the solvent from the emulsion. The solvent is separated in three stages. First, the emulsion is heated to about 40°C and sent to a free water knock-out (FWKO) vessel. A FWKO is a pressurized closed vessel [48] used because it is a simple process and reduces electricity consumption [48]. The FWKO is operated at 200 psi [49], and it is assumed that more than 99 (wt%) of produced water is separated from the emulsion [50]. Moreover, due to the FWKO's operating conditions, the lighter fraction of the solvent (considered to be 10 wt% of the total solvent) is vaporized and separated as distillate from the top of the FWKO along with the produced gases. Water separated from the FWKO goes to the water de-oiling unit. It is assumed that the amount of sloppy water is negligible. Water from the FWKO bottom is heated before entering the de-oiling unit and then sent to a skim tank where suspended matter is separated by skimming. After further treatment in the induced gas flotation (IGF) unit [51] and the oil filter, the de-oiled water is trucked off site for disposal. Meanwhile, the solvent-bitumen emulsion, following water and solvent separation, is sent to the flash system. The flash system is a distillation column maintained at 64°C [52] with top and bottom pressures of 440 [23] and 435 [53] psi, respectively. Because of the temperature of the column, another 10 wt% of the solvent is separated from the tank top at high pressure. The bottom products from the flash system go to the stabilizer. Heat is provided in the stabilizer that causes the rest of the solvent, along with less condensable gases like methane, nitrogen, ethane, etc., to come out. Solvent-separated bitumen is sent to the dilbit storage tank after being cooled to 50°C [54]. In the dilbit storage tank, bitumen is mixed with diluent (naphtha or natural gas condensate) in appropriate proportions and converted to dilbit, which is supplied to the upgrading or refining unit. The key operating parameters for solvent separation are provided in Table 4.

Table 4 - Key assumptions in the solvent separation

Parameter	Values	Comments	Sources
FWKO vessel pressure (psi)	200	-	[48]
FWKO vessel temperature (°C)	40	Temperature is selected based on the propane saturation curve	[45]
Confined water (wt%)	3.5	-	[1]
Flash column pressure drop (psi)	5	-	
Flash column temperature (°C)	64	-	[51]
Stabilizer pressure (psi)	652.7	-	[54]
Stabilizer temperature (°C)	110	-	[48]
Thermal efficiency (%)	90	It is assumed that the FWKO heater, flash column and stabilizer have the same thermal efficiency	[55]
Solvent separation (wt%)	10 (FWKO) 10 (Flash Column) 80 (Stabilizer)	Solvent separation is determined based on the propane saturation curve	[45]

2.4.4. Solvent compression and purification

Gases are produced in the production well during bitumen extraction. Given that the solvent-based process is a new process with limited publicly available data, a wide range for produced gas is considered in this research [47]. Produced gases, along with separated solvent vapor, are compressed in a solvent compressor to 870 psi [35] because of the high pressure requirement in the demethanizer package. There is substantial solvent loss (solvent hold-up) from in situ operations and surface processing. In order to maintain a constant solvent flow rate, additional solvent is supplied from a make-up solvent unit. Solvent, along with gases, is sent to the demethanizer package. The demethanizer package consists of an acid gas removal unit, a glycol dehydrator, and a demethanizer. In this research, the amine process is considered for acid gas removal [35]. Diethanolamine (DEA) is used and regenerated to remove the sulfur and CO_2 contained in the upcoming feed. The K value for a conventional DEA load is 1.45 [57]. After acid gas removal, all gases are sent to the dehydration unit for water removal. Triethylene glycol (TEG) is used in the glycol dehydrator as a desiccant [35]. Equations from the literature were used to calculate energy consumption [35]. The removal of methane from solvent is important because if the amount of methane exceeds a certain limit (> 5 mol%) [21], it will cause solvent poisoning [21]. For this reason, external refrigeration is provided in the demethanizer to condense 100% of the solvent [35] and permit only 1.0 mol % methane in the solvent. The condensed solvent leaves the demethanizer bottom at about 290 psi [58] and then is converted into vapor solvent after further pressure drop. Finally, the solvent is heated in a solvent vaporizer and re-injected into the reservoir. As the amount of less-condensable gases is already low, it is assumed that re-compression work will be supplied by the turbo-expander [57]. The OPGEE model [35] was used to calculate demethanizer energy consumption. The refrigeration system and compressor consume the most energy in the demethanizer [35]. The reboiler at the bottom of the fractionating column also consumes energy by providing heat in the fractionating column [35]. Reboiler efficiency values are shown in Table 5 along with other key operating parameters.

Table 5 - Key assumptions for solvent compression and purification

Parameter	Values	Comments	Sources
Produced gas (m^3/m^3 of bitumen)	1-12	Produced gas will fit in the wide SAGD-produced gas range	[43]
K value of DEA	1.45	-	[56]

Table 5 - Key assumptions for solvent compression and purification			
Reboiler efficiency (%)	80	-	[31]
TEG concentration (wt%)	99	-	[31]
Water removal rate (gal of TEG/lb of H_2O)	2	-	[31]
Gas pressure at compressor outlet (psi)	870.23	-	[57]
Demethanizer pressure (psi)	435.11	-	[56]
Condensed propane pressure (psi)	290	-	[57]
Condensed propane temperature (^oC)	46.11	-	[58]

The critical parameters leading to high heat and electricity consumption were identified from the calculations. Variations in the efficiency of most energy-consuming equipment can result in significantly higher or lower energy consumption. A sensitivity analysis was performed on the energy-sensitive parameters and equipment efficiency. The parameter values were varied within ±30 in keeping with a previous study [5] to identify the most energy-sensitive parameters and equipment. An uncertainty analysis incorporating the most energy-sensitive parameters and equipment was also conducted to determine the feasibility of implementing the modeled simulation. The detailed sensitivity and uncertainty analyses, along with the results, are discussed below.

3. Results and discussion

3.1. Energy and emissions in the unit operations

Energy is consumed in the form of heat, steam, and electricity in bitumen extraction and recovery. Through pumping, bitumen-solvent emulsion is lifted from the reservoir bottom to the top. Natural gas is burned to provide heat in the FWKO heater, flash tank, and stabilizer. Water separated in the FWKO, is heated and then transferred to the water de-oiling unit. Electricity is consumed by the mechanical contractors that agitate the gas bubbles used in induced flotation [60]. The solvents, along with the produced gases, are compressed in the compressor. The compressor energy is calculated using equation (7). The highly compressed gases are then fed into the acid gas removal (AGR) unit to remove all the CO_2 and H_2S. In the AGR unit, electricity is consumed by the booster, reflux, and circulation pumps to remove acid gases and regenerate the amine solution. The amine reboiler is a direct-fired heater that consumes natural gas to provide heating [35]. The aerial cooler needs electricity to cool the amine solution. The sweet gases from the AGR unit go to the glycol dehydrator where all the water contained in the gases is removed. This dehydration is necessary to prevent a reduction in the heating value and solid hydrate formation [35]. In the dehydrator, the reboiler provides heating to regenerate the TEG desiccant. The reboiler consumes natural gas to generate steam. Electricity is consumed by the glycol pump to circulate TEG. In the demethanizer, the propane is condensed by external refrigeration that consumes a significant amount of electricity. The gases separated from the demethanizer are sent to a fuel drum. The produced gases are burned to supplement the heat requirement.

All the equations used to calculate the total energy requirement in the demethanizer package are provided in the Supporting Information. Table 6 shows the overall energy consumption and GHG emissions from each unit operation. The range of values is included because we considered ranges for some input parameters rather than point estimates. The default energy and GHG emissions values correspond to the mean value of the input parameters. The range of output values provides a more conservative estimate of real life implementation compared to a point estimate.

Table 6 - Fuel consumption and GHG emissions in the SEP

	Fuel consumption			Emissions (kg CO_2 eq./bbl of bitumen)		
	Unit	Range	Default[a]	Type	Range	Default[a]
Natural gas	(kg/bbl)	1.5-2.2	2.0	Indirect	4.4-6.5	5.2
	(MJ/bbl)	60.5[b]-89.9	82.1			
Produced gas	(MJ/bbl)	1.5-37.0	19.3	Direct	0.1-2.4	1.2
Electricity	(kWh/bbl)	19.7-19.9	19.7	Indirect	17.4-17.6	17.5
	(MJ/bbl)	70.9-71.6		Venting	0.4-4.3	2.4
				Flaring	-	0.1
				Fugitive	-	0.3

[a] The default is considered the mean value

[b] The natural gas lower heating value (LHV) is considered to be 40700 kJ/kg [24]

The total energy required to extract and recover 1 bbl of bitumen is 132.9-198.5 MJ. The total energy required in the SEP is lower than in the thermal extraction methods (622.1-1003.1 MJ/bbl of bitumen for a SOR_{steam} of around 2.5) reported in the literature [23, 25-28, 61]. In thermal extraction, a huge amount of steam is required to provide heating to dilute and extract bitumen. A significant amount of heat is also lost during extraction because of high operating pressure [8, 21]. On the other hand, the SEP operates at relatively lower pressure and temperature than SAGD [21]. No steam is required in this process, and propane is more effective for removing bitumen's heavy and light components from the reservoir than steam [8]. Due to blowback [8] from previously depleted SAGD chambers, a high amount of steam might go in other directions without coming in contact with bitumen, which will increase the SOR_{steam} tremendously. The blowback problem in SAGD operations can also be eliminated with solvents by controlling the amount of methane in the reservoir. So the SEP not only reduces energy consumption but also provides a better opportunity to control the extraction process.

Table 6 shows that about 39.2-43.5% of the total energy used are through electricity consumption. The amount of electricity consumed in the SEP is higher (approximately 48-144%) than in the thermal extraction processes [5, 25, 26]. Electricity consumption reported in earlier studies [25, 26] varies because of the varying SOR_{steam}, extraction, and surface technologies used to extract and recover bitumen. Still, electricity consumption in the SEP is significantly higher. The reason is the external refrigeration that is required to condense the higher amount of C_2+ compounds in the demethanizer feed, as shown in Fig 2. In the turbo-expansion process, the higher the heavier compounds in the incoming feed, the higher the amount of external refrigeration required [62] to condense the heavier compounds. The feed to the demethanizer can be passed through a membrane-based gas separation process [63, 64] to reduce the amount of C_2+ compounds in the demethanizer feed. Membranes can be used to separate gases without changing the phase by gas permeation (GP). The driving force for membrane separation can be pressure, concentration, temperature, or electrical potential [61]. The distinguishing feature of membrane separation is the additional membrane phase, which improves separation efficiency [61] and reduces energy consumption from separation [59]. The power required for mechanical lifting of bitumen emulsion, running different pumps and coolers in extraction, and surface processing is included in "other auxiliaries."

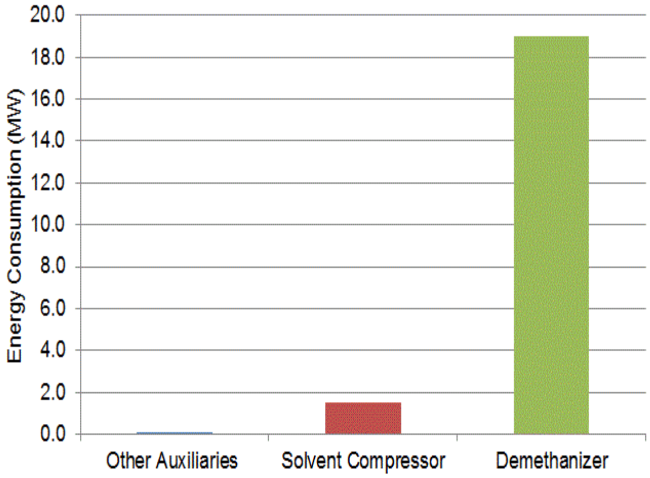


Figure 2-Electricity distribution in extraction and surface processing operations.

Heat energy consumption in different units is shown in Figure 3. The stabilizer consumes the highest amount of heat energy. The majority of non-condensable gases are separated by the heat provided in the stabilizer column. Because of the relatively high operating temperature of the stabilizer, the pressure of the separated solvent increases accordingly. This reduces the work of the compressor. The solvent vaporizer consumes 27.3% of the overall heat energy. The solvent vaporizer is required to boil the condensed bottom product in the demethanizer unit. This is because a large amount of condensed solvent must be superheated before it is re-injected into the reservoir.

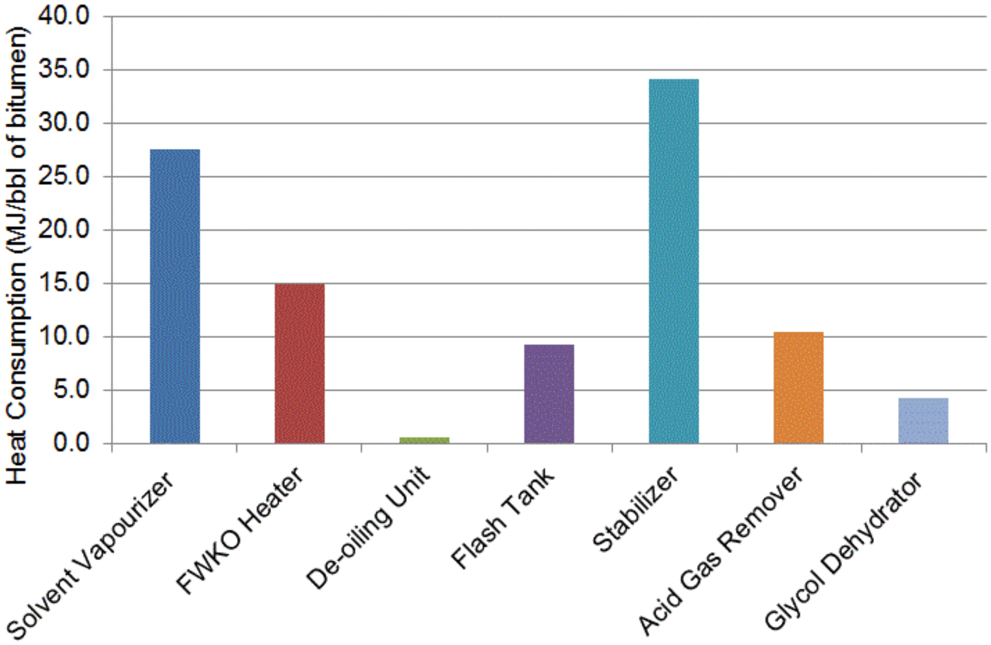


Figure 3-Heat energy distribution in extraction and surface processing units.

Another major heat consumer is the FWKO heater. The FWKO heater increases the temperature of the produced emulsion to ensure that a considerable amount of water is separated in the FWKO drum. In the FWKO drum, the lighter emulsion fractions stay on the top layer and the water-sand slurry remains at the bottom due to the density difference. The volatile fraction (considered to be 10%) of the solvent comes out from the FWKO top. The water-sand slurry is ejected from the FWKO bottom. After the sand has been filtered, almost all the water goes to the de-oiling unit. The amine reboiler in the AGR unit consumes natural gas to provide heating. Heating breaks up the chemical bonds between amine and acid gas [35].

Figure 4 compares GHG emissions results from the SEP with SAGD data found in the literature and other models. The GHG emissions from the SEP are lower than from all SAGD models considering both “no cogeneration” [5, 9, 25-28, 61] and “with cogeneration” [5, 9, 25-28, 61]. GHG emissions from the SEP are significantly lower than from SAGD results reported elsewhere in the literature. The credit goes to the lower energy consumption in the SEP, which reduces emissions. Extraction emissions reported in different SAGD LCA models vary because of differences in system boundaries, assumptions, fuel input, SOR_{steam}, operating conditions, and technology used. The range of GHG emissions presented in this research corresponds to the variations in the input parameters.

It is obvious from Figure 4 that the SEP is less energy and GHG emissions-intensive than the major thermal extraction processes. The GHG emissions ranges estimated in this study are approximately 38-78% less than SAGD emission values reported elsewhere. Also, the produced bitumen has a higher API gravity (14) and lower asphaltene content than SAGD bitumen [65]. So the SEP provides better potential to reduce energy consumption and GHG emissions from oil sands-derived liquid fuel production. As shown in Table 6, 60-71% of the total GHG emissions are from electricity production. If electricity is produced from renewable sources, the GHG emissions will drop further. Cogeneration can also be considered to meet electricity demand. With cogeneration, it is possible to reduce upstream GHG emissions, which will result in lower overall emissions.

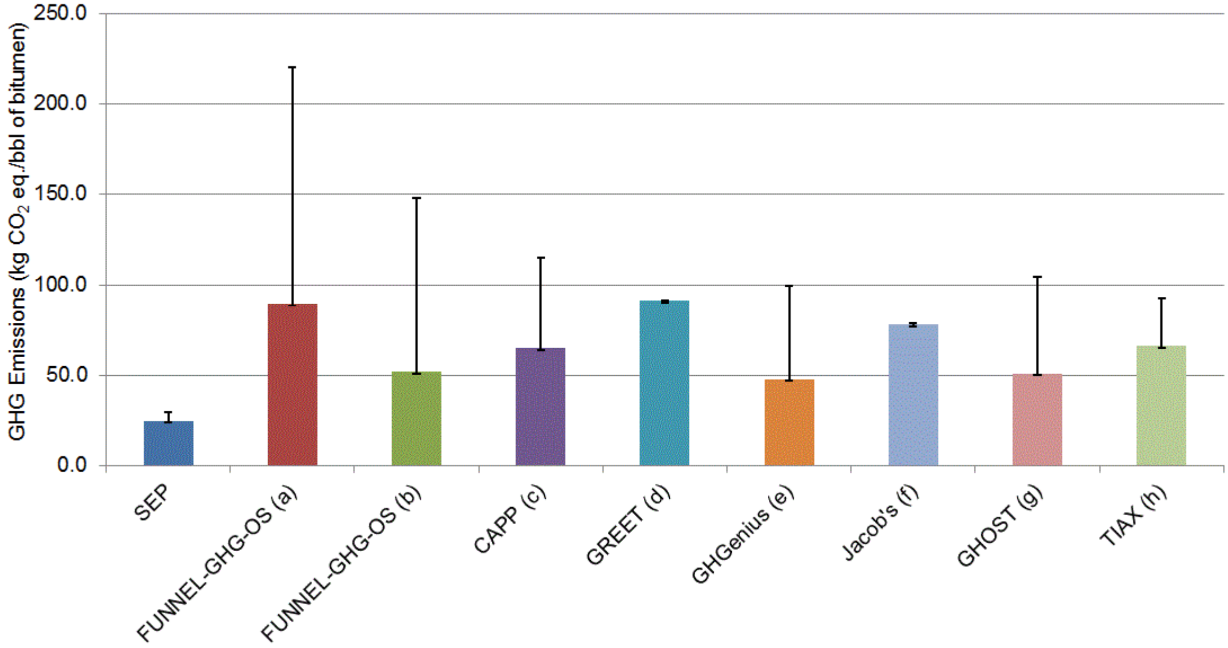


Figure 4-Estimated GHG emissions in SEP compared with existing SAGD models.

(a) [5] Emissions are calculated based on the default values of fuel consumption; no cogeneration is considered (b) [5] Emissions are calculated based on the default values of fuel consumption, and cogeneration is considered (c) [9] The lower value includes cogeneration and the higher value does not include cogeneration (d) [24] Considers cogeneration in its model (e) [23] The lower value corresponds with cogeneration and the higher value with no cogeneration (f) [22] The lower value corresponds with cogeneration and the higher value with no cogeneration (g) [60] The lower value corresponds with cogeneration and the higher value with no cogeneration (h) [25] The lower value corresponds with cogeneration and the higher value with no cogeneration.

3.2 Sensitivity analysis

A sensitivity analysis was performed on the most energy-intensive parameters and on the efficiency of the equipment. The results are given in Table 6. As discussed in section 3.1, the majority of GHG emissions are due to high electricity consumption. The solvent compressor and the demethanizer are the two most power-intensive units. As shown in Figure 3, the solvent vaporizer consumes the highest heat energy. The heating required in the solvent vaporizer depends on the temperature of the condensed solvent from the demethanizer. Also, the higher the amount of solvent recovered from the reservoir, the higher the amount of energy required to process it. So, to see the impact of condensed solvent temperature and the amount of solvent hold-up in the reservoir on energy consumption and GHG emissions, these parameters were included in the sensitivity analysis along with the parameters mentioned above.

As illustrated in Figure 5, the GHG emissions from the SEP are highly dependent on the external refrigeration required in the turbo-expander. External refrigeration can be reduced by transferring all the gases from the compressor to a membrane-based gas separator. As the gases from the compressor will be at a higher pressure, pressure can be used as a driving force to separate C_2+ compounds. As discussed earlier, external refrigeration in the demethanizer is required to condense C_2+ compounds so lowering the amount of C_2+ compounds in the feed will reduce power consumption in the demthanizer significantly. Since the gas pressure at the compressor outlet is slightly sensitive, determining the optimum outlet gas pressure will lower energy consumption and emissions. The solvent hold-up in the reservoir is insensitive to GHG emissions within a ±30 (vol%) variation. This is because the total energy requirement varies inversely with the solvent hold-up in the reservoir but it does not vary significantly per bbl of bitumen. As GHG emissions are related to energy consumption, the GHG emissions' rate also remains insensitive, although total GHG emissions vary. Another noticeable factor is the temperature of the condensed solvent. If the temperature increases more than 10% from the base temperature, GHG emissions drop sharply. This is because if it was possible to separate all the solvents as vapor from the demethanizer, no additional heating would be required in the solvent vaporizer. The energy saved in this process would also save a significant amount of GHG emissions. But with the current technology available, it is not a feasible option.

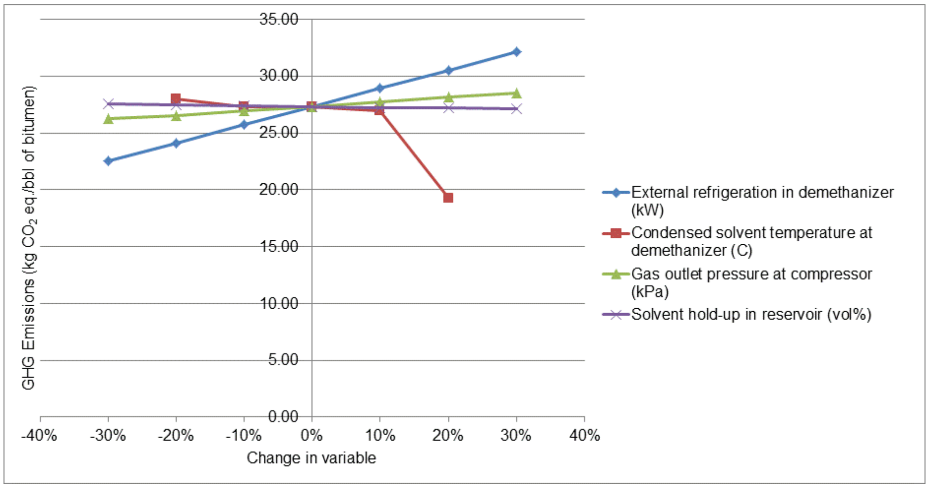


Figure 5-The sensitivity of critical parameters on GHG emissions.

The sensitivity of equipment efficiency is presented in Figure 6. The heat consumption of the SEP significantly depends on the heat exchanger's efficiency. The compressor and the natural gas heater efficiency can be improved to optimize energy consumption. Although the technology of the heat exchanger and steam boiler has matured, their efficiency might drop after a certain period of operation. By optimizing the operating conditions and heat exchanger network (HEN), the efficiency of the heat exchangers can be improved significantly [66]. The fluids inside the heat exchangers deposit suspended and dissolved solids on the heat exchanger surface [67]. After a long period of operation, the deposited solids create an additional layer on the heat exchanger surface, which prevent effective heat transfer. So maintenance should be carried out regularly for consistent performance and to prevent fouling. Compressor performance can also be improved by modifying the design of the compressor blades, as shown by Lee and Kim [68]. Energy efficiency auditing of the heat exchangers, heaters, and compressors might further reduce energy consumption [69].

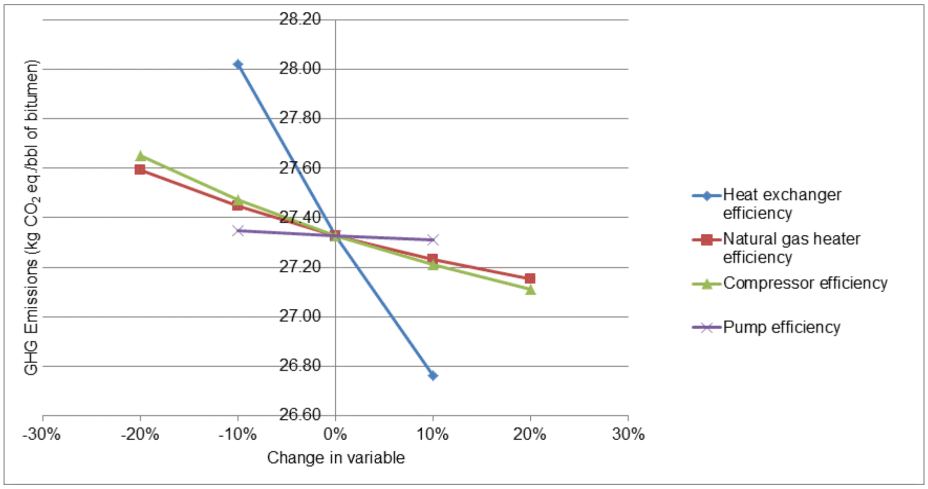
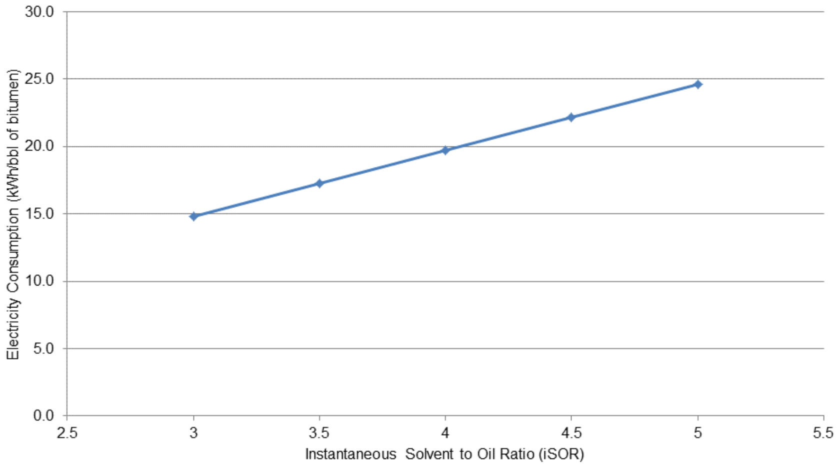
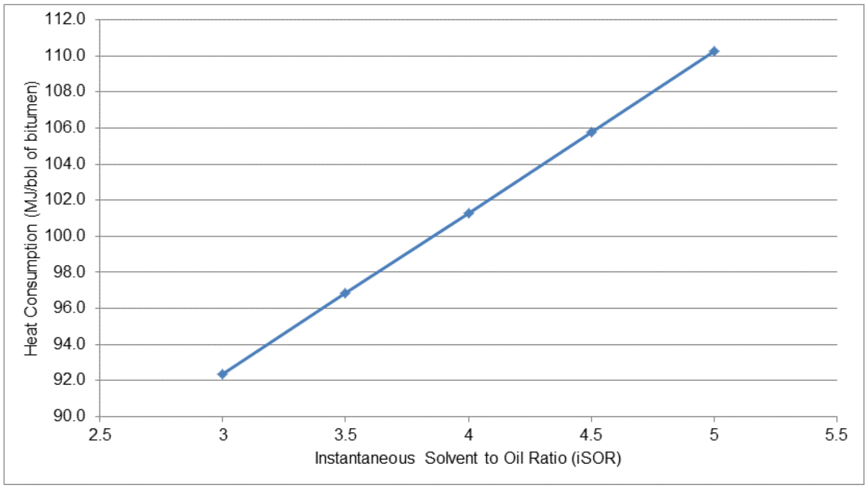


Figure 6-Sensitivity analysis of equipment efficiency on GHG emissions.

Given that the SEP is very sensitive to energy consumption, the effect of changing the instantaneous solvent-to-oil ratio (iSOR) on energy consumption was analyzed. It was found that energy consumption increases linearly with increasing iSOR, as depicted in Figure 7. The change in heat consumption is greater than in electricity consumption. For electricity consumption, the result is reasonable compared to other solvent-based extraction processes [70]. Heat consumption increases because of the additional heat required to heat and process the solvent. Similar analogies have been found for SAGD [5]. Electrical heating techniques like Electro-Thermal Dynamic Stripping (ET-DSP) [71], Enhanced Solvent Extraction Incorporating Electromagnetic Heating (ESEIEH) [72], etc., can be used to reduce the solvent requirement. These techniques use radio frequencies to polarize water molecules [71]. The water molecules then try to align with the electromagnetic field. In the negative half cycle of the microwave, the poles are flipped [73]. The agitation and flipping generate heat. The additional heat can be used to reduce the amount of solvent required to extract bitumen. Using less solvent will reduce the iSOR and total energy consumption.



(a)



(b)

Figure 7-Correlation between (a) electricity consumption and (b) heat consumption with instantaneous SOR in the SEP.

Significant heat is required to separate the solvent from the solvent-bitumen emulsion. To determine how heat consumption varies with the amount of solvent separated in different units, the solvent separated in the stabilizer is decreased with an analogous increase in separation in the flash tank. Solvent separated in the FWKO is kept constant because if a higher amount of solvent is separated from the FWKO at a relatively lower pressure it will increase the work of the compressor. Increasing the compressor work will increase GHG emissions because both compressor efficiency and compressor outlet pressure are sensitive parameters. As illustrated in Figure 8, GHG emissions increase linearly with an increase in the amount of solvent separated in the stabilizer. By looking at the ordinate values, we can infer that the amount of solvent separated in different stages insignificantly contributes to GHG emissions.

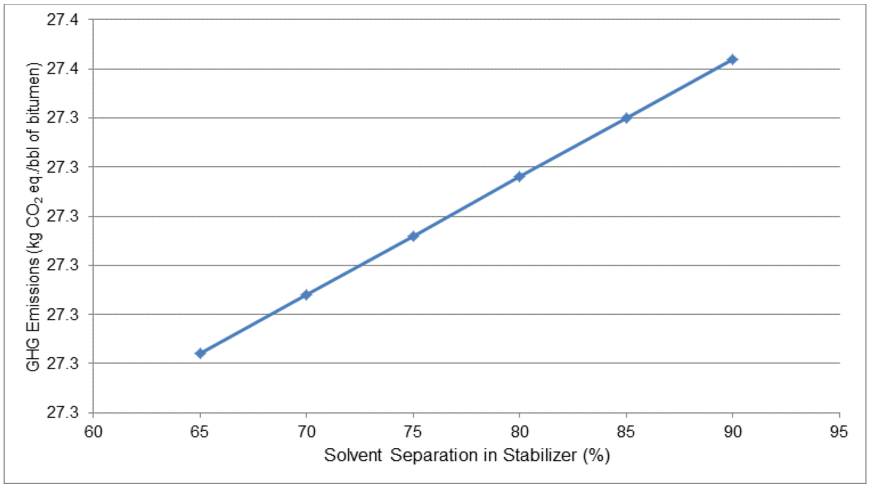


Figure 8-Effect on GHG emissions of variations in solvent separation in the stabilizer.

3.3 Uncertainty analysis

From the sensitivity analysis we determined that the two parameters that impact the emissions most are heat exchanger efficiency and the amount of external refrigeration in the turbo-expander. The amount of external refrigeration depends on the amount of C_2+ compounds in the feed. The feed composition in the demethanizer has significantly higher amounts of C_2+ compound (77.6-87.6 mol%) than usual [62, 74, 75]. In order to make the design robust and allow for flexibility in the demethanizer feed, it was assumed that 90% of the C_2+ feed requires external refrigeration in the base model as a worst case scenario. Using the relation developed by Diaz et al. [62], we found that about 22 mol% C_2+ feed require external refrigeration. This wide range was used to develop the triangular distribution for an uncertainty analysis of external refrigeration. An uncertainty analysis was performed on these parameters along with total electricity consumption and the efficiency of the natural gas (NG) heater. The total electricity consumption was included in the uncertainty analysis to observe the impacts of compressor work and compressor efficiency. A Monte Carlo simulation was used to determine the uncertainty of the input parameters. The simulations were run in ModelRisk [76]. In order to perform the simulations, the statistical distributions of the input parameters are required. Because of limited data, triangular distributions were generated for every parameter except produced gas and venting GHG emissions. A triangular distribution gives conservative results for predictable values as well as a lower standard deviation [77, 78]. For produced gas and venting GHG emissions, it is hard to predict a reliable value as those parameters vary significantly from well to well. This variation is taken into account by choosing a uniform distribution as it gives the most conservative distribution [78] and treats all the input values equally. It is estimated that to keep sampling errors below 0.1 kg CO_2 eq./bbl of bitumen, 100,000 runs are required. Formulas to calculate sampling errors are provided in the Supporting Information. The results are presented for 99% confidence intervals in Figure 9.

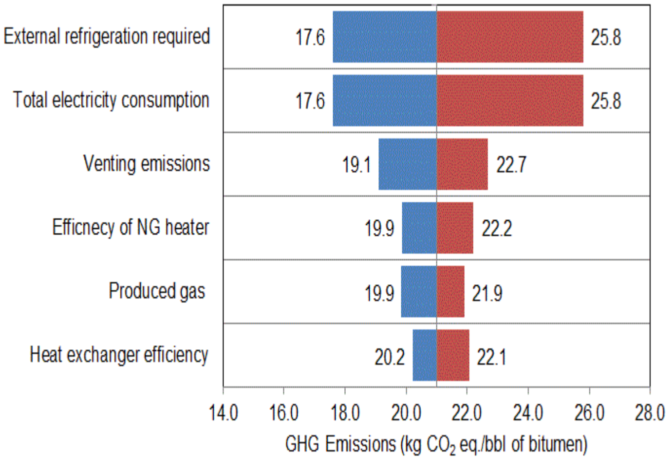


Figure 9-Uncertainty analysis of the most sensitive parameters.

For both external refrigeration and total electricity consumption, the emissions have the same values within the 0.5 and 99.5 percentile. This implies that compressor work and efficiency are relatively insensitive and the highest variations in uncertainty occur because of refrigeration in the demethanizer. The efficiency of the NG heater provides a wider range uncertainty in GHG emissions compared with the efficiency of the heat exchanger, which contradicts the results found from the sensitivity analysis shown in Figure 6. This is because the efficiency of the heat exchanger is considered to be 90 % in this research. As the efficiency of the heat exchanger cannot be higher than 100 %, the efficiency was varied by ±10 percent and the efficiency of the NG heater was varied by ±20 percent. For this reason the uncertainty in emissions for the NG heater (shown in Figure 9) has a wide range. Although a wide range for produced gas from a well is considered in this research, the uncertainties in produced gas emissions have a relatively narrow range.

4. Conclusions

This research presents a data-intensive theoretical model to estimate fuel input, energy consumption, and GHG emissions for a solvent-based oil sands extraction process. Engineering first principles were used to determine mass and energy balances in each sub-unit operation. The total heat consumption is from 62.0 to 126.9 MJ per bbl of bitumen depending on the amount of gas produced from the reservoir. The total electricity consumption is relatively constant, and it is estimated that 19.7-19.9 kWh of electricity is required to extract and recover each bbl of bitumen. It was found that total GHG emissions vary from 24.8 to 29.1 kg CO_2 eq./bbl of bitumen. The total emissions reported in the study are significantly lower than those from steam-based extraction processes. It is also found that, like thermal extraction methods, solvent-based extraction processes are highly sensitive to energy consumption.

More than 92% of the total electricity required is used to condense the solvent in the demethanizer. The SEP is very sensitive to the efficiency of equipment, and among the equipment, the efficiency of the heat exchanger is the most sensitive one. Electricity consumption can be reduced by using low energy-intensive gas separation processes. Improving the HEN and optimizing operating conditions will improve the efficiency of heat exchangers. As the total energy consumption depends on the efficiency of the equipment, proper monitoring with regular maintenance is necessary for consistent performance. Energy consumption varies linearly with the iSOR, as heat consumption is more sensitive than electricity consumption. Energy consumption can be reduced by operating at a lower iSOR.

This modeling approach will help industries find strategic pathways for sustainable oil sands-derived liquid fuel production to meet global energy demands. It will also help policy makers make effective policies considering international market demand, oil price, environmental regulations, etc. that will help the oil sands industry flourish not only in Canada but also around the world.

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Chapter 3

Estimation of energy consumption and greenhouse gas emissions of upgrading and refining bitumen produced by solvent extraction process[2]

1. Introduction

The production and use of transportation fuels account for one-third of the world's total oil consumption [1]. It has been forecasted that the demand for petroleum will be 75 million barrels per day (bpd) by 2020 [1]. To meet the increasing petroleum fuel demand, the production of unconventional oil resources such as oil sands in Canada is projected to grow from 1.95 million bpd in 2013 to 4.81 million bpd by 2030 [2]. Once oil sands are extracted, bitumen is separated from it by surface processing.

Bitumen is a highly viscous crude with an API gravity of less than 10 and a viscosity of over 10^5 centipoise (cp) at standard conditions [3], and for this reason, unlike conventional crudes, the production of transportation fuels from bitumen requires special extraction methods and post-extraction treatment. Because of this, gasoline, diesel, and jet fuels produced from bitumen result in higher life cycle greenhouse gases (GHGs) emissions compared to conventional crudes [4, 5]. The majority of the emissions are from extraction, upgrading, and refining operations.

Only 12% of Alberta's oil sands deposit is surface mineable and the rest lies at a depth of 75-750 m [6], where in situ extraction methods are used. In situ recovery is predominantly achieved by thermal methods. Of the different thermal methods, steam assisted gravity drainage (SAGD) and cycle steam stimulation (CSS) are the major ones [7]. However, steam-based extraction processes are energy- and GHG emissions-intensive [8]. In 2009, the GHG emissions from the oil sands industry were 39.3 metric tonne (MT) of CO_2 eq. and it is estimated by the researchers that with the current extraction methods the emissions will increase to 127 MT of CO_2 eq. by 2035.

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[2] The results of this chapter is prepared for submission as Soiket, M.I.H., Oni, A. O., Kumar, A., "Estimation of energy consumption and greenhouse gas emissions of upgrading and refining bitumen produced by solvent extraction process" in a peer-reviewed journal.

In order to control GHG emissions from bitumen-derived transportation fuel production, energy saving extraction technology such as solvent-based extraction is proposed.

Vapor solvent-based extraction methods have proven to be more effective than steam-based methods [9-12] but suffer from a poor oil recovery rate [10, 11]. The solvent penetration rate increases dramatically with diluted bitumen [13]. Furthermore, the quality of the produced bitumen is enhanced significantly due to high asphaltene precipitation in the reservoir [14]. Rezaei et al. estimated that the vapor solvent extraction process will produce more oils than SAGD [14] while reducing energy consumption and GHG emissions [13]. However, these estimations are based on laboratory scale experiments, which are subject to high uncertainties.
After bitumen is extracted from oil sands by surface processing, diluents such as naphtha or natural gas condensate are mixed with the diluent for easy transportation [15]. As conventional bitumen produced from thermal extraction processes has high density and sulfur content, refineries cannot process bitumen directly [16]. For this reason, bitumen is upgraded and chemically treated to get the higher value synthetic crude oil (SCO) [1]. Commercial upgrading technologies are either thermal cracking-based or hydroconversion-based [3-5]. Upgrading hydrogen-deficient and highly viscous bitumen either by delayed coking or by hydroconversion is energy intensive [1] and results in high GHG emissions. In 2011, 7.8% of Canada's total GHG emissions were generated from oil sands plants and upgraders. It is also projected that by 2020 [2], GHG emissions might be over 100 million tonnes.

Typically, conventional crudes are refined after extraction. But, as mentioned earlier, bitumen is first upgraded and then refined. Because the solvent extraction process causes high asphaltene precipitation, the bitumen produced from solvent extraction is partially upgraded [13]. Since the produced bitumen has an inherently high hydrogen/carbon (H/C) ratio, the upgrading process further improves the quality of the SCO. The quality of SCO supplied to the refinery has a significant impact on refinery energy consumption and GHG emissions [1]. Also, depending on the quality of the feed, refineries produce products with different properties. So, instead of estimating energy consumption and emissions from the refinery alone, it is important to investigate upgrading and refining operations together because refinery energy consumption and GHG emissions are highly dependent on upgrading operations. In order to reduce net GHG emissions from bitumen-derived transportation fuels, life cycle emissions from both upgrading and refining operations first need to be estimated. To lower emissions and to comply with low-carbon fuel regulations around the world [17, 18], it is important to conduct a life cycle assessment (LCA) on bitumen upgrading and refining operations.

Life cycle emissions can be reduced by improving the overall efficiency of the upgrading and refining operations and by capturing produced carbon. The BEST (Bitumen Extraction Solvent Technology) pilot plant demonstrated vapor solvent technology in 2014 [19] and showed that produced bitumen has an API gravity of 14 (compared to 8 in SAGD [20]) and very low asphaltene content [21]. As the bitumen is partially upgraded, it might require little or no upgrading in order to refine it. Also because of upgrading, it is likely that bitumen will produce high-quality SCO that might reduce energy consumption and emissions in the refinery. Alternative project-specific production pathways need to be developed in order to calculate the life cycle emissions of this partially upgraded bitumen from vapor solvent extraction. Bitumen upgrading (through delayed coking or hydroconversion) and then refining compared with bitumen directly refined without upgrading would be potential pathways to investigate the least energy- and emissions-intensive bitumen conversion pathway.

The two most prominent LCA models developed in North America are GREET [22] (Greenhouse Gases, Regulated Emissions, and Energy Use in Transportation) and GHGenius [23]. Both use a top-down approach to estimate upgrading and refining energy consumption and emissions for bitumen produced from thermal extraction methods. These models do not analyze the impact of crude quality on energy consumption and emissions, so it is not possible to determine the upgrading and refinery life cycle energy consumption and emissions of bitumen having significantly different properties with these models as confirmed by Nimana et al. [1]. Other studies [4, 5] have also calculated energy consumption and GHG emissions using bottom-up approach. It is easier in a bottom-up approach than in a top-down approach to trace energy consumption and emissions from each sub-unit operation [24]. However, all these models were developed for certain crude types, and so upgrading and refining energy and emissions can be estimated for the crude provided in those models only. Other studies [25, 26] analyzed the impact of crude quality and refinery configuration but did not consider upgrading and refinery operations together. Still other studies [27, 28] reported energy consumption and emissions range based on confidential industry data for thermal extraction process. The results are specific to the assays provided in the models and are not applicable for other bitumen assays. So, to accurately estimate upgrading and refining energy consumption and GHG emissions, especially for solvent-extracted partially upgraded bitumen and for energy and environmental comparisons with thermally extracted bitumen, process-specific LCA models are required which has also been recommended by other studies [29, 30].

This paper presents a detailed data-intensive simulation model to estimate life cycle energy and GHG emissions from upgraders and refinery operations for partially upgraded bitumen from solvent-based extraction process. Three project-specific production pathways were considered in the model to compare life cycle energy consumption and GHG emissions in each pathway. The specific objectives are to:

- Estimate path-specific energy consumption and life cycle GHG emissions from upgrading and refinery operations
- Determine the best production pathway by comparing final yield, energy consumption, and emissions
- Conduct uncertainty analyses to generate conservative ranges of GHG emissions due to the variations of the most energy- and emissions-sensitive parameters

2. Methodology

2.1 Process description

2.1.1 Upgrading

In upgrading operations, low-value, higher molecular compounds split into high-value, low molecular compounds [3]. The selection of an upgrading technology depends on crude type, techno-economic factors, and the quality of the final product [1]. Upgrading reactions occur in two steps. First, cracking reactions break C-C bonds to convert vacuum residue into distillate products to increase the hydrogen-to-carbon ratio, and then catalytic reactions occur to produce hydrogenated products with lower hydrogen and sulfur contents [3]. The hydrogen to carbon ratio can be increased by either carbon rejection (coking) or hydrogen addition [1]. Coking processes disproportionate the feed [3] and produce coke that is rich in carbon, sulfur, and other contaminants [1], whereas in hydroconversion, hydrogen is added to the feed in the presence of a catalyst to promote hydrogenation and sulfur removal [3].

Energy consumption in sub-unit operations depends on the distillation properties, sulfur content, and API of the bitumen feed. Bitumen assays found in the literature were used as feed in the HYSYS upgrader and refinery models [21]. Bitumen properties are presented in Table 7.

Table 7 - Properties of bitumen assay [23]	
API gravity	14
Density (kg/m^3)	972.51
Sulfur (wt%)	4.6
Asphaltene (wt%)	3
Vacuum residue yield (538^{o}C+) (vol%)	45.4
Metals:	
Nickel (ppm)	30
Vanadium (ppm)	77
Ferrous (ppm)	5

Flow streams are calculated based on mass balance and volume (%) age of distilled products. Distillation fractions for delayed coker and hydroconversion upgraders are provided in the Supporting Information (Appendix A). Figures 10 and 11 shows the system boundaries and sub-unit operations in delayed coker and hydroconversion upgraders, respectively.

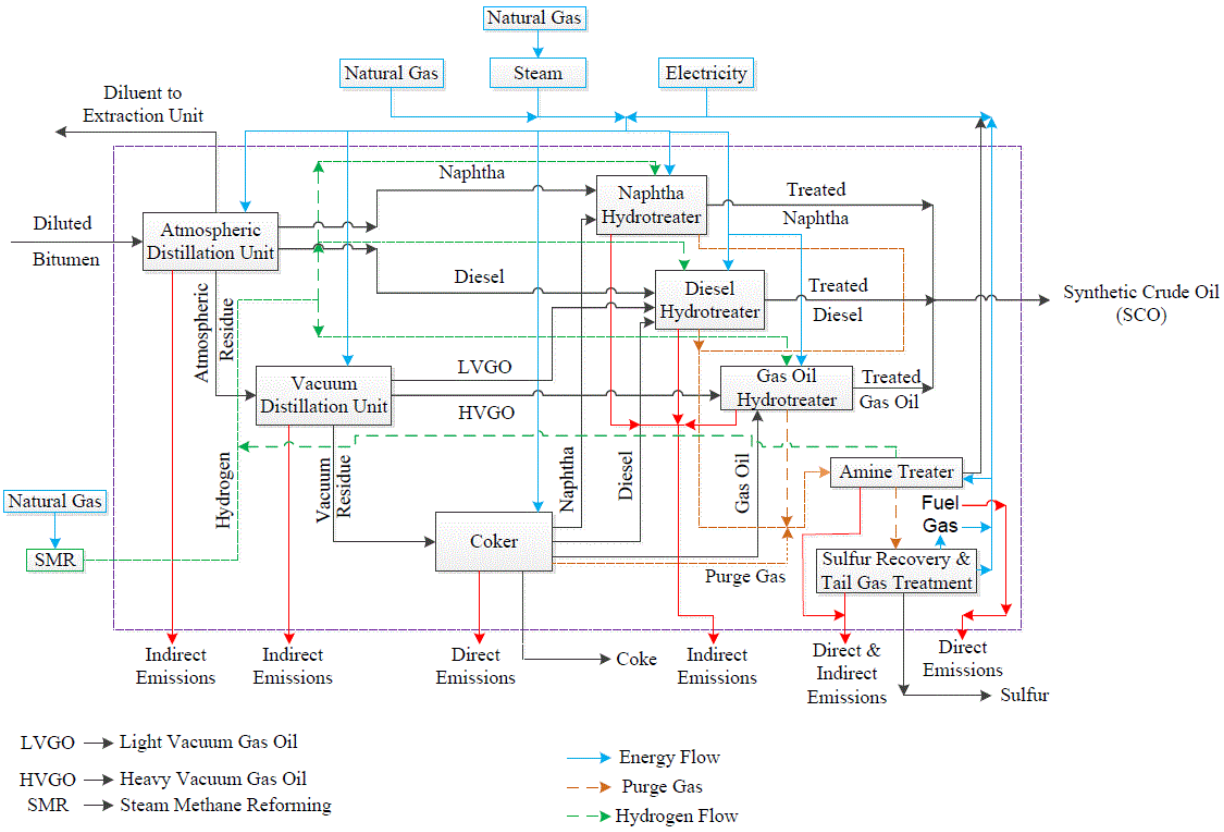


Figure 10-Sub-unit operations in a delayed coker upgrader.

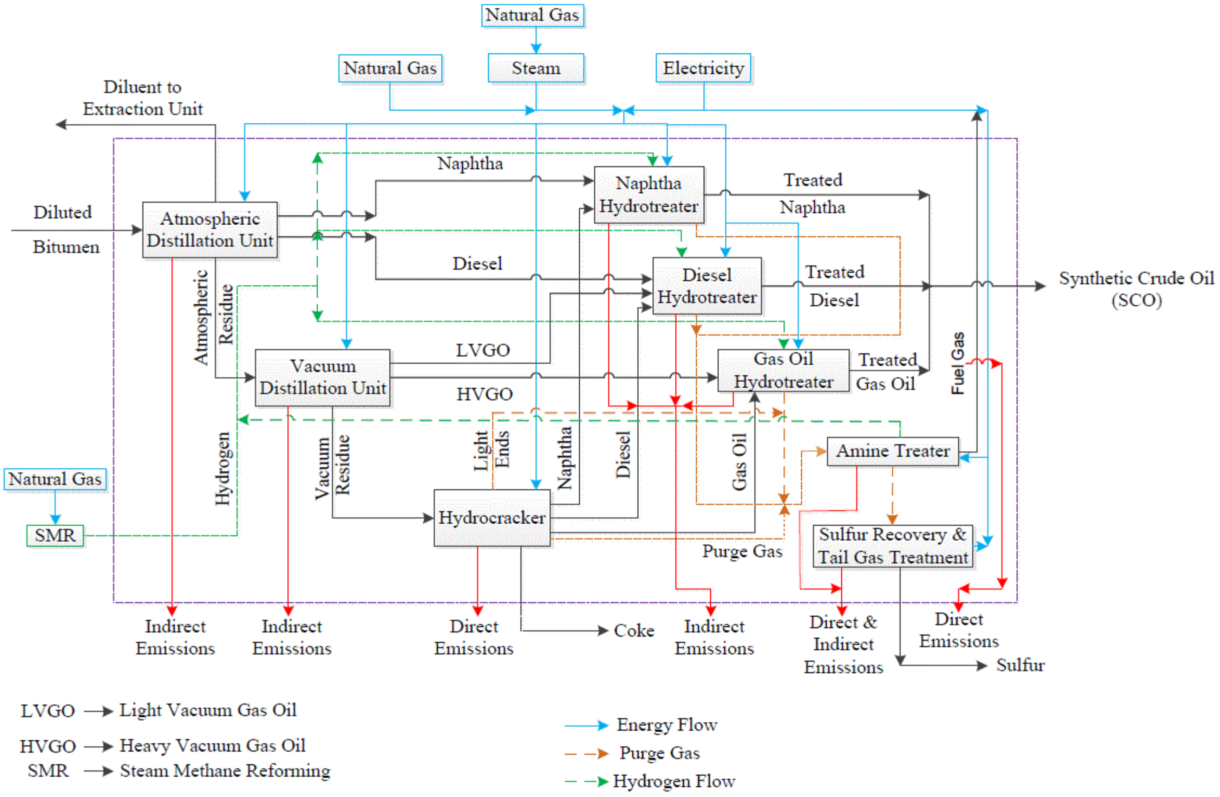


Figure 11-Sub-unit operations in a hydroconversion upgrader.

Energy consumed in the sub-unit operations is in the form of natural gas, steam produced by burning natural gas, purge gas, and electricity from the grid. In distillation towers both steam and natural gas are supplied. Natural gas is burned in the furnace to heat the crude to its vaporization temperature, and steam is required to strip distillation products from fractionating columns [25]. Diluent is separated in the atmospheric distillation unit (ADU) and returned to the extraction unit. For both upgraders, naphtha and diesel are separated from the ADU and sent to naphtha and diesel hydrotreaters, respectively. Atmospheric residue from the ADU bottom goes to the vacuum distillation unit (VDU) and is further fractioned into light and heavy vacuum gas oils (VGOs). Vacuum residue from the VDU fractionating column is fed into a coker unit for delayed coker upgraders whereas in hydroconversion upgraders, the vacuum residue is fed to a hydrocracker. As shown in Figure 10, in a coker the coking process requires a long reaction time (12-14 hours per cycle) in the liquid phase to convert the residue fraction of the feed into gases, distillates, and coke [3]. The highly aromatic produced coke is rich in sulfur, nitrogen, and metals [3]. But in a hydrocracker as depicted in Figure 11, high-pressure hydrogen and a bifunctional acid-cracking catalyst are used to convert the vacuum residue [3]. Hydrocracking processes the feed in two stages: first, the feed is hydrotreated to reduce sulfur and nitrogen levels to make the acid-cracking catalyst effective, and after that actual conversion takes place. An ebullated-bed hydrocracker is assumed in this research because fluidizing the catalyst bed prevents the bed from plugging and catalyst can be replaced online from the bed [3]. Heat exchangers are used to heat intermediate streams between feed and products.

Naphtha, diesel, and gas oils produced in primary upgrading are fed to the hydrotreaters in secondary upgrading. In hydrotreating, heteroatoms are removed selectively with little attendant cracking [3]. The hydrotreater operating temperatures were consistent with those found in the literature [31]. Hydrogen required in hydrotreaters is supplied from on-site steam methane reforming (SMR) plant. A huge amount of hydrogen is also required in the hydrocracker for the hydroconversion upgrader [3]. Hydrogen consumption depends on the type of feed and quality of product [1]. Thus hydrogen consumption is considered a sensitive parameter in this study. Natural gas is supplied in the SMR plant both as feedstock and as fuel to produce hydrogen [32]. The amount of natural gas, steam, and electricity required to produce a per unit volume of hydrogen is taken from the literature [33]. The input data used for developing the upgrader models are provided in Table 8.

Table 8 - Input data used to develop upgrading models

Hydrogen consumption:	Delayed coker	Hydroconversion	Source
Naphtha hydrotreater (scf/bbl)	142	100	[38]
Diesel hydrotreater (scf/bbl)	162	259	[38]
Gas oil hydrotreater (scf/bbl)	736	690	[38]
Hydroconverter (scf/bbl)	-	1218	[38]
Hydrogen production in SMR plant:			
Natural gas (NG) fuel required (m^3/Nm^3 of H_2)	0.0398		[37]
NG feedstock required (m^3/Nm^{3*} of H_2)	0.362		[37]
Electricity consumption (kWh/Nm^3 of H_2)	0.028		[27]
Steam produced (lb/Nm^3 of H_2)	0.86		[27]
Efficiency of equipment:			

Table 8 - Input data used to develop upgrading models		
NG furnace (%)	87	[39]
NG fired boiler (%)	85	[29]
Heat exchanger (%)	90	[40]

Apart from naphtha, diesel, and gas oil, purge gases are also produced as effluent from delayed coking and hydroconversion operations [3]. Purge gases have insufficient amounts of hydrogen and olefins to recover as separate streams [3]. Also, the hydrogenation of oil produces ammonia and hydrogen sulfide (H_2S) from organic compounds. So, ammonia, carbon dioxide, and hydrogen sulfide are removed from the purge gases to use as fuel gas [3]. Ammonia is removed by water wash [3] and then the purge gases go to the amine treater. In this research, diethanolamine (DEA) is assumed to be used to remove the acid gases from the feed. The acid gas pickup rate is provided in Table 9. The fuel gas thus produced is burned to provide heating. The efficiency of the fuel gas burner is considered to be same as in the NG furnace (shown in Table 8). The hydrogen produced in the amine treater is used to supplement the total hydrogen required. All the acid gases are transferred to the sulfur recovery unit to convert H_2S into raw sulfur. A modified Claus process was considered because of its low cost. Since the Claus process is only 92-98% efficient [3], a tail gas treatment unit is used to treat additional sulfur from the effluent gas. Steam is produced as a byproduct from the Claus unit and supplements the total steam requirement.

Table 9 - Input data used for the purge gas recovery process			
Purge gas composition:	Delayed coker	Hydroconversion	Source
Hydrocarbons (mol%)	42.20[a]	24.17[a]	
Hydrogen (mol%)	53.83[a]	70.74[a]	
Acid gas (mol%)	3.97[a]	5.09[a]	
Amine treater:			
Acid gas pickup (m^3/liter of solution)		4.63	[3]
Reboiler heating (MJ/m^3 of DEA)		280	[41]
Electricity consumption (kWh/m^3 of DEA)		2.6	[41]
Claus sulfur recovery plant:			
Electricity consumption (kWh/ton of S)		98	[41]

Table 9 - Input data used for the purge gas recovery process

Steam production (lb/ton of S)	1215	[41]
Tail gas treater:		
Electricity consumption (kWh/ton of S)	463	[41]

[a]Values are obtained from the HYSYS delayed coker and hydroconversion upgrader models

2.1.2 Refining

SCO from upgraders and dilbit from the extraction unit are fed into a deep conversion refinery to obtain gasoline, diesel, jet fuel, and other end products [37]. As depicted in Figure 10, diluent is separated from the ADU of the upgrader or refinery. Refineries are complex process plants and give products based on feedstock, correlations, and processing units [38]. The refinery configuration used in this study is shown in Figure 12.

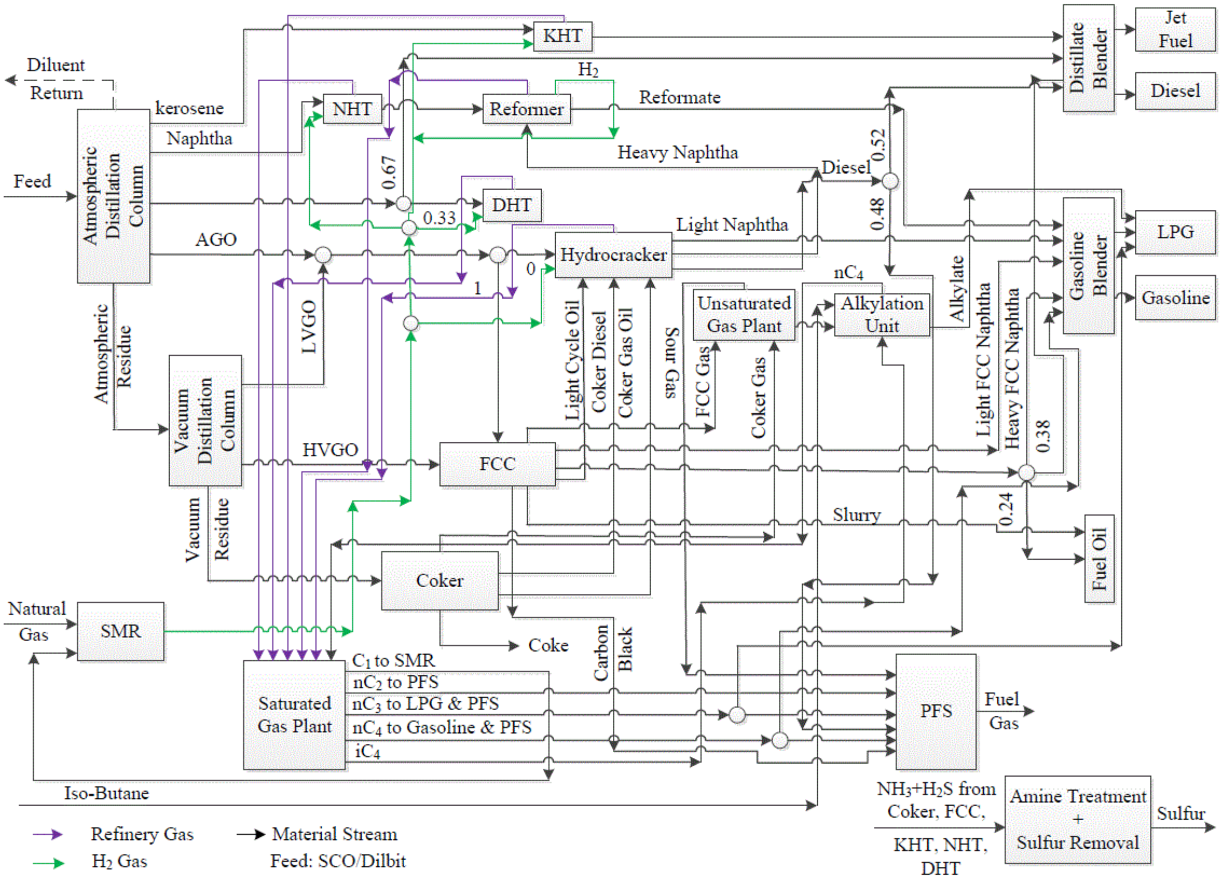


Figure 12-Sub-unit operations in a typical North American refinery.

A typical deep conversion refinery has a coker and a catalytic cracking unit [20]. The distillation curve in the model is determined by Aspen HYSYS [39] based on the boiling point of fractions, density, sulfur content, and carbon residue of the feed [1]. Processing units like hydrotreaters (HTs), fluid catalytic crackers (FCC), reformers, hydrocrackers, and alkylation units are simulated in the petroleum shift reactors, which operate on the delta base-shift concept [39]. All the fractions shown in Figure 12 are calculated in HYSYS using the equations and correlations. The gas streams' containing saturates is directed to the saturated gas plant (SGP). After separation, the methane gas goes to the SMR plant to supplement the hydrogen requirement. The total C_2 and fractions of C_3 and C_4 gases go to the plant fuel system (PFS). The produced fuel gas is burned to generate heat. Unsaturated gases containing olefins from the FCC and coker unit go to the unsaturated gas plant (UGP). From the UGP, ethylene is directed to the PFS whereas propylene and butylenes are transferred to the alkylation unit [40]. Alkylate produced in the alkylation unit is mixed with other components to form liquefied petroleum gas (LPG). Similar to upgraders, the utilities in the refinery are fuel, steam, and electrical power. The model uses base correlations to predict the utility energy consumption values in each sub-unit operation of the refinery.

The total energy consumed in the refinery is obtained from refinery fuel gas, natural gas, steam, electricity, and coke. Fuel oil, used in marine engines, is considered to be a product in this study [41]. Similar to upgraders, natural gas is supplied as fuel and feedstock in the on-site SMR plant to produce hydrogen. The total hydrogen required as feedstock in the SMR plant is supplemented by the methane produced in the SGP. The hydrogen produced in the reformer is of low purity and hence goes to the PFS to produce fuel gas. Steam produced in the sulfur recovery unit supplements the total steam requirement.

2.2 Process simulation

The simulation of the upgrading and refinery operations was done in Aspen HYSYS 8.8 software [39]. The upgrader models were designed using Aspen HYSYS especially for the upcoming bitumen feed (rigorous models). For refining operations, the default deep conversion refining model developed in HYSYS was used because of the scarcity of data. In HYSYS, the dependent variables such as product flowrates, qualities, utilities, etc., are determined by the base correlations specified for different independent variables like feed type and flowrate [39]. In order to adjust variations in the independent variables from a base point, HYSYS uses a set of linear equations that are developed by differentiating the independent variables with respect to the dependent variables at their base points [1]. The derivatives of the independent variables represent the coefficients of the equations [42]. The step-by-step simulation procedures are as follows:

I. A fluid package is selected as input feed. In this study, for bitumen and SCO refinery operations the Peng-Robinson equation of state [43] is considered appropriate
II. Bitumen properties are characterized
III. Upgrading and refining process flow models are developed
IV. Process flows are simulated in models to generate data for energy and emissions analysis

2.3 Production pathways

In this model three pathways were developed to evaluate energy consumption and GHG emissions in upgrading bitumen and refining both bitumen and SCO. As shown in Figure 13, pathways I and III have upgraders, while in pathway II, bitumen is directly sent to a refinery without upgrading. SCO produced from upgrading has properties similar to conventional crudes [3] and can be converted into transportation fuels through refining operations. However, since the bitumen produced from the solvent extraction process is partially upgraded, it would be interesting to observe whether the deep conversion refineries can convert the bitumen into transportation fuels without upgrading. If it is possible, then energy and GHG emissions from oil sands-derived liquid production will be reduced significantly and the production process would be similar to transportation fuels produced from conventional crudes. To investigate whether it is better to upgrade bitumen or directly refine it, pathway II has been considered here. The two upgraders used most in industry, delayed coking and hydroconversion, were considered in pathways I and III, respectively. A deep conversion refinery process model was used to observe refinery operations. It is assumed that the diluents separated from the upgraders and refinery will be transported back to the extraction unit.

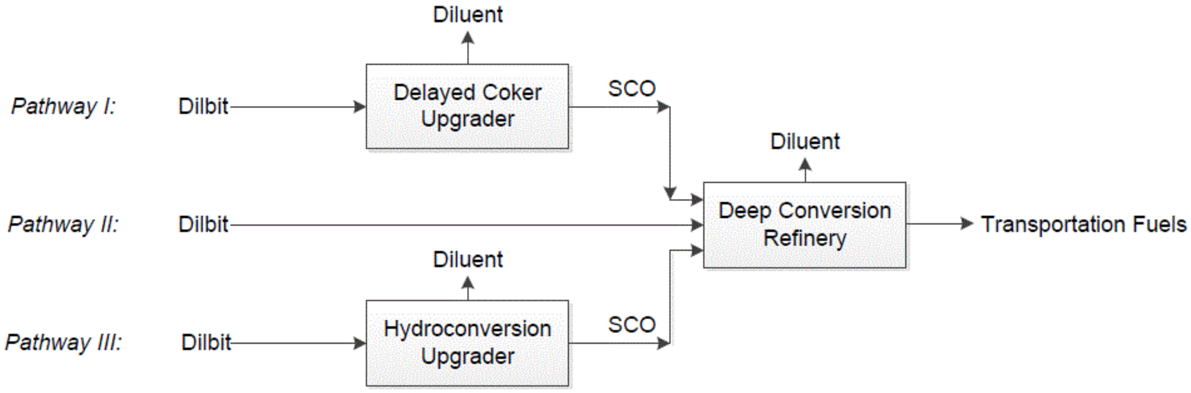


Figure 13-Bitumen to transportation fuel conversion pathways.

The total emissions reported in this model include: 1) direct emissions from the combustion of natural gas and produced fuel gas on site and 2) indirect emissions from the recovery, processing, and transportation of natural gas. It is assumed that all the electricity will be supplied from the Alberta's grid. The upstream and combustion emissions from fossil fuels used to generate electricity were considered in calculating total emissions from electricity consumption. The model considers venting, flaring, and fugitive (VFF) emissions but not land-use emissions. The coke produced in upgrading and refining operations is assumed to be stockpiled.

2.4 Mass and energy analysis

2.4.1 Assumptions

The basic modeling equations are derived based on the following assumptions:

1. The system is in a steady flow condition
2. Changes in kinetic and potential energy are negligible
3. The reference states are T_o = 25^{0}C = 298.15 K, P_o = 101 kPa
4. A change in mol% is equivalent to a change in vol%

2.4.2. Mass and energy balance equations

The upgrading and refinery simulation models were developed based on engineering first principles as presented in chapter 2 (equations 1-3).

The energy balance across the heat exchangers is calculated as [45]:

$$(\dot{E}_{hot,in} - \dot{E}_{hot,out}) - (\dot{E}_{cold,in} - \dot{E}_{cold,out}) = 0 \tag{8}$$

The total heat and steam required in upgrader and refinery models is obtained from HYSYS simulation models. To meet the heat and steam requirement, produced gas and natural gas are burned. To calculate the heat produced from natural and produced gas in upgraders and refineries, equations (4) and (5) are used (see chapter 2).

In produced fuel gas, the amount of C_4 and C_{4+} compounds were less than 5 (vol%) [44] in total so LHV of C_4H_{10} has been used to calculate total heat produced from upgrader fuel gas. For simplicity of calculation, it is considered that all the steam is produced by burning natural gas. The electricity consumed in different sub-units of the upgrader and refinery is determined using correlations from the Prelim model [27].

2.5 Estimation of life cycle emissions

To calculate life cycle emissions from natural gas used (direct and indirect) in upgraders, GHG emission factors are imported from the literature [22]. The LHV of fuels are provided in the Supporting Information. Only upstream emissions have been considered for natural gas supplied as feedstock in the SMR plant. Emission from steam reforming reactions are consistent with those found by Nimana et al. [1]. Netzer [46] estimated an emission factor of 2419.4 g-CO_2 eq. due to burning 1 kg of fuel gas and this emission factor is also used in this study. VFF emission factors are collected from literature [47]. To calculate emissions from Alberta grid, both upstream and combustion emission factors were imported from NIR [48]. The upstream GHG emissions were calculated considering 70% and 30% of the total electricity is produced from coal and natural gas, respectively.

The GHG emission factors to calculate the total refinery GHG emissions are consistent with upgrading units except for grid electricity. The combustion emission factor from the production of 1 kWh electricity is considered as 581 g-CO_2 eq./kWh [1] assuming the refinery is located in the USA and electricity is coming from the local grid. The VFF GHG emissions for refinery operation are also extracted from literature [47].

2.6 Uncertainty analysis

By sensitivity analysis it is possible to observe the impact of input parameters on output results [64]. So a sensitivity analysis has been conducted to determine the impact of energy-intensive parameters on the parameters causing high energy consumption to determine their impact on net GHG emissions due to upgrading and refining. The parameter values have been varied in between ±30% from their base value as consisted with other literature [1]. For some parameters, the variation range is shortened (±10%) to generate meaningful results.

To improve the model reliability and to calculate the uncertainty in GHG emissions, Monte Carlo simulation has been performed in this research to observe the impact of the most sensitive parameters. The sampling error maintained less than 0.1 kg CO_2 eq./bbl of bitumen. To maintain that sampling error sample size is calculated from equation (7) [24]:

Sampling error, $\overline{X} = \frac{z * \sigma}{\sqrt{n}}$ (9)

where σ = standard deviation of the mean and n = number of samples. The Z value is determined based on the confidence interval of the standard normal distribution. The Z values are provided in the Supporting Information (Appendix B).

2.8 Functional unit

To assess LC emissions of oil sands-derived fuels, the functional unit used is one unit volume of bitumen fed into the upgraders and refineries. The functional metric is CO_2 eq./bbl of bitumen. Similar to earlier study [4], to calculate the total CO_2 eq., the three main GHGs (carbon dioxide [CO_2], methane [CH_4] and nitrous oxide [N_2O]) were considered since they have the highest global warming potential (GWP) [49]. However, emissions were also allocated at the refinery sub-process level as recommended by ISO 14041 [50] and presented in g-CO_2 eq./MJ (mega joule) of refined products. The LHV was used to define the energy content, as consistent with GREET [22].

3. Results and discussion

3.1.1 Upgrading

The SCOs produced from hydroconversion upgrading and delayed coker upgrading are 127.2 and 117.9 (vol%) of bitumen, respectively. The SCO produced in hydroconversion upgrading differs in quality from the SCO from delayed coker upgrading. The volume yield from SAGD bitumen ranges from 78%-94% in delayed coking and 95-106% in hydroconversion [1, 27, 28, 51]. A higher SCO yield is obtained from both upgrading units because of the quality of bitumen feed processed.

The total energy consumed to upgrade bitumen depends on the feed quality and the process used [1]. The total energy is estimated to be 0.40 GJ and 0.50 GJ per bbl of bitumen (excluding energy consumption in the SMR plant) for delayed coker and hydroconversion upgraders, respectively. The total GHG emissions calculated (excluding GHG emissions in the SMR plant) for delayed coker and hydroconversion are 54.28 and 80.30 kg CO_2 eq./bbl of bitumen, respectively. Table 10 provides the breakdown of the total energy consumption and GHG emissions in the upgraders.

Table 10 - Upgrading energy consumption and GHG emissions

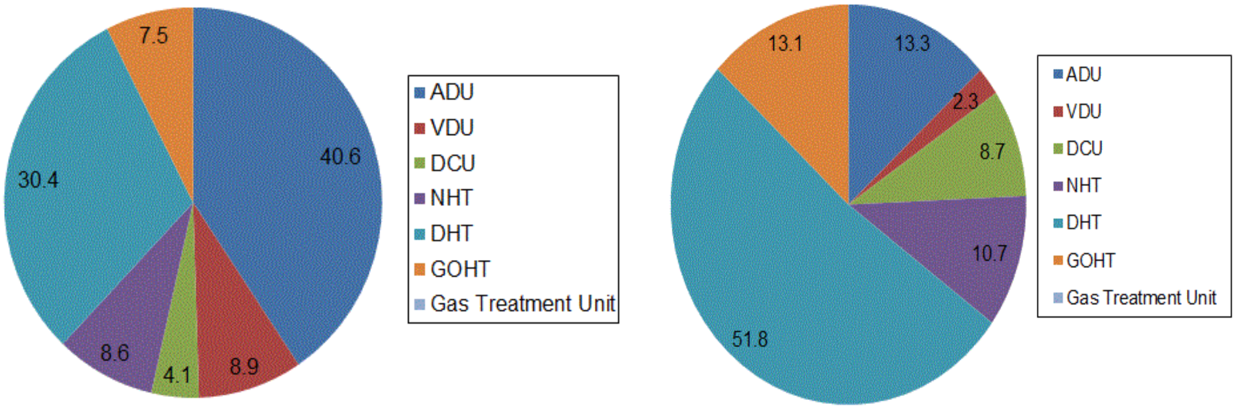
	Units			Delayed coker	Hydroconversion	
SCO produced	bbl/bbl of bitumen			1.179	1.272	
H_2 requirement	Nm^3/bbl of bitumen			7.70	17.70	
	Units	Fuel consumption		Units	Emissions	
		Delayed coker	Hydroconversion		Delayed coker	Hydroconversion
Fuel gas	m^3/bbl of bitumen	0.08	6.18	kg CO_2 eq./bbl of bitumen	11.18	15.14
Natural gas:				kg CO_2 eq./bbl of bitumen	32.13	34.80
1. Heating	kg/bbl of bitumen	8.74	11.86			

Table 10 - Upgrading energy consumption and GHG emissions

2. Steam$^{\alpha}$	kg/bbl of bitumen	2.22	4.23			
	Units	Fuel consumption		Units	Emissions	
Electricity	kWh/bbl of bitumen	6.77	9.07	kg CO_2 eq./bbl of bitumen	5.98	8.01
VFF emissions$^{\beta}$				kg CO_2 eq./bbl of bitumen	4.99	4.99

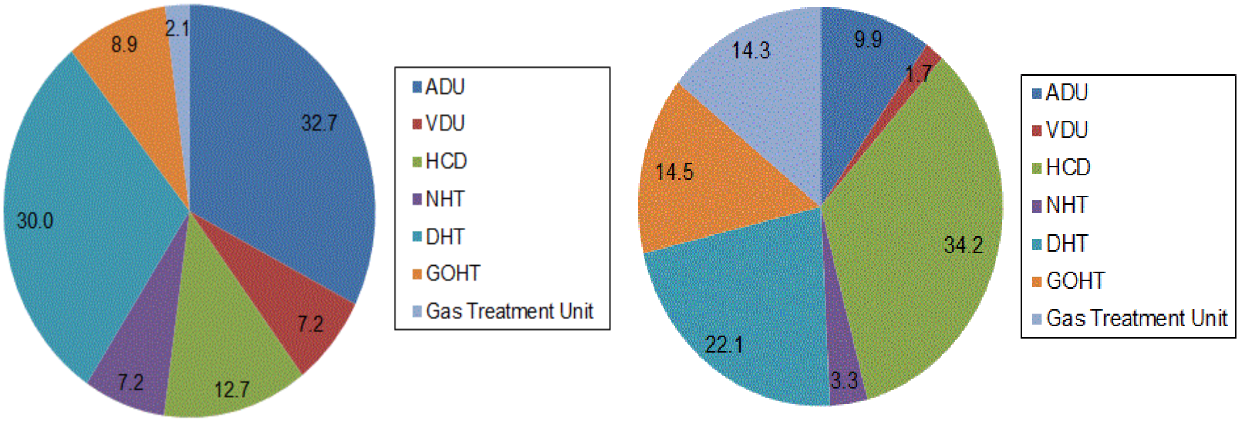
$^{\alpha}$Natural gas required for steam production is determined considering a steam LHV of 2.79 MJ/kg [53] $^{\beta}$VFF emissions are calculated using a bitumen LHV of 6.48 GJ/bbl [22] and emission factors from the NIR [48].

A pinch analysis [53] was performed to reduce the energy requirement by saving energy from the hot streams. The maximum energy recovery (MER) [54] design was obtained for a minimum temperature difference of 21 °C between hot and cold streams in the delayed coking. For hydroconversion, the MER design was obtained at a minimum temperature difference of 18 °C. In coking upgrading, heat is extracted from hot streams at ≥ 215.5°C, and about 46.13% of the total heat energy is recovered through heat exchange between the feed and product streams. In the case of hydroconversion upgrading, the minimum hot stream temperature is 30 °C and the maximum heat energy recovered is 36.81% of the total heat required. Since the design has been optimized and the bitumen fed to the upgraders is partially upgraded, it was found that the energy required in both upgrader types is lower than in SAGD [1]. Of the net energy required, electricity demand ranges from 6.77 kWh/bbl of bitumen in the delayed coker unit (DCU) to 9.07 kWh/bbl of bitumen in the hydroconversion unit (HCU). Total heat and electricity consumption distributions in DCU and HCU sub-unit operations are shown in Figures 14 and 15, respectively.



(a) (b)

Figure 14-Distribution of (a) heat and (b) electricity consumed in delayed coker upgrading (0.40 GJ/bbl).



(a) (b)

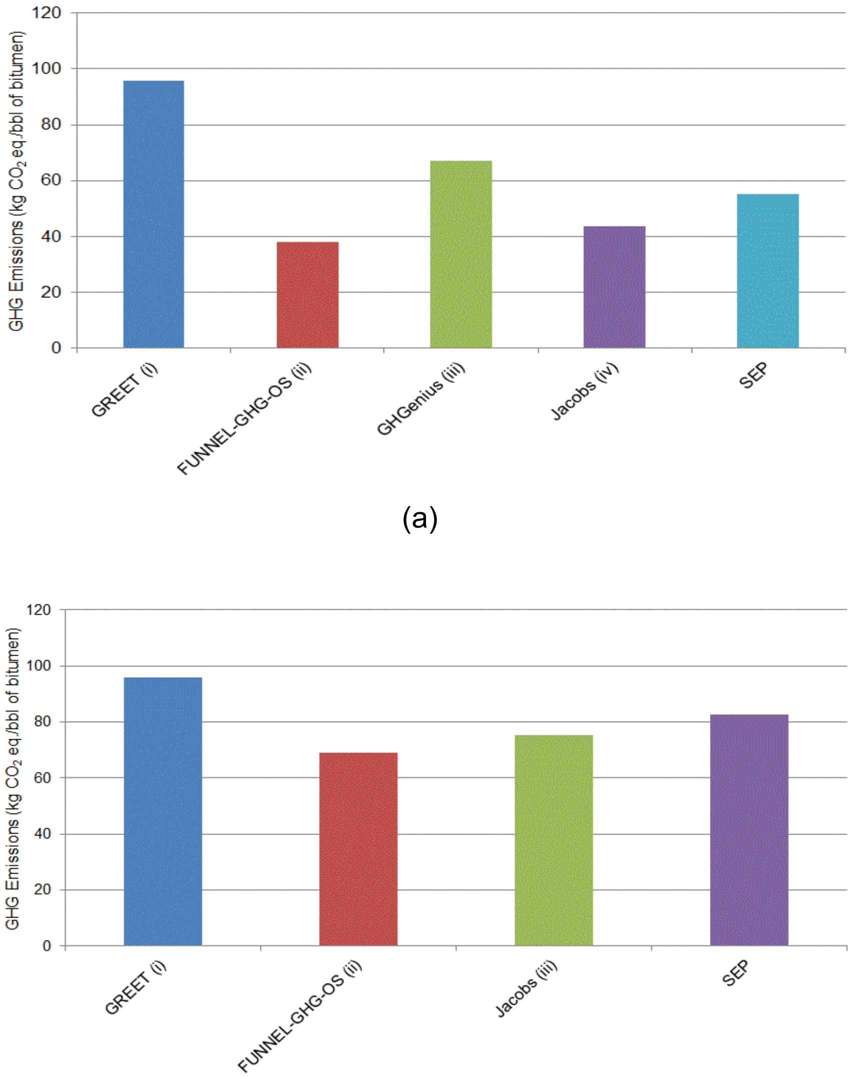
Figure 15-Distribution of (a) heat and (b) electricity consumed in hydroconversion upgrading (0.50 GJ/bbl).

For both types of upgrading unit, the main energy intensive components are the distillation columns (atmospheric + vacuum); this finding is consistent with another study [1]. Among naphtha (NHT), diesel (DHT), and gas oil hydrotreaters (GOHT), the diesel hydrotreater consumes significantly more heat energy than the others. This is because the amount of middle distillate fractions (diesel and light vacuum gas oil [LVGO]) from the ADU and VDU units are significantly higher than other fractions in both cases.

As shown in Table 10, fuel gas production in hydroconversion upgrading is significantly higher than in coker upgrading. That is due to the higher amount of light ends produced in the hydrocracker. As the feed has fewer heavier fractions, high temperature and high pressure hydrocracking [3] reactions break the vacuum residue and produce a significant amount of light ends. The light ends, after treatment, are used as fuel gas in the hydroconversion upgrading process. The emissions factor from upgrader fuel gas is considered to be 2419.4 g-CO_2 eq./kg of fuel gas [20]. VFF emissions depend on the type of reservoir and vary significantly from site to site [55]. Due to the scarcity of site-specific VFF emissions data, Canada's national inventory data were used [56] and are considered to be the same for both upgrading units.

In addition to energy, hydrocrackers and hydrotreaters consume a considerable amount of hydrogen [1]. The on-site SMR plant supplies hydrogen to all the hydrotreating units in coking upgrading and also to the hydrocracking unit in hydroconversion upgrading. More hydrogen is required in the hydrocracking unit than in the hydrotreaters [34], which increases the total hydrogen consumed in hydroconversion upgrading. To produce the hydrogen, natural gas is supplied both as fuel and feedstock. Steam is produced as a byproduct, which reduces the total steam requirement in the upgraders. The amount of natural gas and electricity required and the amount of steam produced from the SMR plant are calculated from the data provided in Table 8. In the SMR plant, emissions occur due to the transportation, combustion, and reforming of natural gas into hydrogen. The upstream and combustion emission factors of NG are taken from the literature [22]. The GHG emissions due to reforming reactions are consistent with FUNNEL-GHG-OS model results [1]. It is estimated that 1.08 kg CO_2 and 2.49 kg CO_2 eq. are emitted to hydrogenate one barrel of bitumen in the delayed coker and hydroconversion upgrading units, respectively.

The GHG emissions from upgrading bitumen produced from the solvent extraction process (SEP) fit within the range of emissions reported in existing models. The results calculated from this research were compared with existing literature and shown in Figure 16.



(a)

(b)

Figure 16-GHG emissions from (a) delayed coking (b) hydroconversion upgrading: (i) [2] (ii) [22] (iii) [25] (iv) [19].

The GREET model [22] underestimated emissions from upgrading Canadian oil sands, so the upgrading emissions were updated later [2]. But the new emissions number reported in the GREET model is higher than in Canadian models. Emissions calculated from the FUNNEL-GHG-OS model did not include VFF emissions [1]. The GHGenius model only considered delayed coking upgrading [23]. The upgrading emissions from SEP bitumen are within 25% of other model results [4, 23]. The variations in emission values reported in the literature are due to differences in production capacity, bitumen feed, emission factor values, and system boundaries.

Since the bitumen from the SEP is partially upgraded, the synthetic crude oil (SCO) produced in both upgraders has a high API gravity and low sulfur content compared with other thermal extraction methods [1, 4, 23]. The API gravity and sulfur content of the produced SCOs are provided in next section.

3.1.2 Upgrading sensitivity analysis

Energy-intensive parameters were selected based on the results in Table 10. The parameters investigated are: heat exchanger efficiency, NG heater and boiler efficiency, sulfur content in the feed, electricity emission factors, and hydrogen required in hydrotreating units. The amount of dry coke produced in delayed coking and the hydrogen required in the hydrocracking unit of the hydroconversion upgrader are also considered as sensitive parameters. The effect of steam conditions and steam energy requirement is reflected in the steam energy parameter.

As shown in Figure 17, changing parameters by ± 30% changes net GHG emissions by ±5.5% in delayed coking. GHG emissions from coking depend mostly on equipment efficiency, steam energy, and electricity emission factors. Hydrogen required in hydrotreaters has an insignificant effect on coking emissions. This might be credited to the inherently higher H/C ratio in the bitumen that reduces the hydrogen requirement in the hydrotreaters.

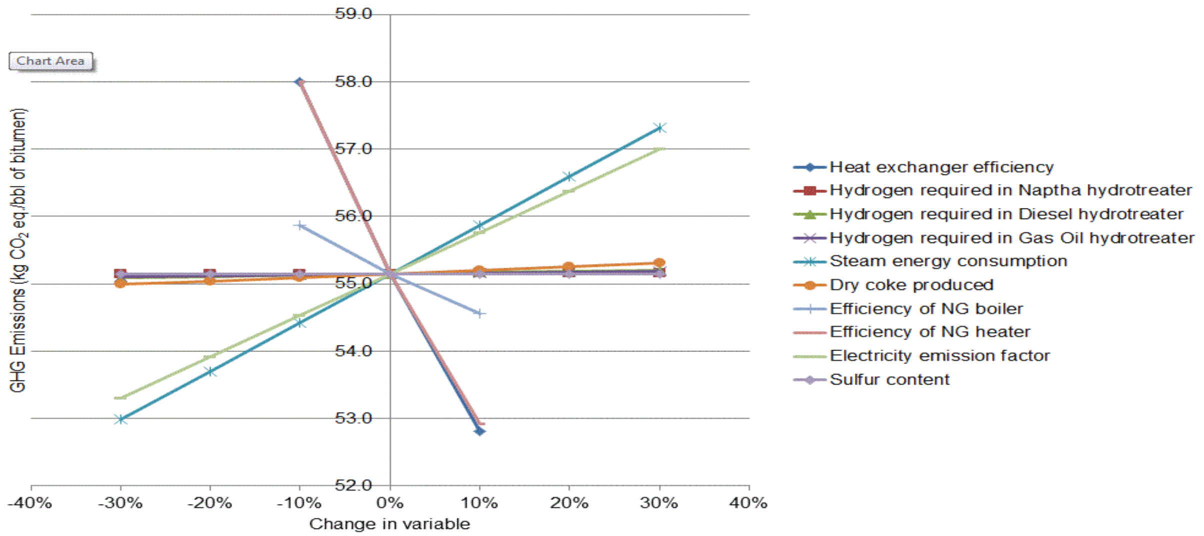


Figure 17-Sensitivity of key parameters on GHG emissions in delayed coker upgrading.

For hydroconversion upgrading, GHG emissions are greatly impacted by steam energy as presented in Figure 18.

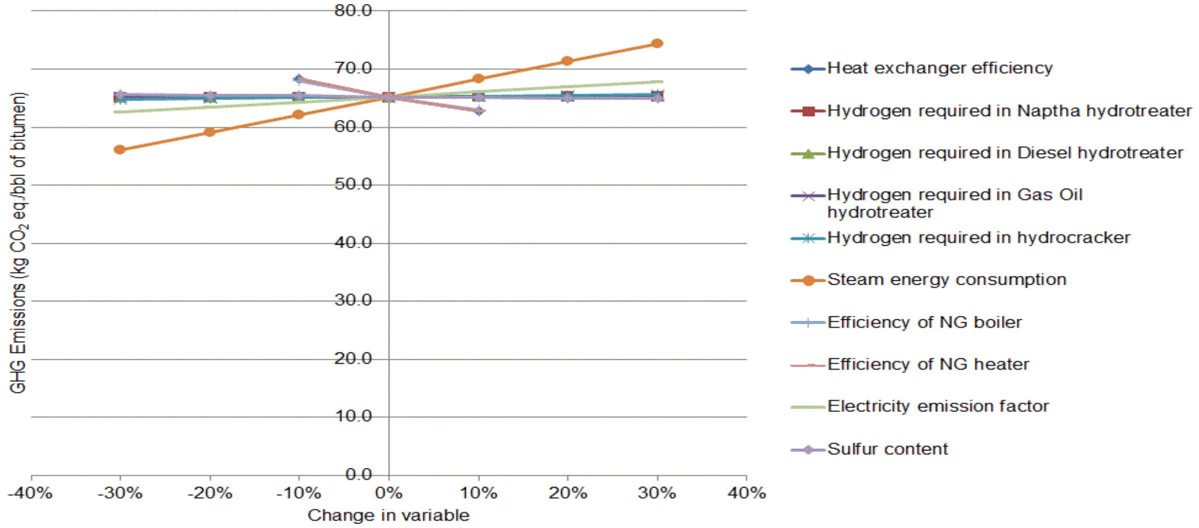


Figure 18-Sensitivity of key parameters on GHG emissions in hydroconversion upgrading.

For a ±30% change in steam energy requirement, GHG emissions vary by ±11.5%. The higher variation range compared to the range used for coker upgrading is because of the steam requirement. As with delayed coking, the electricity GHG emissions factor and NG heater efficiency influence GHG emissions significantly. Unlike assumptions in other models [3, 20], the hydrogen required in the hydrocracker is not significant. This might be because of the better quality of bitumen feed, which requires less hydrogen for hydrocracking.

Although heat exchangers, NG heaters, and boilers have been used in petroleum industries for a long time and their technologies have matured, through friction, wear, and corrosion, their performance deteriorates over time. Regular performance checks and maintenance should be conducted to ensure that the equipment is operating at a desired efficiency level. Better efficiency will result in a low steam requirement. Equally important is to obtain electricity produced with a low emission factor. Using electricity from a less emissions-intensive source like natural gas combined cycle power plants [22] and renewable energy sources like solar, wind, hydroelectric, etc., can reduce emissions from electricity consumption. On-site co-generation plants can also be considered as they will reduce upstream and overall emissions [57, 58]. These options should be assessed economically to determine the feasibility of implementation.

3.2.1 Refining

The deep conversion refinery process model described in Section 2.4 was used to determine the final products, total energy consumption, and associated emissions from processing SCO and bitumen. The API gravity, composition, and sulfur content of SCO obtained from the upgraders are provided in Table 11.

Table 11 - Properties of SCO from upgraders

Properties	DC SCO	HC SCO	SCO produced from SAGD bitumen	Source
API gravity	40.04	37.30	19.6-38.5	[3]
Naphtha (vol%)	20.29	17.16	8-25	
Diesel (vol%)	57.97	59.39	40-59	
Gas oil (vol%)	21.74	23.45	20.1- 40	
Sulfur content (wt%)	0.02	0.01	0.04-0.4	

The SCO obtained from SEP bitumen were compared with the SCO obtained from different SAGD bitumen. As seen in Table 11, the SCO produced from SEP bitumen has a relatively higher API gravity than the average API gravity of the SCO from SAGD bitumen. The sulfur content of both SCOs is significantly lower than that from SAGD bitumen. The results seem reasonable because the bitumen obtained from the SEP has better properties than bitumen obtained from SAGD.

We assumed that the feed is supplied in the refinery at a rate of 25,000 bpd. The yield obtained per bbl of feed is presented in Table 12. The distillation fractions from refinery ADU and VDU are provided in the Supporting Information. SCO is a lighter feed than bitumen [3]. SCO is rich in naphtha, diesel, and kerosene, whereas bitumen contains heavier fractions such as gas oil and residue [1].

Table 12 - Yield obtained from refining per bbl of different feeds

Products	Units	DC SCO	HC SCO	Bitumen
Fuel gas	bbl/bbl of feed	0.51	0.42	0.00
Liquefied petroleum gas (LPG)	,,	0.05	0.04	0.05

Table 12 - Yield obtained from refining per bbl of different feeds

Diesel	,,	0.06	0.12	0.25
Kerosene/Jet fuel	,,	0.05	0.05	0.01
Gasoline	,,	0.37	0.40	0.73
Fuel oil	,,	0.04	0.08	0.18
Coke*	kg/bbl of feed	0.00	0.00	0.00

*Coke formation is almost negligible

As shown in Table 12, the fuel gas produced from refining per bbl of SCO is significantly higher than the fuel gas produced from refining SCO from SAGD bitumen (0-0.15 bbl/bbl of feed) [1, 25]. Table 11 shows that the SCOs produced from SEP bitumen has relatively higher naphtha and diesel contents (close to the upper range of SCO produced from SAGD bitumen) and also significantly less sulfur content. The reason is that in the SEP, the solvent diffusion coefficient is more effective than thermal diffusion coefficient in asphaltene precipitation. Since the produced bitumen has inherently less sulfur, upgrading reduces the sulfur content even further and improves the API gravity of the produced SCO drastically. During distillation in the ADU, synthetic crude oil loses its stability, thereby distilling a significant fraction of SCO produced from both types of upgraders. But bitumen from the SEP has higher heavier fractions than SCO and a negligible amount of fuel gas is produced when bitumen is directly fed into the refinery. As the bitumen is partially upgraded (unlike SAGD bitumen), more liquid petroleum gas (LPG) is produced per bbl of bitumen [1, 25]. Significantly, more gasoline is produced from the upgraded bitumen than from SAGD bitumen (0.54 bbl/bbl of feed) [1, 25], which indicates that the bitumen produced from the SEP has a higher naphtha fraction than conventional SAGD bitumen [25]. Refining HC SCO produces more gasoline and diesel than DC SCO. This is because in hydroconversion upgrading, the feed is hydrogenated and cracked more intensely [1]. Fuel gas is not a desired product, so bitumen produced from the SEP should directly be refined without being upgraded to SCO. A negligible amount of coke is produced from refining both SCO and bitumen. The produced yield fractions from both SCO and bitumen fall within the broad range of yield fractions reported for the wide range of crude assays in the Prelim v1.1 model [59].

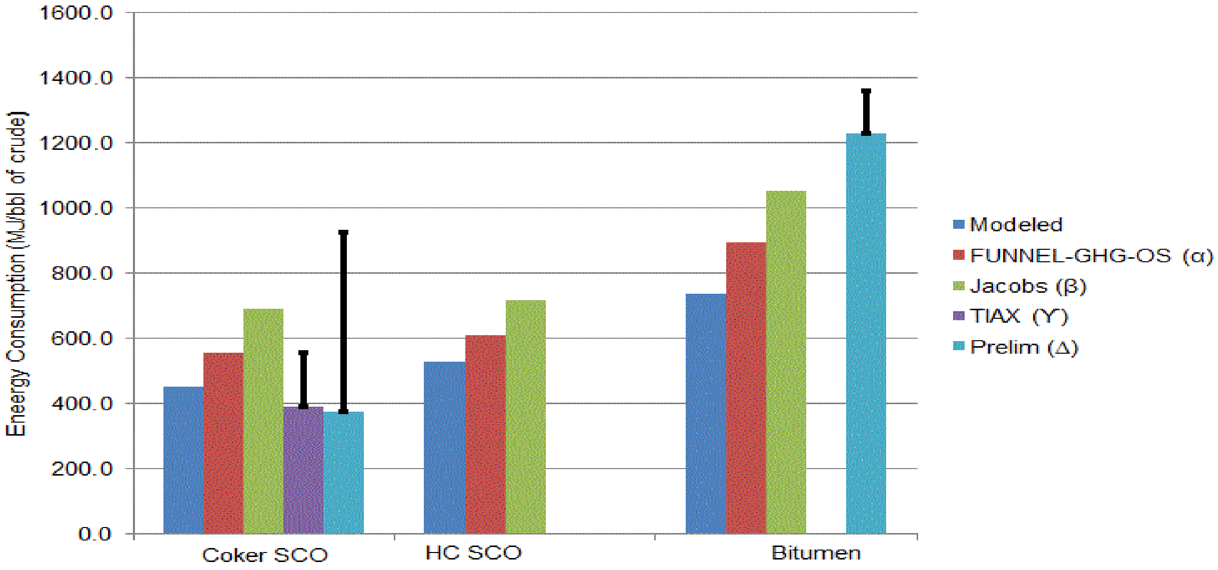


Figure 19-Energy consumption in refining per bbl of crude as modeled compared to other models*.

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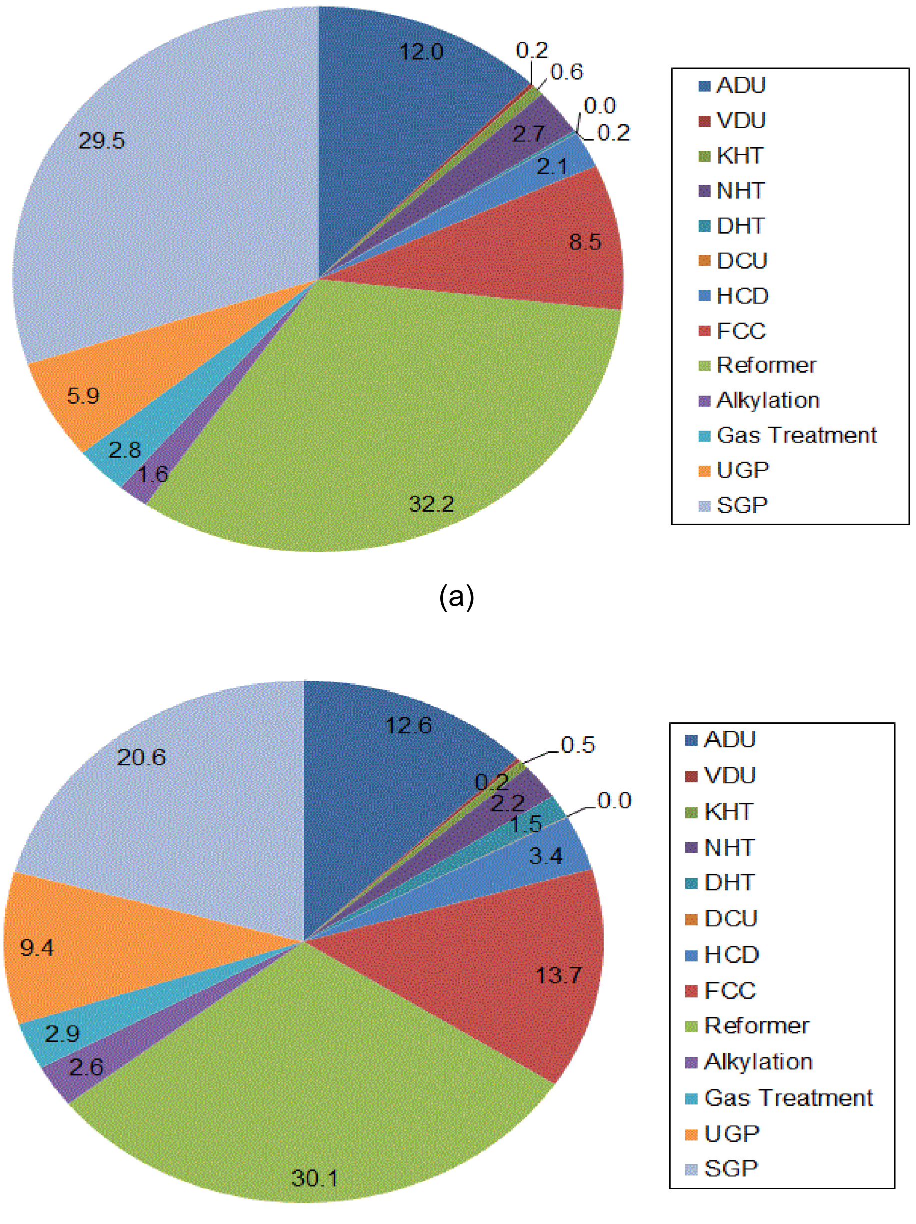
*All the numbers in the literature (α, β, Y, Δ) are for SAGD based bitumen while the modeled numbers are for bitumen extracted through solvent-based processes. (α) The FUNNEL-GHG-OS model estimates energy consumption using the same HYSYS model considered in this study [17] . (β) [19]. (Y) The TIAX model does not differentiate between the energy consumption for SCO from the coker and hydroconversion. The range corresponds to the SCO processed in PADD (Petroleum Administration for Defense Districts) 2, PADD 3, and California. (Δ) PRELIM does not consider the SCO quality produced from the coker and hydroconversion. The range represents energy consumption for different types of crudes processed in different types of refineries [27].

As shown in Figure 19, depending on the crude refined, the total energy consumption in the refinery ranges from 452.8 MJ/bbl to 736.8 MJ/bbl of crude. This is because of the quality of the crude, refinery configuration, and type of desired products [5, 17, 26].

Refining bitumen is the most energy intensive pathway, and energy consumption is estimated to be 68.5% higher than refining coker SCO. This is because distilling bitumen in the ADU and VDU is very energy intensive (energy consumption is more than double) compared to the SCO. Also, SCO (produced from both the upgraders) have significantly higher vapor fractions, which lead to the distillation of fuel gas with very low energy consumption. But the energy consumed in refining solvent-extracted bitumen is almost 21.5 - 84.7% less than SAGD-produced bitumen. 15.1-35.4% less energy is required to refine HC SCO. In case of coker SCO, the energy consumption is within the range of the TIAX and Prelim models [25]. The lower energy consumption reported in the TIAX model is because the TIAX model used an aggregate approach rather than detailed calculations for each sub-unit operation [5]. In the Prelim model, a lower energy consumption corresponds to conventional crudes having better properties (an API gravity as high as 47 or more) compared to coker SCO produced from SEP bitumen [25]. The lower energy consumption in both the TIAX and Prelim models is also influenced by higher production capacities [60]. Increasing plant capacities lowers energy consumption and cost [60]. Energy consumption can be reduced further by increasing plant capacity [4, 5, 25].

The detailed breakdown of energy consumption for refining coker and hydroconversion SCOs and bitumen is shown in Figure 20.



(a)

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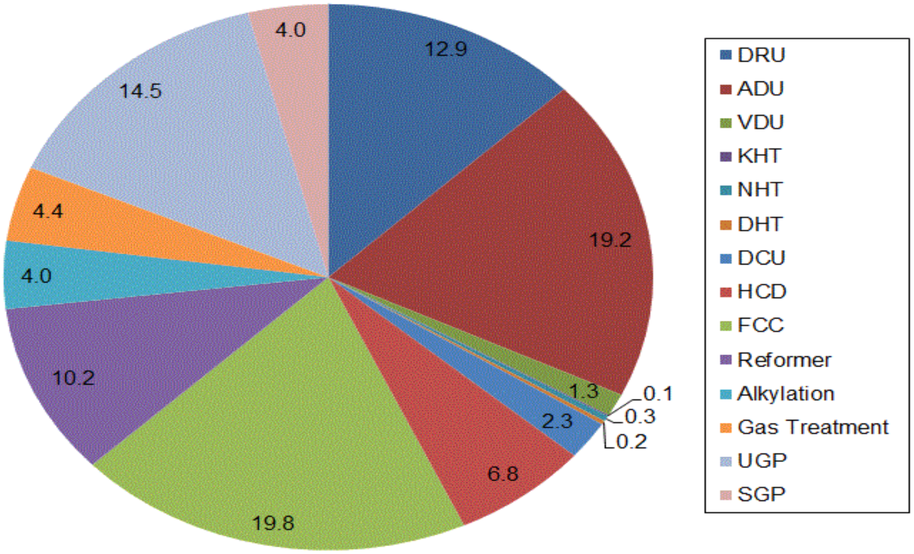

(c)

Figure 20-Energy consumption breakdown in each sub-unit operation of refining (a) coker SCO (b) hydroconversion SCO, and (c) bitumen.

For SCO distillation, 12.3-12.8% of the total energy is required in the distillation columns, but for bitumen, it is more than 20%. As mentioned earlier, a major fraction of the SCOs (both from coker and hydroconversion) is light components (C_4 or less) that distillate at low temperatures, thereby reducing the energy required in SCO distillation. In the case of SCO, the catalytic reformer consumes most of the energy. In a catalytic reformer, energy is required to preheat the reactor beds and to regenerate the catalysts [61]. A significant amount of energy is also consumed in the dehydrogenation and dehydrocyclization reactions (highly endothermic) [61]. So, the higher the feed, the higher the energy required to reform low octane naphthas into high octane reformates. As the SCOs have very high naphtha content, the catalytic reforming is the most energy-intensive operation. This implies that the SCO produced from the upgraders has a relatively higher amount of lighter fractions. For bitumen refining, energy consumption in the reformer is within the range of other studies [1, 25]. A significant amount of energy is also consumed by the SGP unit in refining SCO. The high energy consumption is from treating the high amount of fuel gas produced from SCO as shown in Table 12. As bitumen is the heaviest feed, energy consumption in fluid catalytic cracking (FCC) is higher for bitumen (19.8%) than for SCO (8.5-13.7%). SCO, being lighter than bitumen, requires less cracking to convert heavier fractions into final products [3]. Energy consumption in the UGP ranges from 5.9-14.5%, depending on the feed. The higher production of unsaturated gases from bitumen leads to higher energy consumption than from SCO [1].

As with the upgraders, hydrogen is supplied to the hydrotreaters and hydrocrackers from an on-site SMR plant. The input data used to calculate the total energy required in steam methane reforming are presented in Table 8. Hydrogen produced in the reformer supplements the total H_2 requirement in the refinery. The total energy consumption calculated in the SMR plant is around 7.4%-24% of the total refinery energy consumption. Similar energy consumption results have been reported in the Prelim model [25]. The feedstock required to produce hydrogen comes from the SGP and external natural gas suppliers. Steam produced as a byproduct from the reforming reaction is supplied to the refinery to reduce the refinery steam requirement. Steam produced from the Claus sulfur recovery and tail gas treatment unit also supplement the refinery steam requirement [25].

The total energy required in the refinery comes from steam, electricity, fuel gas, and natural gas. About 25.1%-49.6% of the total energy required is for steam production. More steam is required for bitumen than for SCO because more energy is required to distillate heavier fractions [62]. The total electricity consumption contributes 8.3%-11.5% to the total energy requirement. As from refining both bitumen and SCO, a negligible amount of coke is produced, so all the coke is burned to maintain the catalyst activity in the FCC unit. In the case of refining SCO, the total fuel gas produced is sufficient to meet the heating requirement in the refinery. The heating value of fuel gas is provided in the Supporting Information. The quality of fuel used to meet the total energy requirement has an effect on GHG emissions. To avoid the complexity of fuel quality, it is assumed that 100% fuel gas and 100% natural gas are used to meet energy demand.

The total emissions from processing crude (bitumen and SCO) range from 26.6 kg CO_2 eq./bbl of SCO to 84.3 kg CO_2 eq./bbl of bitumen, as shown in Figure 21. Emissions are proportional to energy consumption [1]. As more energy is required to refine heavier feeds, bitumen refining results in higher emissions than SCO.

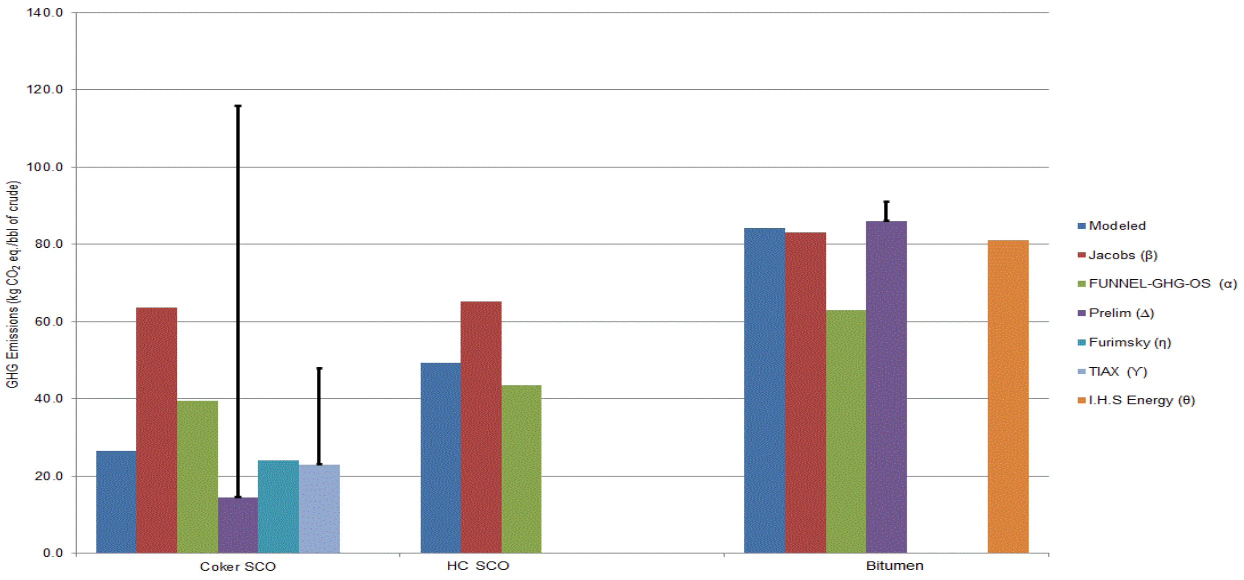

Figure 21-GHG emissions from refining per barrel of crude*.

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*All the numbers in the literature (α, β, Υ, Δ) are for SAGD based bitumen while the modeled numbers are for bitumen extracted through solvent-based processes. (α) FUNNEL-GHG-OS does not include VFF emissions. (β), (Υ) and (Δ) refer to Figure 11. (η) The Furimsky model only considers GHG emissions because of the H2 production required for the refining process. This model did not differentiate between the emissions from coker and hydroconversion upgrading. [64]. (θ) [65].

As shown in Figure 21, the emissions reported in this study are in good agreement with other existing studies [1, 4, 5, 25, 64]. The Furimsky model [63] gave a rough estimate of the total energy consumption in the refinery and only considered emissions from H_2 production. Prelim [25] provides a wide range of emissions from crude refining. This is because the model considers a great variety of crudes. The range of emissions is because of different feed quality and the configuration of the refinery [26, 65].

Since refineries produce different products, proper allocation is required to evaluate the impact of the energy and emissions from the production of individual transportation fuels [50]. For a specific amount of feed, the variation in the production volume of one refined product changes the production volume of other products [1], ultimately affecting the overall energy consumption and emissions. To allocate energy consumption and emissions more accurately to individual products, the ISO recommends allocation at the refinery sub-process level instead of the refinery level [50]. According to Wang [50], the most energy-intensive transportation fuels are gasoline and diesel. Therefore, refinery sub-process level allocation is used to determine the emissions from gasoline and diesel production in this study to compare with other existing models. Figure 22 shows GHG emissions for gasoline and diesel (transportation fuels) at the refinery process level. The results are represented as g CO_2 eq./MJ of gasoline and g CO_2 eq./MJ of diesel for gasoline and diesel, respectively.

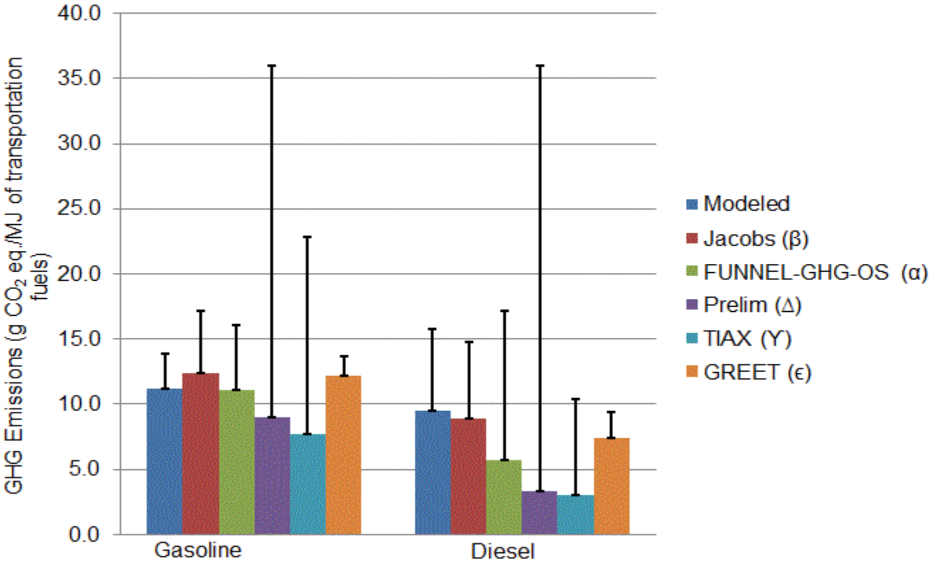


Figure 22-GHG emissions of gasoline and diesel at the refinery process level.

(β) The higher and lower emission values for gasoline and diesel correspond to gasoline and diesel production from bitumen and SCO, respectively [19]. (α) The higher and lower emission values for gasoline and diesel correspond to gasoline and diesel production from bitumen and SCO, respectively. For gasoline, SCO produced from hydroconversion gives the lowest value whereas for diesel, coker SCO gives the lowest emission value [22]. (Δ) Prelim reports gasoline and diesel production emissions from 29 different crudes with 10 refinery configurations [27]. (Ƴ) The higher and lower emission values for gasoline and diesel correspond to gasoline and diesel production from bitumen and SCO, respectively. Gasoline produced from California crude gives the lowest emissions and diesel produced from crudes from PADD (Petroleum Administration for Defense District) 2 and PADD 3 region gives the lowest emissions [18]. (ϵ) The higher and lower emission values for gasoline and diesel correspond to gasoline and diesel production from bitumen and SCO, respectively [2].

As shown in Figure 22, the results calculated in this model are within the range of those found in the literature. The variation in results may be due to differences in the feed rate, relative production fractions of individual fuels, different refinery configurations, and quality of feed supplied to the refinery. The higher range of emissions (represented by the error bar) shown in Figure 22 corresponds to gasoline and diesel produced from bitumen and the lower range is for gasoline and diesel produced from SCO. There is a proportionate relation between energy consumption and emissions [25]. As refining bitumen requires more energy, it also results in higher GHG emissions. GHG emissions from gasoline produced from coker SCO and bitumen

(11.2 g CO_2 eq./MJ of gasoline and 11.6 g CO_2 eq./MJ of gasoline respectively) are almost equivalent but lower than gasoline produced from hydroconversion SCO (14.5 g CO_2 eq./MJ of gasoline). For diesel, however, GHG emissions from bitumen are significantly higher (15.5 g CO_2 eq./MJ of diesel) than from coker (9.5 g CO_2 eq./MJ of diesel) or hydroconversion SCO (14.3 g CO_2 eq./MJ of diesel).

The production of gasoline and diesel from SCO is less energy and GHG emissions intensive than from bitumen. But a significant amount of energy is required in upgrading operations, which results in considerable GHG emissions. Since the GHG emissions from gasoline production are the same for coker SCO and bitumen, pathway II would be less energy- and emissions-intensive than pathways I and III, given that significantly more gasoline is produced than diesel (as shown in Table 12). To justify the above statements a comparative analysis was made by allocating upgrading emissions on a mass basis as described by Wang et al. [50] and adding them with the refinery emissions for pathways I and III. The equations for allocation are provided in the Supporting Information (Appendix B).

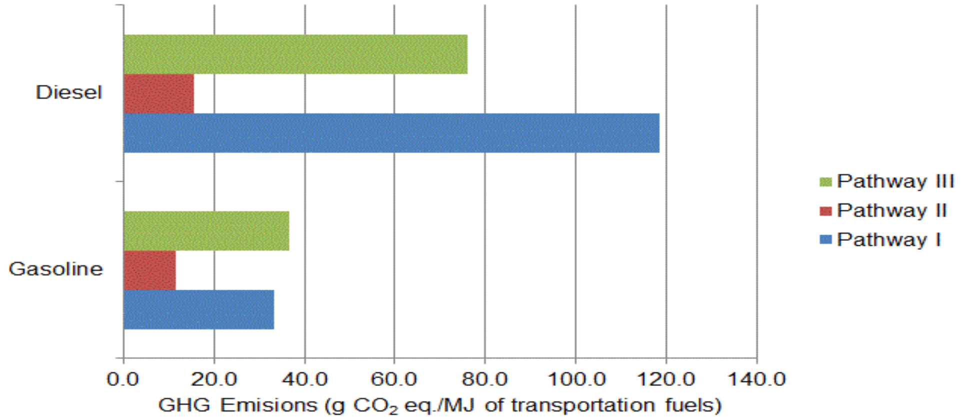
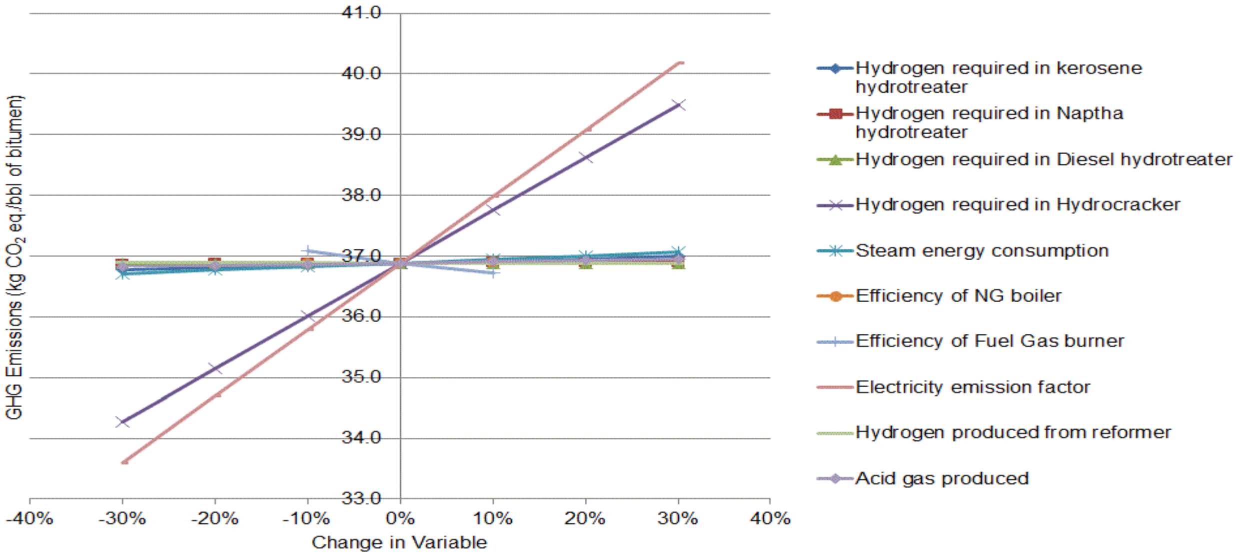


Figure 23-Comparative analysis of GHG emissions from different production pathways.

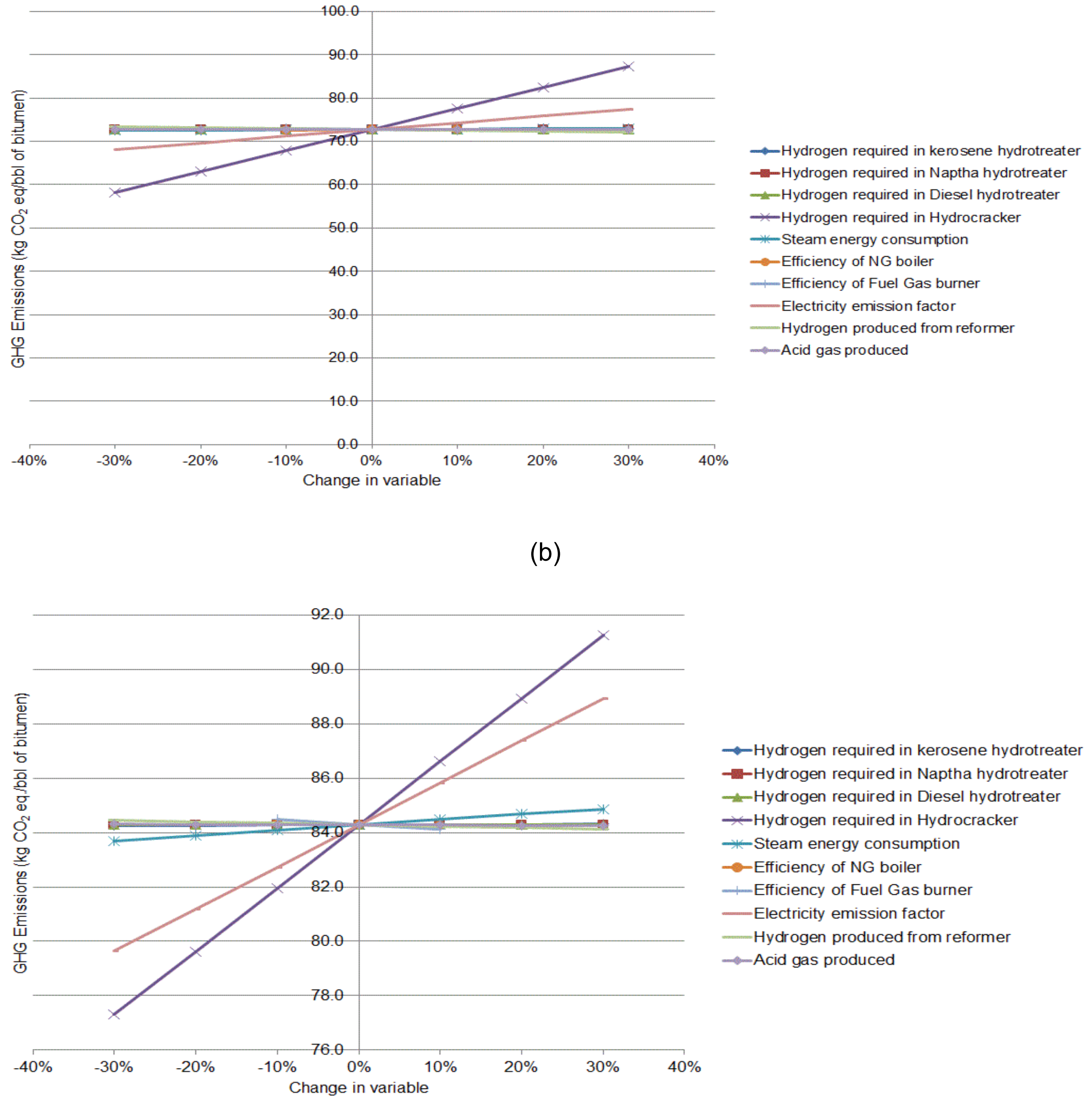
As presented in Figure 23 for gasoline, pathway III is the most GHG emissions intensive and for diesel, pathway I is. Pathway II (refining bitumen) is the least emissions-intensive path. If upgrading is not required and bitumen can be refined directly, energy consumption and emissions will be reduced tremendously and the production path will be similar to the production of transportation fuels from conventional crudes. This production pathway will also reduce transportation fuel production costs significantly because it will eliminate the need to build upgrading units. It is only possible when extracted bitumen is partially upgraded during the extraction process and refineries can handle the bitumen feed without the need to upgrade.

3.2.2. Refinery sensitivity analysis

A sensitivity analysis was performed on the key parameters in the refinery that impact the energy efficiency and performance of refinery operations. The parameters investigated are: the hydrogen required in the hydrotreaters and hydrocracker, the total steam energy consumption, the hydrogen produced from the reformer, the total acid gas produced (CO_2+H_2S), and the efficiency of the equipment. SGP and UGP unit operating conditions were not considered in the sensitivity analysis because the energy consumption calculated in these units was attributed to abnormally higher fuel gas, which is unusual in a refinery. To determine sensitivity, all the parameters were varied by ±30% from base conditions except the efficiency of the equipment.



(a)



(b)

(c)

Figure 24-Impact of key parameters on GHG emissions from refining (a) coker SCO (b) hydroconversion SCO, and (c) bitumen.

The efficiency of the equipment was varied by ±10% from the base condition. As presented in Figure 24, the two most sensitive parameters are the hydrogen required in hydrocracking and the electricity GHG emission factor for electricity production. As mentioned earlier, the hydrogen required in hydrocracking is higher than in hydrotreating, and varying the H_2 requirement in the hydrocracker significantly affects the energy consumption and ultimately the GHG emissions. The electricity emission factor depends on the technology and the type of fuel used to generate electricity. In upgrading, the emission factor due to the on-site combustion of natural gas and the distribution of electricity is considered to be 820 g CO_2 eq./kWh [48]. This emission factor is relatively higher than that for refinery electricity emissions because the upgrading unit is assumed to be located in Canada and the refinery in the USA. But depending on the technology and type of fuel used to generate electricity, emissions can be as low as 428.31 g CO_2 eq./kWh [22]. Selecting electricity from a low-emissions supplier will reduce emissions drastically.

Apart from the two main parameters, the efficiency of the fuel gas burner in the case of refining coker SCO and the total steam consumption in the case of refining bitumen also influence GHG emissions. The total steam consumption depends on steam pressure, quality, and water inlet temperature. Better steam quality results in a higher heating value [66] of steam.

3.3 Uncertainty analysis

Emissions also vary significantly because of changes in key parameters as described in sections 3.1.2 and 3.2.2. In order to accommodate the uncertainties/changes in emissions, we conducted an uncertainty analysis through a Monte Carlo simulation. To conduct a Monte Carlo simulation, the distributions of the input parameters first need to be defined. The range of data considered to develop the input distributions is provided in the Supporting Information. For equipment efficiency and steam heating value, a PERT distribution [67] was used in the Monte Carlo simulation. A PERT distribution emphasizes the most likely value rather than maximum and minimum estimates [67]. A PERT distribution was thus considered for NG heaters, boilers, and fuel gas burners, as their efficiency does not vary extensively. PERT generates an output distribution similar to normal distributions without the input parameter value. As a result, a more conservative range of output values will be obtained, which means that output estimates will not vary significantly from the exact value. For the rest of the sensitive input parameters (electricity emission factors, heat exchanger efficiency, and hydrogen required in the refinery hydrocracker, a triangular distribution was used. Although electricity can be produced from a wide range of technologies, electricity production is shifting from coal to natural gas and renewable energy sources, which will reduce electricity GHG emissions [47, 48]. To obtain more conservative outputs from the most predictable input values and to get a lower standard deviation, a triangular distribution [24] was considered for the heat exchanger efficiency. The hydrogen required in the refinery hydrocracker depends on the feed quality and feed rate to the hydrocracker. As the feed quality causes higher uncertainties in emissions, a triangular distribution with a wider range was generated considering the value calculated here as the mode value. The maximum and minimum values were collected from existing studies [1, 4, 22, 25]. The wide range with the triangular distribution generates an output emission range that emphasizes on the feed quality mentioned in this study.

To ensure the sampling error is less than 0.1 kg CO_2 eq./bbl of bitumen, approximately 100,000 samples are required for each simulation. The samples were simulated in ModelRisk [68]. The uncertainty in upgrading and refining emissions was generated within a 99% confidence interval. In Figure 25, emissions are presented within 5%-95% confidence intervals.

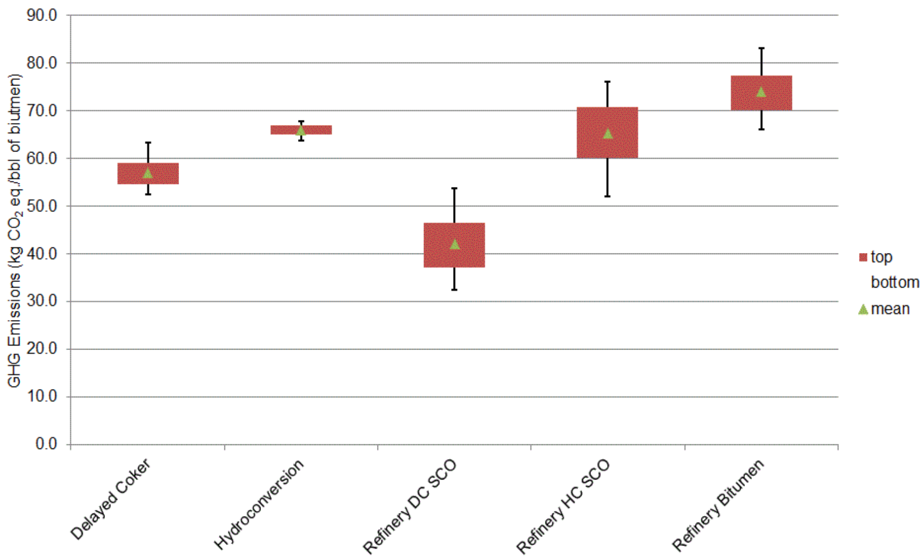


Figure 25-Uncertainty in emissions from upgrading and refining operations.

Detailed uncertainty emissions including the impact of each critical parameter for upgrading and refinery operations considered for all the pathways are provided in the Supporting Information (Appendix B). Only the uncertainty in emissions from upgrading and refining operations is discussed here. The mean is the 50th percentile while the top and bottom of the rectangular boxes are the 75th and 25th percentile, respectively. Accordingly, the top and bottom error bars show emissions at the 95 and 5 percentile, respectively. Refinery operations show a wider range of emissions than upgrading operations. Also, the emission range is higher for refining SCOs than for bitumen. The wider range signifies the wider range of hydrogen required to hydrocrack different qualities of refinery feed (see Supporting Information). For upgrading operations, the uncertainty in emissions is mainly because of the electricity emission factor, which depends on the fuel and technology used to generate electricity. Depending upon the heat exchanger, emissions can vary considerably for coker upgrading, but, as mentioned earlier, the efficiency of the heat exchangers does not vary significantly.

4. Conclusions

A detailed comparative analysis of transportation fuels produced from solvent-extracted bitumen was conducted by developing three production pathways. The GHG emissions from hydroconversion upgrading in pathway III (65.2 kg CO_2 eq./bbl of bitumen) are higher than from coker upgrading (55.1 kg CO_2 eq./bbl of bitumen), but hydroconversion upgrading yields a better quality product. The bitumen yield is significantly higher than from conventional bitumen. The use of electricity produced from less emissions-intensive sources (i.e., natural gas combined cycle power plant or renewable sources) in upgrading operations can reduce emissions significantly.

Refining bitumen consumes 68.5% more energy than refining SCO. But bitumen needs to be upgraded to produce SCO. As emissions are proportional to energy consumption, emissions from refining bitumen (84.3 kg CO_2 eq./bbl of bitumen) are significantly higher than from refining SCO (36.9-72.7 kg CO_2 eq./bbl of bitumen), and upgrading is an energy- and emissions-intensive process that increases overall emissions. By allocating emissions at the refinery process level, an estimated 11.6 and 15.5 g CO_2 eq. are emitted per MJ of gasoline and diesel, respectively, in production pathway II. The emissions in pathway II are comparable to those from gasoline and diesel produced from conventional crudes. So, when the three pathways are compared, pathway II would be the best option to convert bitumen from solvent extraction into transportation fuels. In addition, pathway II eliminates upgrading operations and thereby also reduces production costs. The overall range of uncertainty in refinery operations is wider than in upgrading operations, which is attributed to the higher number of energy- and emissions-intensive parameters in refining than in upgrading operations.

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Chapter 4

A life cycle assessment of oil sands-derived liquid fuel production based on the solvent extraction process (SEP)

This chapter describes the “well-to-tank + combustion” (WTT+C) emissions from oil sands-derived transportation fuels (gasoline, diesel, jet fuels) for solvent-based extraction process. Transportation fuels are produced from synthetic crude oil (SCO) or bitumen. Bitumen is upgraded to SCO in an upgrading unit. The bitumen is obtained from oil sands, which is extracted from the solvent extraction process (SEP). Life cycle inventories are included for each stage of the transportation fuels (recovery and extraction, pipeline transportation, upgrading, refining, fuel distribution, and combustion in vehicles).

4.1 Introduction

According to International Standard Organization (ISO) 14040 [1], “LCA studies the environmental aspects and potential impacts throughout a product’s life cycle (i. e. cradle-to-grave) from raw material acquisition through production, use and disposal.” ISO 14040 [1] and ISO 14044 [2] defined four elements for a standard LCA study. The first element is the “Definition of goal and scope” [3]. The goal defines the objective, interest, and target group of an LCA study [3]. The depth and accuracy also need to be defined while defining the goal of the study [3]. Since the ISO is quite flexible in terms of the details of an LCA study [3], the problem of defining the functional unit, the method and system boundary are achieved by the scope of the study [4].

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*WTT+C ≈ WTW

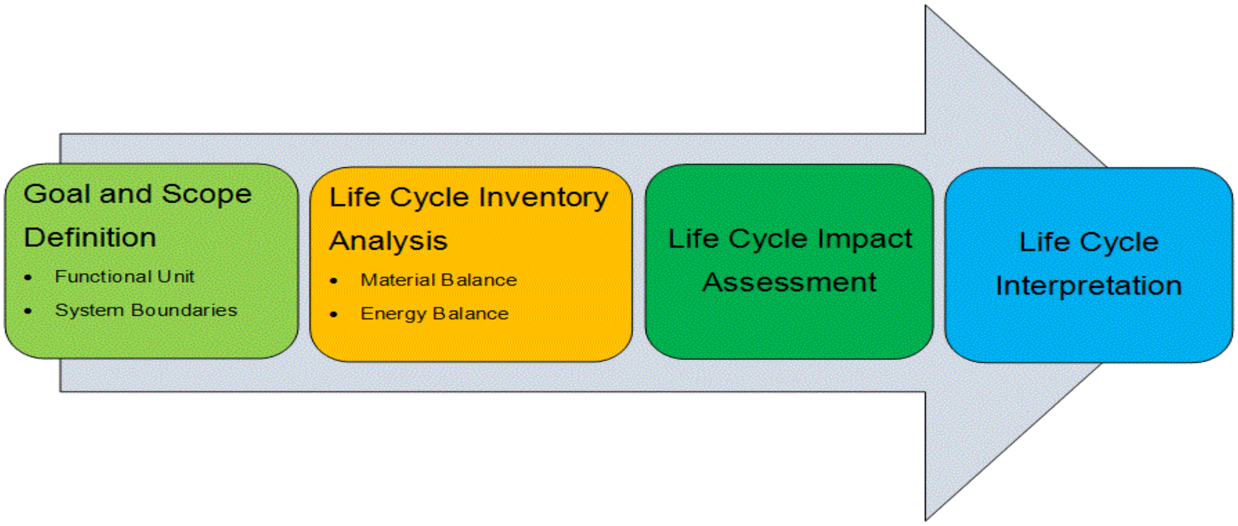

Figure 26-Standard LCA framework as per ISO standards.

As shown in Figure 26, the next element in an LCA is the LC inventory (LCI) analysis [5], a material and energy analysis based on a linear systems analysis following the principles of mass and energy balance [5]. A life cycle impact assessment (LCIA) is the next phase of an LCI [5]. An LCIA aims to understand the impact categories (global warming potential [GWP], human impact, social impact, etc.) and assigns the total environmental impact to relevant impact categories [4]. The results from the life cycle inventory analysis and life cycle impact assessment are combined in the final step, “Life cycle interpretation,” as per the goal of the study, and, finally, conclusions and recommendations are drawn from the results.

4.2 Methodology

To order to assess the LC environmental impact of transportation fuels it is necessary to define the system boundaries, goal and scope, functional unit, collection and allocation of relevant life cycle inventory data, and then conduct an impact assessment [1].

4.2.1 Goal and Scope

The primary goals of this LCA study are:

- To allocate the total GHG (WTT+C) emissions obtained from the SEP simulation model to quantify the LC emissions of transportation fuels from oil sands products, SCO and bitumen;
- To compare the total and allocated emissions of transportation fuels produced from solvent extracted bitumen with bitumen produced from thermal extraction processes;
- To identify the most GHG-intensive processes in the production of transportation fuels by distributing the total emissions; and
- To determine the uncertainty of the model for commercial-scale implementation through a Monte Carlo simulation.

The scope of the study includes all the processes throughout the entire LC from in situ solvent extraction and recovery of bitumen to the combustion of transportation fuels in vehicles.

4.2.1.1 System Boundary

Life cycle GHG emissions consist of well-to-tank (WTT) emissions and vehicle combustion (C) emissions. Three production pathways were considered in this study. To compare the total emissions from transportation fuels, a system boundary was developed and is shown in Figure 27.

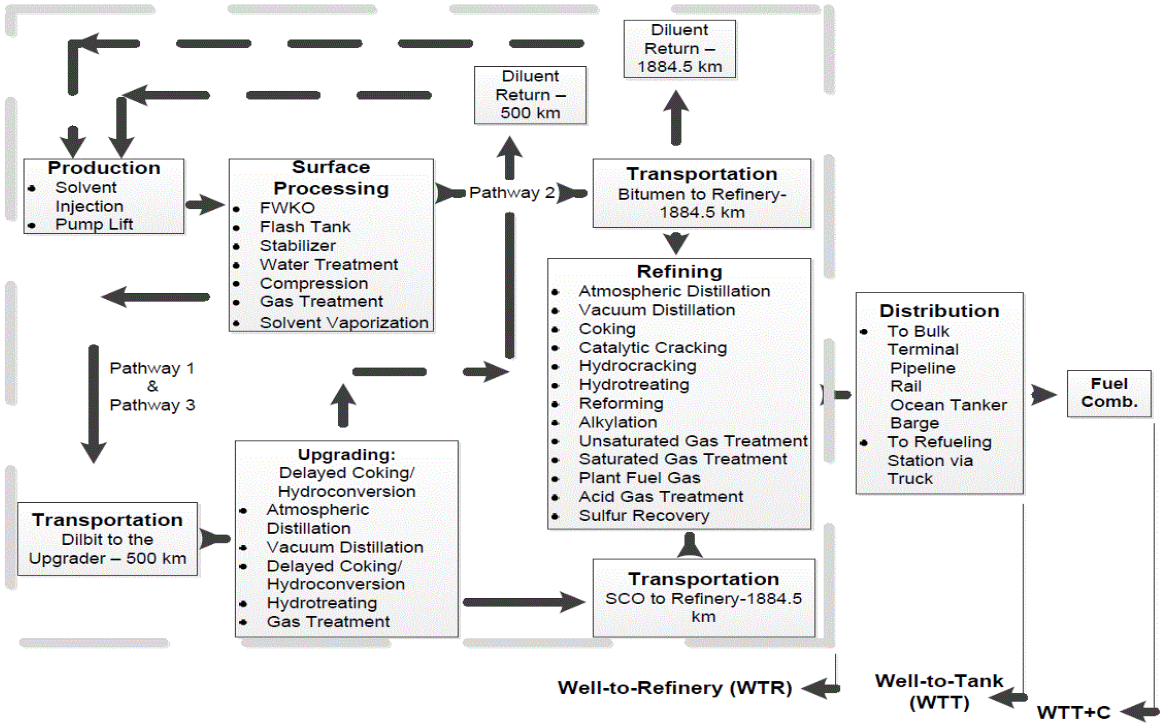

Figure 27-System boundary of the SEP model.

Bitumen, after extraction and recovery, is mixed with diluent and sent as dilbit to the upgrading units in both pathways I and III. For pathway I, bitumen is sent to a delayed coker upgrading unit whereas for pathway III, bitumen is sent to a hydroconversion upgrading unit. The distance from extraction to the upgrading unit is considered to be 500 km, as reported in the GHOST model [6]. In both upgrading units, diluent is separated and sent back to the extraction site. The diluent return line is considered to be inside the system boundary, and so GHG emissions from diluent return were calculated. Bitumen extracted using solvent based extraction method is converted to SCO in the upgrading units, and the SCO is sent to the refinery, where it is converted to transportation fuels. In pathway II, bitumen is mixed with diluent and sent as dilbit directly to the refinery unit without upgrading. In all three pathways, a transportation distance of 1171 miles was considered, the distance of the TransCanada Keystone pipeline [7]. In pathway II, diluent is recovered from the refinery and sent back to the extraction site. Instead of being returned, diluent can also be sold in the local market or processed in upgrading and refinery units along with bitumen to increase yields. So studying diluent that is returned from different places to the extraction site will give insights into transportation energy consumption and emissions and will assist in considering other options from economic and emissions perspectives. In Figure 27, the boundaries are defined at different levels to give more insight into the upstream and downstream emissions.

4.2.1.2 Functional Unit

A bottom-up approach is used to quantify the mass and energy balances at each life cycle stage. A functional unit of kg CO_2 eq./barrel of bitumen is used for pre-refinery emissions and g-CO_2 eq./MJ of gasoline/diesel/jet fuel is used for WTT+C emissions. The GHG emissions include the impact of other major GHGs such as N_2O and CH_4. To define the energy content of fuels, a lower heating value (LHV) consistent with that reported in the literature [8] was used.

4.2.2 Life Cycle Inventory (LCI)

The LC bitumen production pathways involve the following unit operations:

- Recovery and extraction (SEP)
- Transportation of dilbit to the upgrading unit
- Upgrading bitumen in the delayed coker or hydroconversion unit
- Transportation of SCO and bitumen into the refinery

- Refining of oil sands products
- Fuel transmission and distribution
- Combustion of gasoline and diesel in vehicles

First, oil sands are extracted from the reservoir using vapor solvents. Through surface operations, bitumen is recovered from bitumen-solvent emulsion (see chapter 2 for details). The main energy inputs in solvent extraction and recovery are natural gas and electricity. As described in chapter 2, bitumen extracted through the SEP has a higher API gravity and lower asphaltene content than the main in situ thermal extraction processes, SAGD and CSS. Three pathways were developed (see Figure 27) to determine the best production pathway for the high-quality bitumen. In two paths (I and III), bitumen is upgraded to SCO. SCO is a light oil with low sulfur and asphaltene content [4] that can easily be transported into a refinery via pipeline. In the third path, bitumen is sent directly to the refinery. In order to meet pipeline specifications (as outlined by Gray [9]), the bitumen is mixed with natural gas condensate or naphtha called diluent. The diluent is mixed with bitumen in a sufficient amount (approximately 22.4:77.6 [vol%]) to achieve the appropriate pipeline viscosity and API gravity. In the pathways I and II, diluent is separated from dilbit in the upgrading units and recycled (assuming no loss) back to the extraction site, and in pathway III, diluent is separated in the refinery. It is assumed that the refinery is located 1171 miles from both the extraction and upgrading units. Both bitumen and SCO are processed in a deep conversion refinery [10]. Transportation fuels such as gasoline, diesel, and jet fuel are produced in the refinery, transported and distributed to retail locations via ocean tankers, barge, rail, and pipeline, and combusted in vehicles.

Finding quality LCI data is difficult and it also depends on the method used to obtain it. To overcome this problem, models were developed for the three production pathways. In these models, mass and energy balance are used to determine the LCI data for energy consumption in extraction and recovery operations. Three types of process energy (heat, steam, and electricity) are required for upgrading and refining operations. It is assumed that all the required steam is produced from the natural gas boiler. The total heat required in the extraction unit comes from both produced and natural gas. The natural gas requirement and GHG emissions are calculated based on an instantaneous solvent-to-oil ratio ($iSOR_{solvent}$) using heat and mass transfer equations (details in Appendix C). To meet upgrading and refining heat requirements, the produced fuel gas is burned along with natural gas. The efficiency of the fuel gas and natural gas burner is considered the same (87%) [11]. The natural gas boiler efficiency is considered to be 85% [6].

It is assumed that all the electricity is supplied from the Alberta grid and all of it is produced from coal and natural gas. Details on electricity consumed in the major units, along with the emission factors, are provided in chapters 2 and 3. The hydrogen required in upgrading and refining is produced from an on-site SMR plant using natural gas. Steam is also produced as a byproduct from the SMR plant and supplements the steam requirement in upgrading and refining operations. The amount of natural gas required in hydrogen production is calculated based on the correlations provided in chapters 2 and 3. Emissions from electricity and natural gas consumption and hydrogen production were calculated through detailed equations (see Appendix C).

4.2.2.1 Feedstock Transportation

The transportation of bitumen to the upgrading and refining units is a very important stage in the life cycle of transportation fuels because generally upgraders and refineries are located far away from the extraction site. The refined products also need to be transferred to the bulk terminals, from where gasoline, diesel, and jet fuel are distributed to refueling stations. Depending on the mode of transportation and distance, the required energy consumption varies, which results in different amounts of GHG emissions. The following section describes the emissions associated with bitumen transportation.

Although bitumen produced from the SEP has better properties than thermal extraction (described in chapter 2), it does not fulfill pipeline requirements [9]. Hence bitumen is mixed with lighter hydrocarbons like naphtha or natural gas condensate to meet the pipeline density (API gravity > 19 [9]) and viscosity (<= 350 centistokes [cSt] [9]). This mixture is called dilbit. The distance between the extraction site and upgrading facility is considered to be 500 km, which is the distance between the extraction site located in Fort McMurray and the upgrading unit in Fort Saskatchewan [4] (see Appendix C). It is assumed that the refineries are 1884.5 km from both the upgrading and extraction units. This distance represents the Keystone pipeline that transports bitumen from Hardisty, Alberta to the American Midwest market in Illinois and Oklahoma [12]. A pipeline transportation model was developed to estimate the energy consumption and GHG emissions from transporting dilbit and SCO including diluent return to the extraction site. The Keystone pipeline can transport 590,000 bpd of feed [12].

First, the diluent ratio (DR) is calculated based on the specific gravity of dilbit, diluent, and bitumen (the equations are provided in Appendix C). Then the target velocity and crude supply are used to determine the actual velocity and approximate pipe diameter [13]. The approximate pipe diameter has been compared to a list of API 5L standard pipe diameters. The designed capacity of the pipeline system is calculated based on diluent ratio and shipped volume of feed. Fluid velocities are calculated considering standard pipe diameter above and below the approximate pipe diameter. Finally, the standard pipe diameter for which the calculated fluid velocity matches best with the target velocity was selected.

Pipe friction reduces the pressure from the fluid. To calculate the pressure drop, the friction factor is calculated. If the Reynolds number of the feed is less than 2100, the flow is laminar and the friction factor is determined by $f = 64/\mathrm{Re}$, where Re is the Reynolds number. But if the Reynolds number is higher than 2100, the flow becomes turbulent and there is no exact formula to calculate the friction factor for turbulent flow. So numerical formulas like the Haaland friction factor formula [14] are used to calculate the initial friction factor value. To obtain the exact friction factor, the Colebrook friction factor formula was used [15]. Since the Colebrook equation is an iterative formula, the equation is iterated several times until almost the exact value is obtained (a difference of less than 10^{-5} between the input and output values). Once all the parameters listed above are calculated, the pressure loss due to pipe friction is calculated using the following formula:

$$P_{friction} = \frac{fL\rho}{2D} v^2 \quad \text{...}(10)$$

where L is the pipeline length (m), ρ is the density of the shipped volume (kg/m^3), D is the pipeline inner diameter (m), and v is the fluid velocity (m/s).

The pressure drop due to elevation change is calculated from the following formula:

$$P_{elevation} = h\rho g \quad \text{...} \quad (11)$$

where h is the change in elevation (m) and g is the gravitation acceleration (9.81 m^2/s).

The change in elevation from Alberta to refineries in the American Midwest is considered to be 632 m, a figure used in the pipeline model described by Nimana et al. [13]. The elevation change from Fort McMurray to Fort Saskatchewan is 350 m [16, 17]. Once total pressure loss has been calculated, pipeline pumping energy intensity is calculated (see Appendix C). In pipeline transportation, only electricity is consumed to drive the pumps [6]. The total GHG emissions from pipeline transportation are calculated considering the energy intensity and GHG emission factors. The GHG emission factors are taken from literature [8]. The properties of the feeds and pipeline specifications are provided in Table 13.

Table 13 - Feed properties and pipeline specifications

Parameters	Dilbit	Diluent	SCO	Sources
Shipped volume (bpd)	590,000	132336.2$^{\alpha}$	590,000	[12]
API	21.4	55	40.04 (coker), 37.30 (hydroconversion)	[4, 13] (SCO API is obtained from the HYSYS model
Fluid velocity (m/s)	1.4	1.4	1.4	[13]
Pipe inner diameter (inch)	39.124	18.5	39.124	Calculated
Pump efficiency (%)	85	85	85	[13]
Outlet pressure (bar)	1	1	1	[13]
Relative roughness	0.000046	0.000046	0.000046	[13]
Friction factor	0.008	9.68E-03	0.008	Calculated

$^{\alpha}$Diluent amount is calculated based on a diluent ratio (DR) of 22.43:77.57 of diluent and bitumen

The GHG emissions from the pipeline transportation of bitumen and SCO and to return diluent to the extraction site are shown in Figure 28. Returning diluent is the more emissions-intensive than transporting bitumen and SCO. This is because a smaller pipeline is used to transport diluent due to the lower shipping volume. A smaller pipe causes more friction, and thus more energy loss. Transporting dilbit to the refinery is more energy- and emissions-intensive than SCO because SCO is lighter and less viscous than dilbit. The results are consistent with the results presented by Nimana et al. [13]. It is also noticeable that with the increase in distance, energy consumption and emissions also increase.

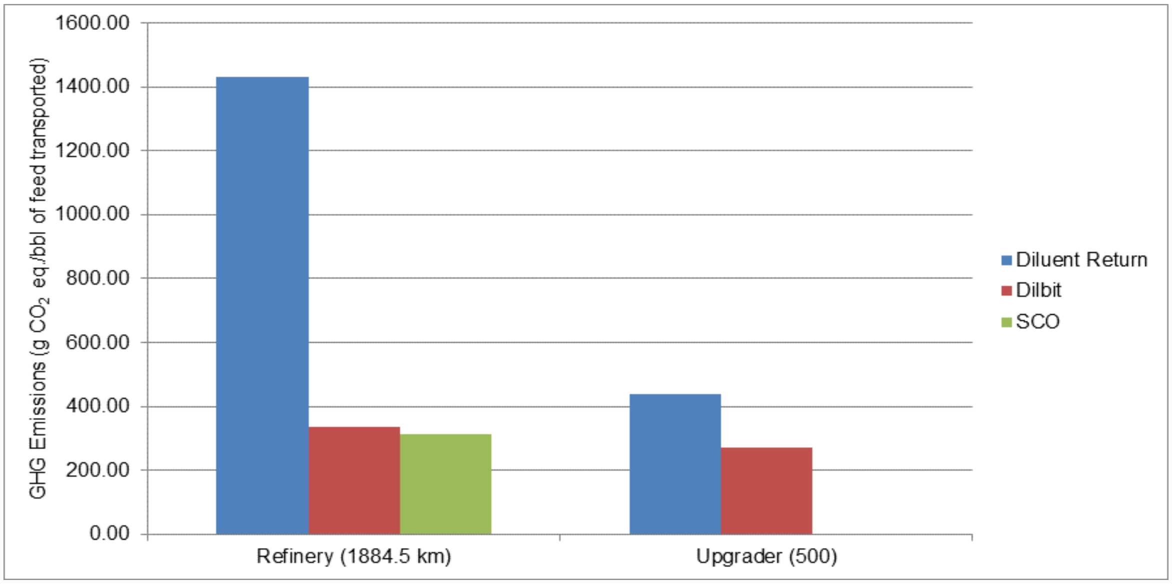

Figure 28-GHG emissions from the pipeline transportation of feed to the upgrader and refinery.

4.2.2.2 Refining

The GHG emissions in refining bitumen and SCO are calculated based on the energy consumption values from the simulation model developed in chapter 3 [10]. In order to calculate GHG emissions per bbl, is it important to know the refinery yield. Wang et al. recommend that as refineries produce various products in different amounts, process-level emissions should not be presented in an aggregated manner but that refinery sub-process level allocation be used to track emissions through the refinery to calculate each product's share of the total emissions [18]. The mass-based allocation GHG emissions results are provided in chapter 3. The GHG emissions factors used to calculate total life cycle emissions are provided in Table 14.

Table 14 - Emission factors for life cycle assessment

Fuel	Unit	Value	Source
NG as fuel	g-CO_2 eq./kJ	0.072	[8]
NG as feedstock	g-CO_2 eq./kJ	0.005	[4]
NG reforming	g-CO_2 eq./gm of NG	2.75	[4]
Produced gas	g CO_2 eq./kJ	0.064	[8]
Upgrader fuel gas	g-CO_2 eq./kg of fuel gas	2419.4	[4]
Refinery fuel gas	g-CO_2 eq./kJ	0.061	[4]
Upstream electricity emissions	g CO_2 eq./kWh	62.941	[19]
Alberta grid electricity	g CO_2 eq./kWh	820	[20]
Grid electricity for refinery	g CO_2 eq./kWh	581	[20]
Grid electricity for pipeline transportation	g CO_2 eq./kWh	741	[13]
Fuel	Unit	Value	Source

Table 14 - Emission factors for life cycle assessment

FCC coke	g-CO_2 eq./MMBTU	10200	[8]

4.2.2.3 Transportation and Distribution

The final petroleum products are transported and distributed from the refinery to the end users through refueling stations. First, the products are supplied to the bulk terminals and from there the products are trucked to refueling stations. As tracing the flow of each product is difficult, the GREET model [8] is used to estimate the transportation and distribution GHG emissions of the refined products.

Table 15 - GHG Emissions data for transportation and distribution emissions [8]

Mode of transport	Gasoline		Diesel		Jet fuel	
	Distance (miles)	Share (%)	Distance (miles)	Share (%)	Distance (miles)	Share (%)
Ocean tanker	2600	3	1300	4	1300	4
Barge	340	31.2	200	48.5	200	48.5
Pipeline	129	67.6	110	46.4	110	46.4
Rail	150	2.2	490	5.1	490	5.1
Transportation emissions (g-CO_2 eq./MJ of transportation fuel)	0.358		0.290		0.287	
Distribution[ρ] emissions (g-CO_2 eq./MJ of transportation fuel)	0.136		0.138		0.136	

[ρ] All the transportation fuels are distributed by truck from the bulk terminal [8]

The LCI inventory data are provided in Table 16.

Table 16 -LCI data for extraction, upgrading, transportation of intermediate feed, refining, transmission and distribution, and combustion emissions for gasoline and

Extraction:					
	Units	Energy Consumption		GHG Emissions (kg CO_2 eq./bbl of bitumen)	
		low	high	low	high
Natural gas	kg/bbl of bitumen	1.80	2.23	5.28	6.56
Produced gas	kJ/bbl of bitumen	1.51	37	0.10	2.36
Electricity	kWh/bbl of bitumen	19.73	19.74	17.42	17.43
Venting emissions	-	-	-	0.36	4.33
Flaring emissions	-	-	-	0.14	
Fugitive emissions	-	-	-	0.27	
Upgrading:					
	Units	Energy Consumption & Yield		GHG Emissions (kg CO_2 eq./bbl of bitumen)	
		Delayed Coking (DC)	Hydro conversion (HC)	Delayed Coking (DC)	Hydro conversion (HC)
SCO produced	bbl/bbl of bitumen	1.18	1.27	-	-
Hydrogen requirement	Nm^3/bbl of bitumen	7.70	17.70	1.08	2.49
Fuel gas	m^3/bbl of bitumen	0.08	6.18	11.18	15.14
Natural gas				32.13	34.80
(i) Heating	kg/bbl of bitumen	8.74	13.55		
(ii) Steam	kg/bbl of bitumen	2.22	4.23		
Electricity	kWh/bbl of bitumen	6.77	9.07	5.98	8.01
Venting emissions				3.54	3.54
Flaring emissions				1.09	1.09
Fugitive emissions				0.14	0.14
Transportation of SCO^{α}-1884.5 km	kWh/bbl of SCO	0.423	0.423	0.369	0.398

Table 16 -LCI data for extraction, upgrading, transportation of intermediate feed, refining, transmission and distribution, and combustion emissions for gasoline and

Transportation of Dilbit$^{\alpha}$-500 km	kWh/bbl of dilbit	0.365	0.365	0.435	0.435
		Delayed Coking (DC)	Hydro conversion (HC)	Delayed Coking (DC)	Hydro conversion (HC)
Transportation of Diluent$^{\alpha}$-500 km	kWh/bbl of diluent	0.593	0.593	0.127	0.127
Dilbit Transportation to Refinery		Energy Consumption		GHG Emissions (kg CO_2 eq./bbl of bitumen)	
Transportation of Dilbit$^{\alpha}$-1884.5 km	kWh/bbl of dilbit	0.455		0.435	
Transportation of Diluent$^{\alpha}$-1884.5 km	kWh/bbl of diluent	1.932		0.414	
Refining:					
	Units	Energy Consumption			
Gasoline		DC SCO	HC SCO	Bitumen	
Heat energy required	MJ/bbl of bitumen	165.41	198.13	229.15	
Steam energy required	MJ/bbl of bitumen	73.62	90.61	180.22	
Electricity required	kWh/bbl of bitumen	5.60	7.02	10.52	
Hydrogen required	kg/bbl of bitumen	1.47	4.31	7.93	
Diesel		DC SCO	HC SCO	Bitumen	
Heat energy required	MJ/bbl of bitumen	4.65	17.37	39.69	
Steam energy required	MJ/bbl of bitumen	9.55	25.23	155.89	
Electricity required	kWh/bbl of bitumen	1.84	1.81	5.41	
Hydrogen required	kg/bbl of bitumen	1.32	7.54	7.49	
Diluent Separation for Bitumen	Units	Energy Consumption			
Steam required	MJ/bbl of bitumen	91.49			
Electricity required	kWh/bbl of bitumen	1.06			

Table 16 -LCI data for extraction, upgrading, transportation of intermediate feed, refining, transmission and distribution, and combustion emissions for gasoline and

	Units	GHG Emissions		
		DC SCO	HC SCO	Bitumen
Gasoline	g CO_2eq./MJ of gasoline	11.82	14.46	11.61
Diesel	g CO_2eq./MJ of diesel	9.48	14.32	15.50
Transportation and distribution of fuels:				
		Gasoline		*Diesel*
g-CO_2eq./MJ of transportation fuel		0.49		0.42
Combustion of fuels:				
		Gasoline		*Diesel*
g-CO_2eq./MJ of transportation fuel		72.71		74.91

[α]Based on a transportation scale of 590,000 barrels of bitumen and SCO; 132,336 bpd of diluent

4.2.2.4 Combustion

The combustion of the transportation fuels in vehicles is the last stage of the life cycle assessment. Fuel combustion emits gases like CO_2, CH4, N_2O, SO_x, and NO_x along with particulates and volatile organic compounds (VOCs). But in this study only the emissions of the major gases like CO_2, N_2O, and CH_4 are considered. Combustion emissions from gasoline, diesel, and jet fuels are established and do not vary much depending on the vehicles. The combustion GHG emission factors are taken from the GREET model [8]. The GHG emission factors are collected by running the simulation model for passenger cars and aircraft (single aisle). The emission factors are:

	Conventional Gasoline	Conventional Diesel	Jet Fuel
g-CO_2 eq./MJ	72.71	74.91	72.80

Due to differences in system boundaries and assumptions, variations in the LCI data are inevitable. Because of that, instead of point estimates, a range of inputs is used, and this results in a range of outputs and gives more conservative results.

4.2.2.5 Sub-process Level Allocation

All the production pathways shown in Figure 27 depict the production of more than one type of transportation fuel. This makes it difficult to allocate the environmental impact of processing one particular type of fuel. To resolve this problem, the ISO advocates allocating life cycle GHG emissions at the refinery sub-process level instead of the aggregated level [18]. In previous studies, allocations have been done based on mass, energy, market value, or hydrogen content [18, 21-23]. In this study, GHG emissions are allocated at the refinery sub-process level based on mass. The reason to use the mass fraction as a weighting factor is that the mass distribution is proportional to energy consumption [18]. GHG emissions from hydrogen production are allocated based on how much hydrogen is required in each unit operation. The GHG emissions for each sub-unit operation are allocated according to equation (12) [4]. The GHG emissions from one unit operation are added to the GHG emissions from the next sub-unit.

Emissions allocated to product (i) (g-CO_2 eq./MJ)

$$= \textit{Emissions in sub-unit operation}\left(\frac{g-CO_2eq.}{MJ}\right)x\left(\frac{M_i}{\sum_{i-j,k,l........} M_i}\right) \tag{12}$$

where M_i = mass of the product *(i)* produced and *j,k,l,……* are the products of each sub-unit operation.

Table 16 shows the energy consumption and GHG emissions in each life cycle stage. But the data are provided in different units. Thus necessary conversions were made to present the LC GHG emissions in a common unit for each pathway. Here the unit considered is in g-CO_2 eq./MJ of gasoline, diesel, and jet fuel. All the GHG emissions from extraction and recovery, transportation, and upgrading are allocated to the total thermal energy obtained from gasoline, diesel, and jet fuel [4].

Upstream emissions allocated to product (i) (g-CO_2 eq./MJ)

$$= \textit{Emissions in each unit operation x } \frac{1}{\sum_{i=j,k,l} E_i} \ \textit{(g-}CO_2\textit{ eq./MJ)} \tag{13}$$

where E_i = total energy content of the product *(i)* produced per day and *j,k,l* are gasoline, diesel, and jet fuel.

4.2.2.6 Uncertainty Analysis

Uncertainties in extraction and in upgrading and refining emissions as detailed in chapters 2 and 3, respectively, were combined to estimate total uncertainties in the major unit operations (extraction, upgrading, and refining). To maintain a sampling error of less than 0.1 kg CO_2 eq./bbl of bitumen, 100,000 samples were used for each scenario (see the uncertainty analyses in chapters 2 and 3 for details). The results are reported within the 5th-95th percentiles to capture the extreme estimates.

4.3 Results and Discussion

4.3.1 Life Cycle Impact Assessment (LCIA)

The LC GHG emissions range from 92.39 to 120.00 g-CO_2 eq./MJ of gasoline, 103.56 to 248.94 g-CO_2 eq./MJ of diesel, and 289.90 to 465.54 g-CO_2 eq./MJ of jet fuel, depending on the pathway. The wide GHG emission ranges were obtained because of the wide ranges of GHG emissions in oil sands operations, as shown in Table 16. The higher GHG emissions ranges for diesel and jet fuel are from pathways I and III. Diesel and jet fuel have higher GHG emissions ranges than gasoline because less diesel and jet fuel are produced from SCO obtained from coker and hydroconversion upgrading (yield fractions are provided in chapter 3). The sub-process level gasoline and diesel GHG emissions are provided in Figures 29 and 30, respectively.

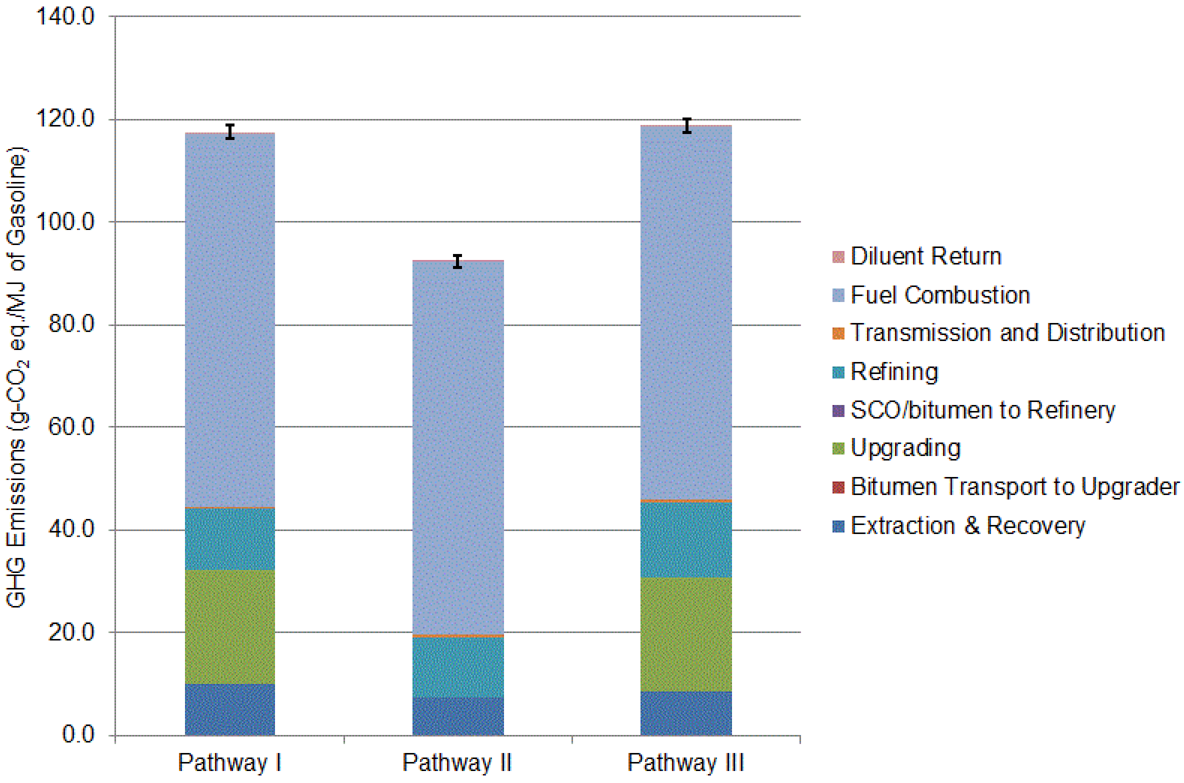

Figure 29-WTT+C LC GHG emissions from gasoline production.

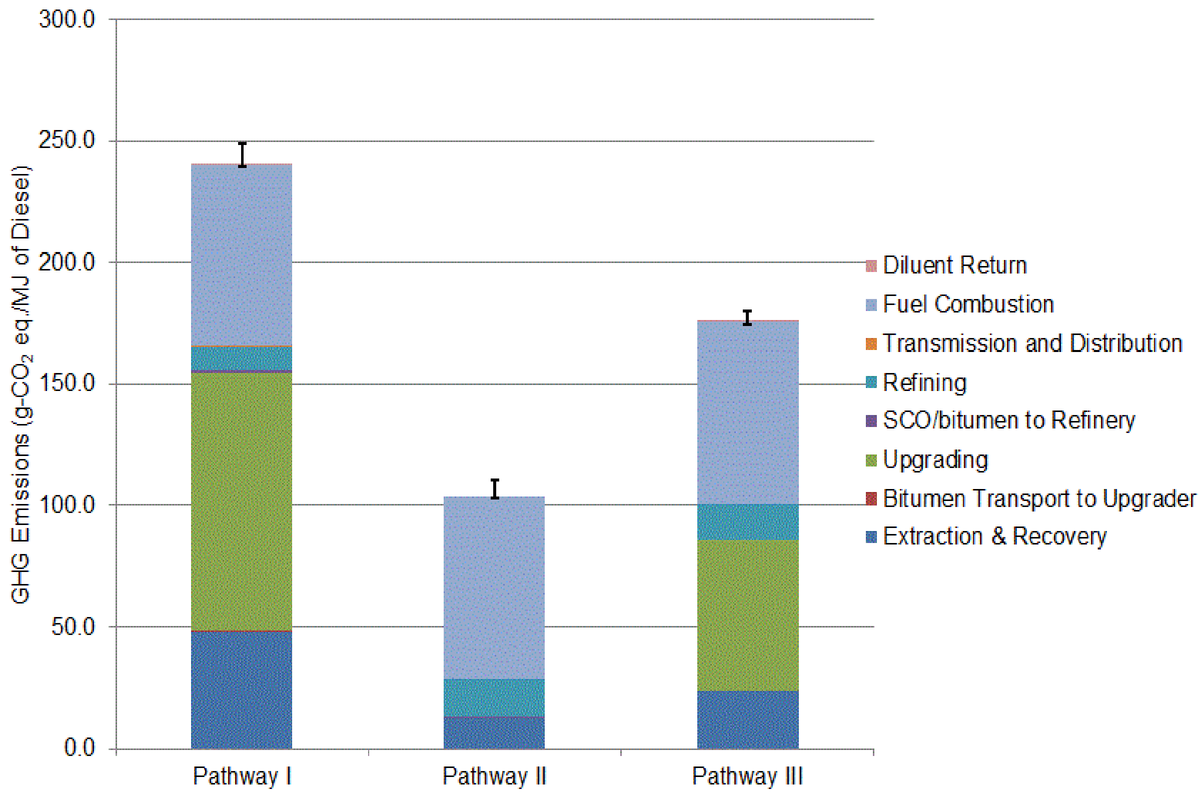

Figure 30-WTT+C LC GHG emissions from diesel production.

As shown in Figures 29 and 30, in pathway II the LC emissions of gasoline (92.39-93.66 g-CO_2 eq./MJ of gasoline) and diesel (103.56-110.09 g-CO_2 eq./MJ of diesel) are significantly lower than in the other pathways. This is because of the GHG emissions credit from upgrading operations. If the bitumen produced is already upgraded and results in better yields from refining, then there is no need to upgrade bitumen to SCO. Refining bitumen directly will also significantly save the cost of building the cost-intensive upgrading units [24]. As discussed in chapter 3, the SCO produced from SEP bitumen is lighter and loses its stability in the distillation columns of the refineries; less SCO is obtained than from refining bitumen directly. So, pathways I and III would not be economical due to their lower yields. As energy consumption is proportional to emissions, pathway II also requires less energy to produce gasoline and diesel.

Figures 29 and 30 show that the gasoline production is less GHG intensive than diesel and jet fuel production. On the contrary, gasoline produced from refining SCO (in case of SAGD bitumen) is more GHG intensive than diesel and jet fuel [18, 21] because the produced bitumen has different properties than SCO and refining produced bitumen yields considerably less amount of diesel and jet fuel (mass basis) [4]. So, lower mass fractions of diesel and jet fuel result in higher GHG allocations for diesel and jet fuel, which lead to higher emissions (see Appendix C). The mass basis allocation factors are provided in Table 17.

Table 17 - Mass fractions at the refinery sub-process level (mass basis)

	Gasoline	Diesel	Jet fuel	Source
Coker SCO	0.45	0.09	0.07	Aspen HYSYS model
Hydroconversion SCO	0.46	0.16	0.06	Aspen HYSYS model
Bitumen	0.53	0.23	0.01	Aspen HYSYS model

As presented in Table 17, jet fuel produced from bitumen has a significantly lower yield than from SCO. Hence it is not a good choice to produce jet fuel from SEP bitumen with the refinery configuration used in this study.

As shown in Figures 29 and 30, emissions from fuel combustion in vehicles constitute the highest portion of emissions (approximately 60-80% for gasoline, 30-70% for diesel, and 17-25% for jet fuel). Transportation and distribution emissions constitute a negligible amount of the total emissions (≥ 0.6%). In pathways I and III, 9-23% of the total gasoline, diesel, and jet fuel LC emissions are from extraction and recovery whereas in pathway II, 9-78% of the total LC emissions are from extraction and recovery. This is because there is no upgrading unit in pathway II. Refinery emissions are also higher in pathway II than in the other pathways. The transportation of bitumen and SCO to the refinery and bitumen to upgraders has minimal impact.

4.3.2 Comparison of Transportation Fuels LC Emissions with those from Other LCA Studies

The LC emission results calculated in this study were compared with those from other LCA studies. As shown in Figure 31, LC emissions estimated for gasoline produced from SEP bitumen are lower than those from the gasoline produced from SAGD bitumen as reported in several major studies [8, 25-27]. Diesel emissions are within the ranges provided in other studies. Because refining SCO or bitumen produces more gasoline than diesel [4, 25], transportation fuels produced from the solvent extraction process will reduce overall LC GHG emissions of transportation fuels. Also, refining bitumen without upgrading it will significantly reduce transportation fuel production costs.

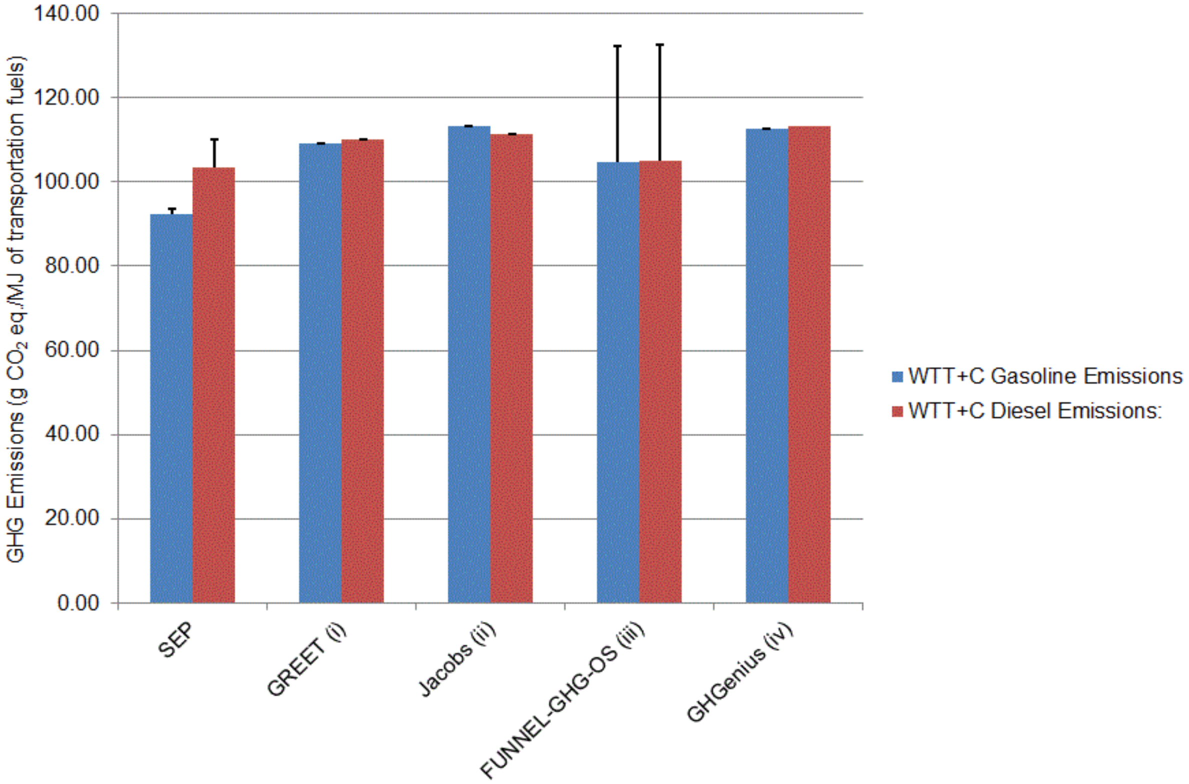

Figure 31-Comparison of modeled WTT+C GHG emissions of gasoline and diesel with other LCA studies*.

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*All the numbers in the literature are for SAGD based bitumen while the modeled numbers are for bitumen extracted through solvent-based processes. (i) The GREET model does not differentiate between delayed coker and hydroconversion upgrading [8]. (ii) The lower and upper values of gasoline emissions are provided for reformulated gasoline blendstock for oxygen blending (RBOB) and conventional gasoline blendstock for oxygen blending (CBOB), respectively. The diesel emissions are provided for ultra-low sulfur diesel (ULSD) [25]. (iii) The wide emissions range is provided considering the 6 pathways developed for gasoline and diesel production [4]. (iv) GHGenius .[27].

4.3.3 Total Uncertainty in Emissions from Major Operations

Figure 32 shows the total GHG emissions from extraction, upgrading, and refining for the three pathways. Pathways I and III provide wider ranges of uncertainty in total emissions compared to pathway II because for pathway II, uncertainties in upgrading emissions are not included as bitumen is directly refined without upgrading. The lower part of uncertainty in emissions in pathway III overlaps with the higher part of emissions in pathway I, and the total emissions for pathway II do not overlap with pathway III.

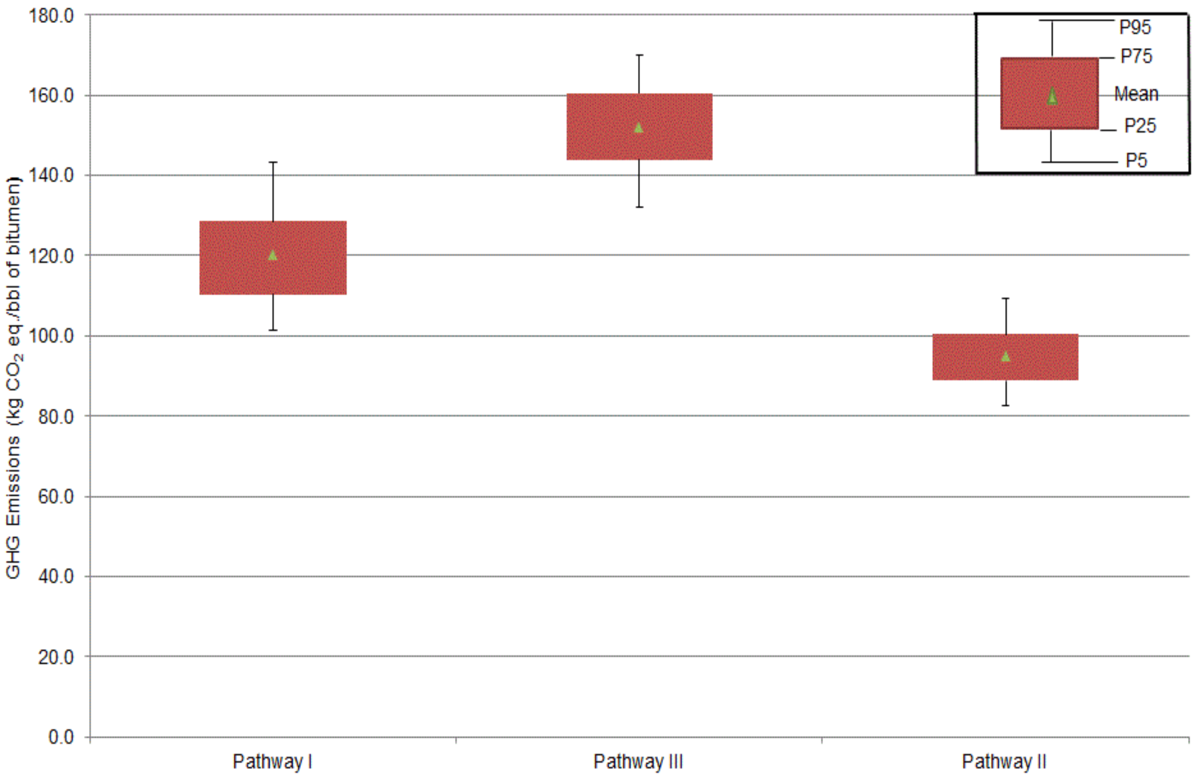

Figure 32-Total uncertainty in the major unit operations (extraction, upgrading, and refining).

It is clear that pathway III is the most energy- and GHG-intensive pathway. This is because of the higher hydrogen requirement in hydroconversion upgrading. The lower portion of pathway I overlap with the higher portion of pathway II. The difference in GHG emissions between pathway I and II reflects GHG emissions due to delayed coking. Pathways I and II overlap which means that the sensitive inputs in extraction and coker upgrading have a significant effect on final emission results.

4.4 Conclusions

A comprehensive WTT+C life cycle assessment of transportation fuels like gasoline, diesel, and jet fuels was performed considering three different production pathways. In all three pathways, bitumen is produced from the solvent extraction process. A data-intensive model was developed based on engineering first principles. Instead of providing point estimates as has been done in previous studies, the results are given in ranges, which increase the ability of the model to incorporate variations in input parameters and also improve the reliability of the model. To minimize energy consumption and GHG emissions and produce the greatest yield, partially upgraded bitumen from the solvent extraction process should be refined directly without upgrading. The LC GHG emissions in pathway II range from 92.39-93.66 g-CO_2 eq./MJ of gasoline, 103.56-110.09 g-CO_2 eq./MJ of diesel, and 406.12-465.54 g-CO_2 eq./MJ of jet fuel. The main contributor to GHG emissions is the combustion of fuels in vehicles. The allocation of co-products based on mass also has a significant impact on LC GHG intensity.

From the uncertainty analysis, it was found that pathway III has the most GHG emissions (132.21-169.91 kg CO_2 eq./bbl of bitumen) and its uncertainty range is higher than that of pathway II. The largest sources of uncertainty are from external refrigeration in the demethanizer to condense propane gases, the source of electricity, and the hydrogen required to refine bitumen. To reduce uncertainty in GHG emissions, power consumption in refrigeration should be reduced. Electricity should be supplied from low GHG emission sources like natural gas combined cycle power plants, renewable energy, etc. The cogeneration of electricity can also be considered as an alternative source of electricity. Hydrogen should be produced from low GHG emissions-intensive sources.

The production pathways developed in this study will help oil producers to determine the best production pathway for the solvent-based extraction process. The uncertainty analysis will give readers insight into the impact of assumed input values on WTT+C emissions and will also assist policy makers in decision making. Also, the uncertainty analysis helps to determine the potential areas of GHG reduction that will make solvent extraction a sustainable production process.

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Chapter 5

Conclusions and Recommendations for Future Work

5.1 Conclusions

In this study, a data-intensive vapor solvent-based oil sands extraction simulation model was developed for a 25,000 bpd capacity to investigate the potential of the solvent-extraction process. Three project-specific WTW pathways were developed that incorporate the transportation of feedstock from one unit to another to determine the best production scenario. In pathways I and III, bitumen produced from solvent-extraction was sent to the upgrader to produce SCO. In pathway II, bitumen is directly refined. For bitumen upgrading, two comprehensive upgrading models, one for delayed coking and one for hydroconversion, were developed. The upgrading models calculate the amount of SCO produced from a unit volume of bitumen. To investigate refining operations, a process simulation model was used. The refinery model estimates the yield from a particular feed. The simulation model developed was used to estimate the net energy consumption and GHG emissions in all three pathways based on engineering first principles by taking into account the technical parameters in each unit. Adding an uncertainty analysis to the developed model helped determine the most energy- and GHG emissions-intensive parameters and provided a more realistic representation of the life cycle energy consumption and GHG emissions from solvent extraction process.

Natural gas and electricity are consumed in the conversion of oil sands into transportation fuels (gasoline, diesel, jet fuel, etc.). Natural gas is burned to generate heat and steam according to the requirements of extraction, upgrading, and refining operations. Natural gas is also used in steam methane reforming as both fuel and feedstock to meet the hydrogen requirement in upgraders and refineries. The energy consumption in hydroconversion upgrading is more than coker upgrading but results in a higher yield than coker upgrading. About 46.13% and 36.81% of the total heat required in the delayed coker and hydroconversion upgrader, respectively, are met by heat recovered from different streams. Refining bitumen requires more energy than refining SCO. SCO produced from solvent-extracted bitumen loses its stability upon refining and produces a very high amount of fuel gas. So, higher amounts of valuable products are obtained from refining solvent-extracted partially upgraded bitumen than from SCO. But refining bitumen causes 84.28 kg CO_2 eq./bbl emissions, which is 15.86% and 128.49% higher than hydroconversion and delayed coker upgrading, respectively. In terms of feedstock transportation in the refinery, dilbit requires more energy than SCO. Diluent return from the upgrader or refinery to the extraction site is GHG intensive; however, diluent return uses pipelines that are smaller in diameter than those used to transport dilbit and SCO.

5.1.1 LCA GHG WTW emissions

A comprehensive WTW LCA was conducted for all three pathways to estimate the upstream and end-use GHG emissions of solvent-extracted bitumen. The results showed that the well-to-refinery (WTR) GHG emissions are 117.49-122 kg CO_2 eq./bbl in pathway I, 109.74-114.71 kg CO2 eq./bbl in pathway II, and 180.79-185.76 kg CO_2 eq./bbl in pathway III. The WTR emissions reported in this study are significantly lower than those from the main thermal extraction processes like SAGD and CSS. Since no upgrading is considered and bitumen is directly refined, pathway II is the least energy- and GHG emissions-intensive pathway. The high GHG emissions in pathway III are attributed to the hydroconversion upgrading, which emits significantly more GHG emissions than delayed coking followed by upgrading. After emissions are allocated at the refinery sub-process level, WTW emissions ranges for gasoline are calculated: 117.21-119.20 in pathway I, 92.33-93.80 in pathway II, and 124.37-126.06 kg CO_2 eq./MJ in pathway III. For diesel, WTW emissions range from 240.30-249.89 (pathway I), 103.47-110.49 (pathway II), and 192.03-196.73 kg CO_2 eq./MJ (pathway III). The GHG intensity in each pathway is affected by the individual yield in each pathway and the allocation method used. From the results, it is clear that pathway II represents the best production and conversion pathway for solvent-extracted bitumen. In pathway II, the WTW emissions due to gasoline production from solvent-extracted bitumen are also significantly lower than from thermally extracted bitumen.

5.1.2 Uncertainty in the LCA GHG WTW emissions

Through energy and GHG emissions calculations, we identified the most energy and GHG emissions-intensive parameters. The GHG emissions-sensitive parameters were identified through a sensitivity analysis. If a ±10% change in a unit's input value leads to a 1% change in the overall GHG emissions of that unit, it is considered to be a GHG emissions-intensive/critical parameter. The uncertainty analysis is conducted by incorporating all the critical parameters and using a Monte Carlo simulation.

Overall, the uncertainty in the combined extraction, upgrading, and refinery operations GHG emissions varied by a maximum of +19.5% to a minimum of -15.9% from the default operating conditions for each pathway. Pathway I has the widest uncertainty GHG emissions ranges because it has more critical parameters than the other pathways. The uncertainty in pipeline transportation was not considered because pipeline GHG emissions are almost negligible compared to extraction, upgrading, and refinery GHG emissions. As tank-to-wheel (TTW) GHG emissions are almost constant, the uncertainty in upstream major unit operations provides a better representation of the overall WTW GHG emissions and helps identify the parameters critical to upstream GHG emissions.

This study clearly states that the vapor solvent extraction process is a less energy- and emissions-intensive process than thermal extraction processes. Because the produced bitumen is partially upgraded, it can be refined in a typical deep conversion refinery in North America with upgrading. Throughout the WTW life cycle, the solvent extraction process has a high potential to reduce energy consumption and emissions from oil sands-derived transportation fuel production. Another unique factor of this study is the uncertainties in emissions. The more the number of factors sensitive to GHG emissions, the wider the emissions range become. This study will assist policy makers by providing a more accurate representation of the life cycle emissions with a reliable uncertainty emissions range from solvent-extracted bitumen.

5.2 Recommendations for Future work

Further research is recommended in the following areas.

Improvement of the existing model:

- <u>Integrated in situ extraction and upgrading operations</u>: In the current study, it is considered that the upgrader unit is located 500 km from the extraction site. But some companies have an upgrader unit adjacent to the extraction site. The upgrader location has an impact on life cycle energy consumption and GHG emissions. If the upgrader is close to the extraction site, less energy is required to transport bitumen. Moreover, the upgrader might have a combined cogeneration plant to supply surplus electricity and fuel gas to meet electricity and heat energy demand in the extraction unit. A detailed investigation might show a further reduction in life cycle GHG emissions.

- Fluid bed coking: In the current study, the two most widely used upgrading technologies, delayed coker and hydroconversion, were modeled. Another promising upgrading technology, fluid bed coking, is currently employed in companies like Syncrude. Unlike delayed coking, fluid coking is a continuous coking process that uses the produced coke in the coker to meet the heat requirement. Fluid bed coking is a better technology than delayed coker, especially when the feed has high amounts of coke and residue. A project-specific pathway can be developed in order to investigate energy consumption and GHG emissions in this upgrading configuration.
- Comprehensive refinery model: This study used a generic deep conversion refinery model built in Aspen HYSYS, a simplistic model that uses petroleum shift reactors. The model calculates energy use and product yield based on simple linear correlations. To improve the model's accuracy and to get better results, a rigorous refinery model should be developed using Aspen HYSYS.

Inclusion of land-use and infrastructure emissions: In the current study, emissions from land use and infrastructure construction were not included due to lack of data. Although land-use and infrastructure emissions are supposed to be minor, these emissions need to be included in the system boundary to observe the impact of land-use and construction emissions.

Impact of refinery configuration: In this study, it is assumed that the partially upgraded bitumen produced from the solvent extraction process and SCO is refined in a typical deep conversion refinery. Since the SCO produced from bitumen has high lighter fractions, it is worth investigating to SCO in a medium conversion or a hydroskimming refinery. These refinery configurations have different rates of energy consumption and produce different mass yields of transportation fuels than deep conversion refineries. The use of a medium conversion or hydroskimming refinery might produce higher yields and might result in life cycle GHG emissions even lower than what is reported in this study.

Effect of allocation methodologies: The method used to allocate emissions to individual transportation fuels produced from bitumen significantly impacts on the resulting life cycle GHG emissions from a particular transportation fuel. The ISO recommends that emissions be allocated at the refinery sub-process level instead of the refinery level. A mass base refinery sub-process level allocation was made in the current study. Other allocation methods such as energy base sub-process level allocation and allocation based on the amount of fuel hydrogen content can also be used. As different studies use different allocation methods, it would be helpful for policy makers to determine which basis they prefer.

Venting, flaring, and fugitive (VFF) emissions: VFF emissions vary significantly from site to site and depend on different factors such as well completion and servicing; gases produced along with bitumen, the type of equipment used for extraction and recovery, oilfield waste management facilities, etc. Due to the scarcity of site-specific VFF emissions data and in order to avoid model complexity, we used industry average VFF emission factors. An attempt should be made to develop strategies to calculate site-specific VFF emissions based on fundamental engineering principles. Analyzing well completion technologies and waste management facilities would be a good starting point. Otherwise, site-specific VFF emissions data can be collected for proper quantification of the VFF emissions.

Dilbit refinery: In the current study, it is assumed that bitumen is transported in the refinery as dilbit and then diluent is separated from it. Instead of separating diluent, dilbit can be directly refined, which might produce a higher yield and fewer emissions compared with refining bitumen. So, a project-specific pathway needs to be developed in order to calculate WTW life cycle energy consumption and GHG emissions considering dilbit refining with upgrading.

Source of electricity: It is considered in this study that all the electricity required in bitumen extraction and conversion operations will be supplied from the Alberta grid. However, some extraction sites have cogeneration plants and produce on site the electricity required for extraction and recovery operations. Incorporating a cogeneration unit in the extraction site will prevent electricity loss during transmission and distribution from the grid. On-site produced gas can be used to generate electricity. The impact of electricity generation from renewable sources like hydro, wind, solar, geothermal, nuclear, etc. can be investigated. So, further research should be conducted to examine bitumen extraction and conversion operations considering electricity supply from renewable sources.

Technological advancements in oil sands operations: As mentioned in previous chapters, the solvent extraction process might be incorporated with electrical or electromagnetic extraction processes like ESEIEH, ET-DSP, etc., in order to improve the solvent-to-oil ratio ($SOR_{solvent}$). But reducing the $SOR_{solvent}$ might result in higher heat energy consumption. The quality of bitumen produced from the combined solvent and electromagnetic heating process is also a critical factor. As the technologies are still in the pilot stage, more detailed research is required to implement these processes for commercial-scale implementation.

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APPENDIX A

Appendix A contains supporting information for chapter 2.

Table A1 – Composition of produced gases [1]

Gas	Amount (mol%)
CH_4	63.6
N_2O	1.3
H_2S	0.13
CO_2	30
H_2	0.3
C_2H_6	1.63
C_3H_8	1.98
C_4H_{10}	0.3
C_{5+}	0.88

Table A2 – Upstream and combustion emission factors

Natural gas (NG) emissions (g CO_2 eq./kJ of NG):	
Upstream emissions	0.008 [2]
Combustion emissions	0.064 [2]
Electricity emissions (g CO_2 eq./kWh)	
Upstream emissions	62.94 [2]
Production emissions (includes transmission emissions)	820 [3]
Combustion emissions from produced gas (g CO_2 eq./kJ of produced gas)	0.064 [2]

Equations for calculating energy consumption in the acid gas removal (AGR) unit

All the equations were imported from the OPGEE model [4].

The heat duty in the amine reboiler:

$$\Delta H_g = \frac{24 * 72000 * 0.00378541 * Q_{amine}}{1055.87 * 10^6} * 1.15 \qquad \textbf{(A1)}$$

ΔH_R: heat duty (MJ/day); Q_{amine}: amine flow rate (m^3/min)

The amine flow rate is calculated as $Q_{amine} = 100 * K * 0.00378541 * (Q_{H_2S} + Q_{CO_2})$ **(A2)**

Here the K value is considered to be 1.45 (gallons per minute-d/100MMscf) [5]; Q_{H_2S}: H_2S removal (MMscf/day); Q_{CO_2}: CO_2 removal (MMscf/day).
Power required in the amine cooler:

$$BHP_F\ (hp) = 0.36 * Q_{amine} \quad \textbf{(A3)}$$

Power required in all the pumps are calculated as follows:

$$BHP_{RP} = 0.06 * Q_{amine} \quad \textbf{(A4)}$$

$$BHP_{BP} = 0.06 * Q_{amine} \quad \textbf{(A5)}$$

$$BHP_{CP} = 0.00065 * 6.89476 * Q_{amine} * P_d \quad \textbf{(A6)}$$

BHP_{RP}: reflux pump brake horse power (hp); BHP_{BP}: booster pump brake horsepower (hp); BHP_{CP}: circulation pump brake horsepower (hp); and P_d: pump discharge pressure (kPa).

Equations for calculating energy consumption in the gas dehydration unit

All the equations were imported from the OPGEE model [4].

The regeneration duty is estimated using the formula:

$$\Delta H_{GD} = 900 + 966 * 2327.7968 * q_{TEG} * (\frac{1}{10^6}) \quad \textbf{(A7)}$$

ΔH_{GD}: reboiler heat duty (MJ/kg of H_2O) and q_{TEG}: triethylene glycol (TEG) circulation rate (m^3 of TEG/kg of H_2O). In this research, q_{TEG} is considered to be 0.017 (m^3 of TEG/kg of H_2O) [6].

The horsepower required in the glycol pump in the dehydration process is calculated using the formula:

$$BHP_{GP} = \frac{Q_{TEG} * \Delta P}{1714 * \eta_{GP}} * 0.00378541 * 6.89476 \quad \textbf{(A8)}$$

BHP_{GP}: glycol pump brake horsepower (hp); Δp: pumping pressure (kPa); Q_{TEG}: TEG circulation rate in gallons per minute (m^3/min) and η_{GP}: pump efficiency (90%) [7].

Equation for calculating energy consumption in the demethanizer unit

The refrigeration brake horsepower required in the demethanizer is calculated using the following formula [4]:

$$BHP_{RS} = \frac{1}{24} * e_{RS} * Q_{g_{in}} \qquad \textbf{(A9)}$$

BHP$_{RS}$: refrigeration system brake horsepower (hp); *e*$_{RS}$: energy factor, for the refrigeration system energy factor is considered to be 3.6 (bhp-hr/kmol$_{cond}$) [4]; and Q$_g$: gas condensed in the demethanizer (kmol/day).

Equation for calculating the sampling error for the Monte Carlo simulation

The Monte Carlo sampling error determines the error that occurs between simulations and can be calculated using the following equation [8]:

Sampling error, $\overline{X} = \frac{z * \sigma}{\sqrt{n}}$ **(A10)**

where σ = standard deviation of the mean and n = number of samples. The Z value is determined based on the confidence interval of the standard normal distribution.

Table A3 – Z values for different confidence intervals

Confidence Interval (%)	Z value	Sources
90	1.645	[9]
95	1.96	[9]
98	2.33	[9]
99	2.58	[9]

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APPENDIX B

Appendix B contains supporting information for chapter 3.

Table B1 – Distillation fractions from ADU and VDU of upgrading

Fractions*	Upgrading (vol%)
Naphtha	5.31
Diesel	43.04
LVGO[i]	5.87
HVGO[ii]	7.03
Vacuum Residue (VR)	38.77

*Distillation cut temperatures are consistent with Gray [1], Netzer [2]. [i]Light Vacuum Gas Oil, [ii]Heavy Vacuum Gas Oil.

Table B2 – Distillation fractions from ADU and VDU of refining

Fractions	Refining (vol%)		
	Coker	Hydroconversion	Bitumen
Fuel Gas	50.85	42.13	0.21
Naphtha	27.18	24.67	6.00
kerosene	4.85	4.68	1.35
Diesel	3.66	4.62	11.48
LVGO	0.85	0.62	8.27
HVGO	12.57	23.18	66.82
VR	0.04	0.08	11.74

Table B3 – Lower heating value (LHV) of fuels

Fuel	LHV (MJ/kg)	Source
Natural Gas (NG)	40.70	[3]
Refinery Fuel Gas	88.69	[3]
Steam	2.79	[4]
Gasoline	41.74	[3]
Diesel	42.79	[3]
Upgrader fuel gas		
CH_4	28.74 (kJ/m^3)	[3]
C_2H_6	48.70 (kJ/m^3)	
C_3H_8	70.84 (kJ/m^3)	
C_4H_{10}	88.94 (kJ/m^3)	

Equation for allocating refinery emissions at the refinery process level

g CO_2 eq./MJ of transportation fuel [5] =

$$\frac{kg\ CO2\ eq.}{bbl\ of\ bitumen}\ x\ \frac{bbl\ of\ bitumen}{kg\ of\ bitumen}\ x\ \frac{kg\ of\ bitumen}{kg\ of\ SCO}\ x\ \frac{kg\ of\ SCO}{kg\ of\ transportation\ fuel}\ x\ \frac{kg\ of\ transportation\ fuel}{MJ\ of\ transportation\ fuel} \quad \textbf{(B1)}$$

Transportation fuels : gasoline, diesel etc.

Mass fractions (SCO/bitumen): for delayed coking 0.88 and for hydroconversion 1.01.

Table B4 – Range of values for developing the input distributions

Parameter	Minimum	Maximum	Most likely (mode)
Efficiency of NG Heater (%)	60 [6]	100 (theoretical highest value)	87 [7]
Heat Exchanger Efficiency (%)	60 [6]	100	90 [8]
Steam Heating Value (MJ/kg)	1.66 [9]	3.59 [10]	2.79 [4]
Electricity Emission Factor (g CO_2 eq./kWh)	428.31 [3]	1047.62 [11]	882.94 [3, 11]
Efficiency of NG boiler (%)	60 [6]	86 [12]	85 [13]
Hydrogen required in refinery hydrocracking (kg/bbl):			
Delayed Coker SCO	0.27 [6]	25.96 [14]	7.80 (Modeled)
Hydroconversion SCO	0.35 [6]	25.96 [14]	25.01 (Modeled)
Bitumen	1.03 [6]	22.89 (Modeled)	22.89 (Modeled)

The lower hydrogen consumption reported by Nimana et al. [6] reflects the effect of plant capacity.

Table B5 – Z values for different confidence interval [15]

Confidence Interval (%)	Z value
90	1.65
95	1.96
98	2.33
99	2.58

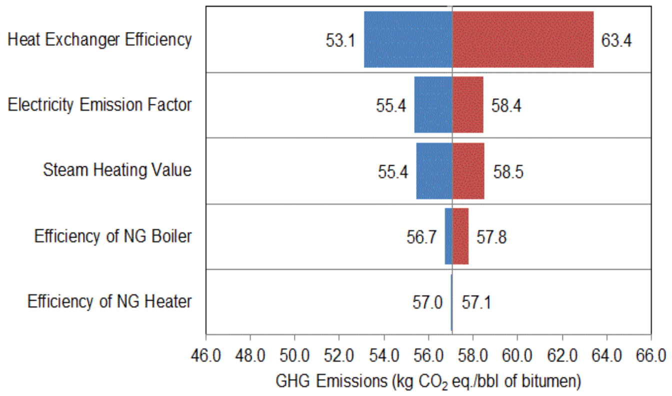

Figure B1 - Uncertainty in emissions in coker upgrading.

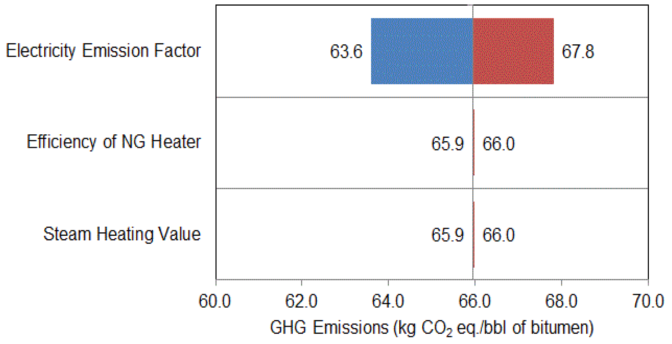

Figure B2 – Uncertainty in emissions in hydroconversion upgrading.

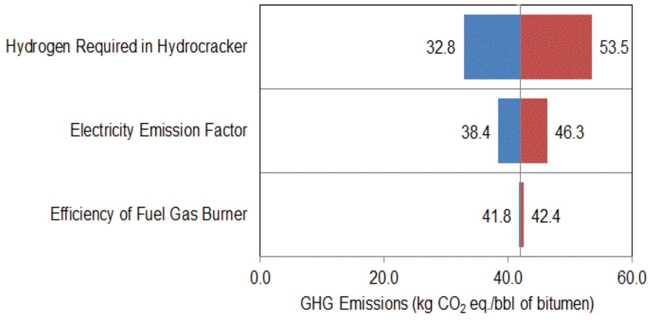

Figure B3 – Uncertainty in emissions due to refining coker SCO.

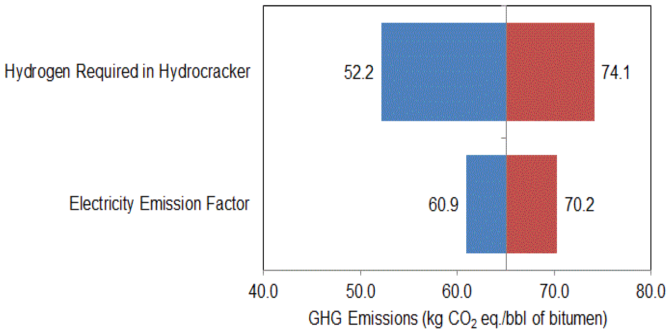

Figure B4 – Uncertainty in emissions due to refining hydroconversion SCO.

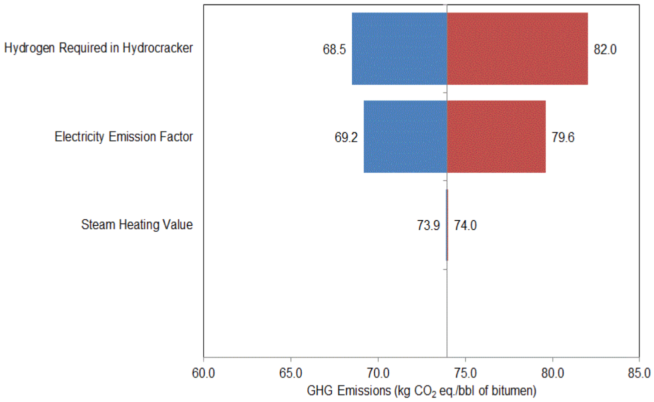

Figure B5 – Uncertainty in emissions due to refining bitumen.

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APPENDIX C

Appendix C contains supporting information for chapter 4.

Equations used to calculate pipe size

The diluent ratio is calculated using the following equation [1]:

$$\textit{Diluent Ratio (DR)} = \frac{SG_{dilbit} - SG_{bitumen}}{SG_{diluent} - SG_{bitumen}} \qquad \textbf{(C1)}$$

here, *SG* means specific gravity.

The shipped volume (m^3/day) is calculated from the shipped capacity using the equation below [1]:

$$\textit{shipped volume, } \dot{V}_{shipped} = \frac{\dot{V}_{capacity}}{1 - DR} \qquad \textbf{(C2)}$$

where $\dot{V}_{capacity}$ is the designed system capacity (m^3/day) and *DR* is the diluent ratio.

The approximate pipe diameter (inch) is calculated from equation (C3) [1]:

$$D_{approximate} = \left\lfloor \sqrt{\frac{\dot{V}_{shipped}}{\frac{24hr}{1d} * \frac{3600s}{1hr}} x \frac{4}{\pi * v_{target}}} \right\rfloor * \frac{1in}{0.0254m}$$

(C3)

here v_{target} is the target velocity of the feed (m/s).

From the standard API 5L diameter (inch), the actual fluid velocity (m/s) is calculated from equation (4) [1]:

$$\text{Actual fluid velocity, } v_{fluid} = \frac{\dot{V}}{\frac{24hr}{1d} * \frac{3600s}{1hr}} * \frac{4}{\pi * (D_{inner} * \frac{0.0254m}{1in})^2} \qquad \textbf{(C4)}$$

Equations used to calculate pipe friction factor

The Reynolds number is calculated from the equation (C5) for pipe flow [1]:

$$\mathrm{Re} = \frac{\rho * v_{fluid} * D_{inner}}{\nu} \qquad \textbf{(C5)}$$

here, ρ is the density of shipped products (kg/m^3) and ν is the dynamic viscosity of fluid (Pa.s)

The initial friction factor is calculated from the Haaland friction factor [2]:

$$\frac{1}{f_{in}} = -1.8\log_{10}\left[\frac{(e/D_{in})}{3.7}\right]^{1.11} + \frac{6.9}{\text{Re}} \quad \textbf{(C6)}$$

here, *e* represents relative roughness.

From the initial friction factor (*f*$_{in}$), the exact friction factor is determined from the Colebrook friction factor [3]:

$$\frac{1}{\sqrt{f_{out}}} = -2.0\log_{10}\left[\frac{(e/D_{in})}{3.7}\right]^{1.11} + \frac{2.51}{\text{Re}\sqrt{f_{in}}} \quad \textbf{(C7)}$$

where f_{out} is the iterative friction factor. The iteration is continued until the difference between the input (f_{in}) and output (f_{out}) friction factors is negligible (> 10^{-5}).

Equations used for calculating pipeline pumping energy intensity

The working power of the pump (W) is calculated from pressure loss due to pipe friction ($P_{friction}$) and change in elevation ($P_{elevation}$) using the equation below [1]:

$$W_{pump} = (P_{friction} + P_{elevation}) * \text{[illegible]}_{mp} * \frac{1d}{24hr} * \frac{1hr}{3600s} \quad \textbf{(C8)}$$

here η_{pump} is the pump efficiency.

From pump working power, pumping energy intensity is calculated [1]:

$$E_{pump} = \frac{W_{pump}}{\dot{V}_{shipped}} * \frac{1kW}{1000W} * \frac{24hr}{1d} \quad \text{……}\textbf{(C9)}$$

Figure C1. Distance between Fort McMurray and Fort Saskatchewan [4].

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