Life Cycle Assessment of Lignocellulosic Biomass Conversion Pathways to Hydrogenation Derived Renewable Diesel

by

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Abstract

Renewable fuels standards introduced in various jurisdictions aim at increasing the use of biofuels. There has been limited work on the life cycle assessment of the production of HDRD in terms of overall environmental impacts. This study is focused on conducting an LCA on the production of hydrogenation-derived renewable diesel (HDRD) from lignocellulosic biomass available in western Canada, especially Alberta, to fill the gap in knowledge. The focus of the study is on assessments of the life cycle greenhouse gas (GHG) and water requirement for the HDRD production pathway from lignocellulosic biomass. HDRD has better properties than biodiesel in terms of its use in colder climates like Canada and can be produced from lignocellulosic biomass. The GHGs emitted from the fossil fuel energy used in the HDRD production pathway are assessed for three types of feedstocks, whole tree, forest residues, and agricultural residues. The results reveal that the GHG emissions and net energy ratio (NER) (the energy output per unit fossil fuel energy input) for fast pyrolysis-based processes followed by processing lie in the range of 35.4 - 42.3 gCO_{2,eq}/MJ HDRD and 1.55 - 1.90 MJ/MJ, respectively. HDRD from agricultural residues produces the least emissions and highest NER followed by whole tree feedstock, with forest residues having the most emissions and lowest NER. In addition to assessing the amount of GHG emissions and fossil-derived energy input, the life cycle water use requirements of HDRD production were also determined. This water use impact is extended to hydrothermal liquefaction (HTL) to study and compare two different types of conversion pathways. The water use requirements for whole tree and forest residues are 579.5 L H₂O/MJ HDRD and 438.1 L H₂O/MJ HDRD through fast pyrolysis and HTL, respectively. Agricultural residues had a lower water use requirement than whole tree and forest residues,

valued at 83.7 L H₂O/MJ HDRD and 59.1 L H₂O/MJ HDRD through fast pyrolysis and HTL, respectively. Water use from biomass production make up almost all of the total water use required to produce HDRD; therefore agricultural residues, requiring less water for growth, have a lower water use requirement than the other two feedstocks. Another factor that affects the water use required for HDRD production is the HDRD yield. Biomass going through HTL followed by hydroprocessing gives a higher HDRD yield than biomass going through fast pyrolysis followed by hydroprocessing; therefore, a lower water use is required per unit MJ of HDRD for HDRD produced by HTL and hydroprocessing. The results of the study are helpful in making investment decisions and policy formulation associated with HDRD production from lignocellulosic biomass in Alberta.

Preface

This thesis is an original work by Alain Jian Lin Wong. No part of this thesis has yet been published, but it is expected that two papers will be published based on the research work in this thesis.

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List of Symbols

Avg	Average
AR	Agricultural residue
bar	Bar (pressure)
°C	Degrees Celsius
CH ₄	Methane
CO ₂	Carbon dioxide
D	Distance
eq	Equivalent
Ein	Energy input
Eout	Energy output
FR	Forest residue
g	Gram
GHG	Greenhouse gas
GJ	Gigajoule
ha	Hectare
H ₂ O	Water
HDRD	Hydrogenation-derived renewable diesel
hr	Hour
HTL	Hydrothermal liquefaction
IEA	International Energy Agency
IPCC	Intergovernmental Panel on Climate Change
K ₂ O	Potassium oxide
kg	Kilogram
km	Kilometer
kW	Kilowatt
kWh	Kilowatt-hour
L	Liter
LCA	Life cycle assessment
LUC	Land use change

m ³	Cubic meters
MJ	Megajoule
mm	millimeter
MPa	Megapascal
MWe	Megawatt (electricity)
Ν	Nitrogen
N ₂ O	Nitrous oxide
NaOH	Sodium hydroxide
NER	Net energy ratio
P_2O_5	Phosphorous
r	Length of the radius of the circular harvesting area
r _{avg}	Average transportation displacement
RFS	Renewable fuels standard
S	Sulphur
ULSD	Ultra-low sulphur diesel
WT	Whole tree
wt%	Weight%
yr	Year
Σ	Summation

Chapter 1: Introduction

1.1 Background

Fossil fuel combustion has led to rising greenhouse gases (GHG), which in turn have caused climate changes [1]. As seen in paleoclimate data, climate is highly sensitive to climate forcings in the long-term [2]. Moreover, the current global carbon dioxide concentration of 385 ppm is considered to be at a threatening level [2]. These observations put increased emphasis on environmental issues and energy sustainability, which in turn lead to greater focus on the importance of alternative fuel sources.

Carbon-rich material such as biomass could be used as an energy source to produce fuels, especially transportation fuels due to the similar properties of biofuels to conventional gasoline and diesel. Because the carbon obtained from biofuels is originally derived from the carbon dioxide (CO₂) in the atmosphere when a plant absorbs CO₂ during photosynthesis, biofuels are considered to be nearly carbon-neutral [3].

In an effort to promote wise use of energy and responsible development, Alberta's Renewable Fuels Standard (RFS) introduced in 2011, requires an average of 2% renewable diesel in diesel fuel sold in Alberta, and the renewable fuels used should provide a reduction in GHG emissions of at least 25% compared to equivalent petroleum fuel [4]. Following the implementation of RFS, the demand for diesel for transportation increased by approximately 4 - 6% between 2010 and 2013 [5]. The International Energy Agency (IEA) and Intergovernmental Panel on Climate Change (IPCC) predicted that biofuels will make up 10 - 20% of transportation fuel by 2030 [6]. The demand for diesel is high in Alberta's transportation sector and is expected to continue to grow [7]; thus, it will be important to meet the growing demand for renewable diesel in a sustainable manner to mitigate GHG emissions.

Hydrogenation-derived renewable diesel (HDRD) is one of the biofuels (e.g. ethanol, methanol, bio-oil, biodiesel) available. Produced from biomass through thermochemical conversion

processes such as pyrolysis and hydrothermal liquefaction followed by hydro-deoxygenation process, HDRD gives a higher cetane number and better cold flow properties than biodiesel [8]. Although HDRD serves as a good alternative fuel to fossil diesel and a better choice for blending with ultra-low sulphur diesel (ULSD) than biodiesel, production of HDRD in Canada has not been commercialized at the moment [8, 9].

Lignocellulosic biomass is available in Alberta in large quantities and is commonly available in the form of agricultural residues when harvesting of grains takes place, forest residues when logging operations take place, and also whole trees when they are entirely used for biomass after clear cutting of the forest [10, 11, 12]. These kinds of biomass, except for whole tree, not only do not interfere with food production, but also do not get used in Alberta currently on large scale. The adoption of lignocellulosic feedstock for HDRD production could be an option of using renewable resource available in Canada.

Apart from GHG emissions and reliance on fossil fuel energy in the conversion process of biomass to HDRD, water is also directly and indirectly required for the production of HDRD. As clean water is an important resource, having a water efficient conversion pathway to produce HDRD is of importance to reduce impact on the environment. In addition, Canada's semi-arid prairies have limited water availability, and this is a factor to consider for biomass production to ensure consistent supply of biomass [13, 14]. Understanding the amount of water use required for HDRD production could then allow future water use planning to take place when demand for HDRD increase.

There are studies done on HDRD production from wood [15, 16], ethanol from switchgrass and corn stover [17], and biodiesel from palm oil [18]. The studies were conducted on different type of biofuels, feedstocks, or geographical locations that are not in Canada. Studies on water use for biofuels production from various types of biomass are also found [19, 20, 21]. However, these studies on water use either focus on biomass production only i.e. not on the life cycle footprint or their scope was based on United States. With the literature covering many aspects of biofuel production from biomass and their environmental impacts, but not HDRD production from lignocellulosic biomass in western Canada, this study is aimed at filling this gap in knowledge.

1.2 Objectives of the study

The overall objective of this research is to investigate the environmental sustainability of producing HDRD from lignocellulosic biomass over the life cycle. This study develops comprehensive data-based models that use Alberta-based data inputs for lignocellulosic biomass, such as whole tree, forest residues, and agricultural residues, that is converted to HDRD. The specific objectives are as follows:

- Determine the biomass conversion pathways to produce HDRD;
- Develop a data-intensive model to estimate the energy required for each unit operation in HDRD production and find out the net energy ratio (NER) (the ratio of the output energy produced in the process to the input energy required [\sum E_{out}/\sum E_{in}]);
- Develop and estimate the GHG emissions of each unit operation over the life cycle of HDRD production;
- Develop a framework to assess the water footprint for all unit operations in the HDRD production life cycle for two pathways. The two pathways are:
 - Conversion of lignocellulosic biomass to bio-oil through fast pyrolysis followed by conversion of bio-oil to HDRD through hydroprocessing
 - Conversion of lignocellulosic biomass to bio-oil through HTL followed by conversion of bio-oil to HDRD through hydroprocessing;
- Develop models to estimate direct and indirect water use required of unit operations in the life cycle of HDRD production;
- Estimate the effect of uncertainties of variables on the results obtained in the study by conducting a Monte Carlo simulation on results;
- Compare results with fossil fuel diesel to assess sustainability;

• Compare results among feedstocks to identify the major variables affecting results.

1.3 Scope and limitations of the study

LCA of biomass conversion to HDRD involves the following unit operations: harvesting and fertilization, transportation of biomass, fast pyrolysis, transportation of bio-oil, hydroprocessing of bio-oil to produce HDRD. In Chapter 2, GHG emissions and fossil fuel energy input for each unit operation is computed to estimate the total amount of GHG emissions and NER to produce 1 MJ of HDRD. The GHG considered in this study are CO₂, CH₄, and N₂O. The data inputs were from various sources of literature, consultation with industry experts, and development through calculations.

Similarly, estimation of water use requirements in Chapter 3 follows the same unit operations of LCA. Direct water (e.g. cooling water, water for irrigation, precipitation) and indirect water (e.g. water required to produce fossil fuel and fertilizer) are derived for each unit operation to estimate the total water use required to produce 1 MJ of HDRD. Chapter 3 extended the study of water use requirements to another conversion pathway that adopts hydrothermal liquefaction in place of fast pyrolysis. The differences between the two conversion pathways are identified and separate input data are used to ensure accuracy.

Direct inputs, such as fertilizers, energy, used in the processes to produce HDRD are considered for the LCA study while the indirect inputs, such as lubricants and manufacturing of equipment and plant, are not considered. In this study, assumptions such as nutrient and carbon content of the soil does not change over time are made; hence, the impact of changes in nutrient and carbon content of soil are not considered.

1.4 Organization of the thesis

This thesis is in paper-based format. This thesis consists of independent chapters, with each chapter being a paper, are intended to be read separately. This thesis consists of four chapters.

Chapter 2 covers the GHG emissions factors and fossil fuel energy required for HDRD production from lignocellulosic biomass through fast pyrolysis and hydroprocessing. A comparison is conducted between three feedstocks, whole tree, forest residues, and agricultural residues. Sensitivity and uncertainty analyses are also conducted to understand the effects of variables and their uncertainties on the results of study.

Chapter 3 evaluates the water requirements for production of lignocellulosic biomass and its conversion to HDRD through fast pyrolysis or HTL followed by hydroprocessing. The water requirement factors are then compared and analyzed between feedstocks and the two different bio-oil production pathways. Sensitivity and uncertainty analyses are conducted to understand the effects of variables and their uncertainties on the result of study.

Chapter 4 concludes the study and provides recommendations for future work.

Chapter 2: Life cycle assessment of renewable diesel from lignocellulosic biomass¹

Chapter 2 investigates the GHG emissions and fossil fuel energy required to produce HDRD from three feedstocks, whole tree, forest residues, and agricultural residues, by following the methodology of an LCA.

2.1 Introduction

Fossil fuel combustion has led to an increase of carbon dioxide to a concentration of 385 ppm, causing global warming [2, 22]. Global warming issues caused by greenhouse gas (GHG) emissions from fossil fuels can be mitigated through the use of biofuels. Biofuels are considered to be nearly carbon-neutral as the carbon generated from combustion of biofuels is originally derived from the carbon dioxide (CO₂) in the atmosphere when a plant absorbs CO₂ during photosynthesis [3]. In an effort to promote wise energy use and responsible development, the governments of various countries, such as the United States of America, the United Kingdom, and Canada, have come up with renewable fuel regulations [23, 24, 25]. Although biofuels are regarded as carbon-neutral, the biofuel production process produces GHG emissions and has other environmental impacts. Biofuels characteristics and environmental impacts vary based on conversion pathways and biomass type, and these variations result in different amounts of energy use and GHG emissions [26, 27].

Lignocellulosic biomass from forests and agricultural land provides a source of biomass for HDRD production sufficient to meet the demand initiated by the various renewable fuel regulations in various jurisdictions [23, 24, 25]. Although biodiesel is able to fulfill government regulations, the chemical composition between biodiesel and HDRD is different [8]. Biodiesel is

¹ Wong A., Zhang H., Kumar A. Life cycle assessment of renewable diesel production from lignocellulosic biomass. Bioresource Technology, 2015 (to be submitted).

produced through transesterification and contains straight-chain fatty acid alkyl esters, while HDRD is produced through hydroprocessing and contains components such as alkanes, aromatic compounds, and alkyl side chains [28]. These chemical structures of biodiesel and HDRD determine the physical properties of biodiesel and HDRD [28]. Due to the chemical composition differences between biodiesel and HDRD, biodiesel has a higher cloud point than HDRD, and this poses a problem for blending with fossil fuel diesel, especially in colder climates [8]. Furthermore, the cloud point of HDRD can be lowered by altering the isomerization or hydrocracking process to make it ideal for blending with fossil fuel diesel [8]. Besides the cloud point of fuel, other physical properties, such as cetane number and cold flow properties, make HDRD a more suitable alternative to fossil fuel diesel than biodiesel [8]. Therefore, this study focuses on HDRD instead of biodiesel due to its more favorable physical properties to allow this study to be applicable to colder climates. Biofuel use is expected to grow further as a means of mitigating GHG emissions [6, 7]; thus it will be important to increase our understanding of the environmental impact of HDRD production from lignocellulosic biomass if HDRD is to help meet the growing demand for biofuels.

Studies based on various technologies currently available have been done on converting biomass to renewable diesel. Papong et al. looked into the net energy ratio (NER) (the ratio of energy output to fossil-fuel energy input) of biodiesel from palm oil; this biodiesel has a NER of 2.5 MJ/MJ, making the production of this biodiesel efficient in terms of energy [27]. However, this study did not include an environmental impact analysis. Peters et al. simulated the fast pyrolysis and hydro-upgrading processes to convert poplar into HDRD using data specific to Spain [30]. In their study, both processes showed 54.5% GHG reductions compared to fossil gasoline and diesel [30]. Peters et al. also mentioned biomass drying as the major energy consumer while direct emissions from pyrolysis and hydroprocessing plants were the main GHG emissions contributors [30]. Han et al. performed a life cycle analysis on the well-to-wheel process of forest residues and corn stover conversion to gasoline and diesel via pyrolysis and hydroprocessing based on research data specific to United States of America [31]. In their study, pyrolysis yields from woody biomass range from 50-70% while yields from agricultural residues

range from 30-60% [31]. Han et al. also concluded that GHG emissions reductions range from 55-64% when natural gas is used to produce hydrogen for hydroprocessing [31].

With relatively few LCAs conducted for lignocellulosic biomass conversion to HDRD and no Canada-based research, this paper serves to fill this gap in the literature. The overall objective of this research is to conduct the LCA of HDRD production from lignocellulosic biomass for Canada. The specific objectives are:

- To develop a data-intensive model to estimate the energy input for producing HDRD from lignocellulosic biomass in Canada.
- To quantify GHG emissions for each stage of lignocellulosic biomass harvesting to delivering produced renewable diesel to consumers.
- To conduct an uncertainty analysis of the results based on the Monte Carlo simulation.
- To develop a sustainability parameter for producing HDRD from Canada's available lignocellulosic biomass to assist the oil refining industry and government in making decisions on future implementations of HDRD.

2.2 Methodology

The LCA conducted in this study followed the four steps given in ISO 14040: a goal and scope definition, life cycle inventory analysis, life cycle impact assessment, and life cycle interpretation [32]. The goal and scope of the paper are clearly defined by stating the intended audience as well as the system boundary set for the study. A detailed inventory of GHG emissions and energy inputs for lignocellulosic biomass to HDRD are compiled for the assessment required in the second and third steps of a life cycle assessment. Subsequently, global warming potentials are allocated to the respective GHG emissions for an accurate impact assessment before further interpretation of the results is done, and shared, in the results and discussion section of the paper.

This study made several assumptions. First, the locations of pyrolysis plants and hydroprocessing plants are based on the locations of biomass availability and the current locations of oil and gas processing facilities. Traveling distance is then determined according to these designated locations. Second, it is assumed that soil nutrient content and carbon concentration remain the same following fertilization, reforestation, and cultivation of agricultural crops.

2.2.1 Goal and scope

The first step of an LCA, goal and scope, states the objective, boundary and the functional unit of the study.

2.2.1.1 Goal

The LCA model developed in this study, a well-to-wheel approach, helps analyze whether it is more environmentally friendly to use HDRD than its conventional fossil fuel alternatives. With site-specific data and pathways, this model is more precise than LCA models currently available in the public domain. The amount of GHG emissions from the production of HDRD from forest biomass and agricultural residues is estimated (in the model) in order to quantify the feasibility of using the biomass available in Alberta, a province in Western Canada, as feedstock in an effort to mitigate GHG emissions. As part of the LCA, the net energy ratio (NER) is estimated to determine the ratio of energy output to fossil fuel energy input ($\Sigma E_{out}/\Sigma E_{in}$). The NER quantifies the effectiveness of energy use in HDRD production from forest biomass and agricultural residues [33]. The values of GHG emissions and the NER derived in this LCA can then be used as a reference to benefit industry for the commercialization of HDRD plants.

2.2.1.2 Scope

Emissions and energy use are calculated for the following key stages: (i) logging trees, harvesting forest and agricultural residues, (ii) transportation of whole trees, forest residues, and agricultural residues in the form of chips and bales, (iii) pyrolysis of biomass, (iv) transportation of bio-oil to the hydrotreating plant, distillation, and hydrocracking plant, (v) HDRD production, (vi) transportation of HDRD to the refinery for blending and finally delivery to consumers, and

(vii) combustion of HDRD by consumers. Carbon emissions from the combustion of biomass are absorbed during plant growth, rendering the emissions from the combustion of biomass carbon-neutral [3].

2.2.1.3 System boundary, functional unit, and GHGs

A detailed illustration of the system boundary is provided in Figure 2-1. The system boundary encompasses the direct inputs of fossil fuel in each stage of HDRD production for the whole life cycle assessment. The indirect inputs (i.e., manufacturing trucks for transporting feedstock and building factories for feedstock conversion) are not considered in the study as these are a small percentage of the overall emissions [33]. The functional unit, the unit used as the basis for analysis, is a unit of energy (1 MJ) of the renewable diesel produced based on lower heating value. The GHGs considered in terms of their contribution to global warming are CO₂, CH₄, and N₂O, which have global warming potentials (GWP) (CO_{2, equivalent}) of 1, 25, and 298, respectively; these figures are based on a 100-year time horizon and adopted by Intergovernmental Panel on Climate Change (IPCC) and Alberta Government [22, 34].

2.2.1.4 Allocation method

An allocation method is needed to distribute the inputs and outputs of each product in the system and its respective environmental impact [35]. Energy allocation, an allocation method wherein environmental impacts are allocated based on the energy contents of products formed in the system studied, is used here because HDRD and co-products are energy sources and are used as products for their energy content. Energy allocation is widely used as an allocation method for bioenergy-related LCAs [36]. Furthermore, energy allocation does not change with time as calorific values of products are not dependent on time [37]. In addition, comparisons between our work and other published energy allocation-based results can be made. Other methods such as displacement and economic allocation are not applicable as, in the first instance, there is no prevalent equivalent product in the market for displacement, and the second applies when economic concerns are the main driver [38].



Figure 2-1: System boundary of LCA of HDRD production

2.3 Life cycle inventory

This inventory encompasses the necessary direct energy inputs, GHG emissions, and the materials required for all unit operations from the production of biomass to its conversion to HDRD.

2.3.1 Availability of biomass

The large areas of Alberta covered by forests provide a sufficient amount of trees for a biomass feedstock supply if sustainable forest management practices are carried out. The main harvests in Alberta's forestry industry are coniferous and deciduous trees, and thus this study focuses on these tree types [39]. To fully tap the resources of the forest, the entire tree is used for biomass feedstock. This includes the tops and branches, which constitute around 15-25% of the tree biomass [40]. The harvest of forest residues such as branches and tree tops contributes about 3.29 million dry tonnes of wood biomass generated predominantly from logging operations [33]. To increase the energy density of forest residues, the residues can be densified through pyrolysis to bio-oil, before stabilization and hydrocracking, followed by conversion into gasoline and diesel blend components [41].

Pyrolysis plants are assumed to be located in the center of a circular biomass collection area; hence the locations of pyrolysis plants in Alberta depend on the availability of biomass. With respect to whole tree feedstock, regions within Alberta's Land-use Framework where the province's main timber harvesting activities occur are the Lower Peace, Upper Peace, Lower Athabasca, and Upper Athabasca [10]. Similarly, forest residues are primarily available in the Lower Peace and Upper Athabasca [11]. Based on statistics available from Alberta Environment and Sustainable Resource Development, the Lower Peace and Upper Athabasca regions are able to meet biomass demand for a 2000 dry tonnes/day capacity pyrolysis plant [10, 11]. Therefore, locations of pyrolysis plants for wood chips are assumed to be in the Lower Peace and Upper Athabasca regions.

In Alberta, wheat and barley constitute the bulk of the agricultural harvest [42]. From 1997 to 2008, the combined average annual yield of wheat, barley, and oats was approximately 12.72 million tonnes/year [12]. With straw-to-grain ratios of 1.1 for wheat, 0.8 for barley, and 1.1 for oats [43], a large amount of straw can be used as biomass for HDRD production. This straw is normally left in the fields to decompose and in the process releases CO₂ into the atmosphere. That said, a portion of agricultural residues must be left in the fields to prevent soil erosion, some agricultural residues are used for animal feed and bedding, and machines are too inefficient to collect all the straw from the field. For an average grain production of 6.9 million tonnes/yr, 5.1 million tonnes/yr, and 0.72 million tonnes/yr during the period 1997 - 2008 for wheat, barley, and oats, respectively, an average straw yield of 2.70 tonnes of straw/ha is available in the field [12]. With an additional 0.75 tonnes/ha of the residues left in the field to prevent erosion, harvesting equipment capable of harvesting 70% of the residues available in the field, and 0.66 tonnes/ha to be used as feedstock and bedding, 0.517 dry tonnes/ha is available for biomass conversion to HDRD [43].

For a 2000 dry tonnes/day agricultural residue biomass pyrolysis plant, the south-east region of the province (demarcated by Statistics Canada), according to Alberta Agriculture and Rural Development, is able to supply that demand with agricultural straw [12, 44]. A location in south-east Alberta is assumed for a pyrolysis plant using agricultural straw as feedstock. The collection of agricultural residues is assumed to be done based on a square-shaped collection area of farmland in the middle of which the pyrolysis plant is located. A square collection area is assumed because of the farmland layout and existing roads.

2.3.2 Biomass harvesting and collection

In whole tree harvesting, operations involved are felling, skidding, and chipping. Whole trees are felled with a harvester at a fuel consumption of 0.67 L of diesel/m³ of wood before they are skidded by grapple skidder to a roadside chipper over an assumed skidding distance of 150 m at fuel consumption of 0.75 L of diesel/m³ of wood [33, 40]. Both harvesting and skidding use Ultra-low sulphur diesel (ULSD) and have an energy coefficient of 45.25 MJ/L diesel and a GHG emissions coefficient of 2727 gCO_{2,eq}/L [45, 46]. The roadside chipper chips the trees into

chips that are transported to a pyrolysis plant at 3.33 L of diesel/dry tonne [33]. After the removal of the trees, nitrogen fertilizer is applied to the soil with an energy consumption of 50 MJ/ha to encourage growth of saplings and to minimize nitrogen loss in soil [47]. Productivity and ULSD use in each of these sub-unit operations is calculated to obtain the amount of fossil fuel used and the corresponding GHG emissions. Table 2-1 shows the input quantities for each sub-unit operation based on a pyrolysis plant with a capacity of 2000 dry tonnes/day. The input quantities of fossil fuel and its corresponding emissions coefficients given in the table can be used to derive the values of GHG emissions ($gCO_{2,eq}$)/functional unit of the sub-unit operations. Similarly, using the energy coefficients, the same input quantities of sub-unit operations can be converted to their corresponding values of NER.

Forest residues refer to tops and branches and are considered to be leftovers from cut-to-length logging operations. In Alberta, 80% of harvested trees are skidded to the roadside where they are delimbed and topped [40]. These residues are piled at the roadside for burning [40]. To make the discarded forest residues usable, the residues are forwarded to a roadside chipper with a fuel consumption of 0.52 L of ULSD/m³ and chipped with a fuel consumption of 3.93 L of ULSD/dry tonne by the roadside chipper (see Table 2-2) [33]. Because forest residues differ from whole trees in terms of size and compactness, the chipping efficiency is lower for forest residues than whole trees. Like whole trees, forest residues are transported in the form of chips to the pyrolysis plant. When forest residues are removed, nitrogen is removed from the soil. As with whole tree feedstock, nitrogen fertilizer is applied to the soil with an energy consumption of 50MJ/ha to return nitrogen to the soil for sapling growth [47].

Whole tree											
Operation	Input quantity			Energ	Energy coefficient			Emission coefficient			Emissions
	Used value	Units	Ref	Used value	Units	Ref	Used value	Units	Ref	MJ/MJ	$\begin{array}{l}gCO_{2,eq} \\ MJ \end{array}$
Felling (diesel) ^a	0.67	L/m3	[33]	45.25	MJ/L	[45]	2727	gCO _{2,eq} / L	[46]	0.005	0.31
Skidding (diesel) ^a	0.75	L/m3	[33]	45.25	MJ/L	[45]	2727	gCO _{2,eq} / L	[46]	0.006	0.34
Chipping (diesel) ^a	3.33	L/dry tonne	[33]	45.25	MJ/L	[45]	2727	gCO _{2,eq} / L	[46]	0.009	0.53
Transportation of chips (diesel) ^a	0.24, 0.33	L/km	[48]	45.25	MJ/L	[45]	2722	gCO _{2,eq} / L	[46]	0.003	0.20
Road construction ^b	700	km	[33]	1731	GJ/km	[49]	403845	kgCO _{2,eq} /km	[49]	0.006	1.34
Nitrogen replacement	0.61	wt% N	[41]	49.45	MJ/kg	[50]	201.3	gCO _{2,eq} / kg	[50]	0.018	0.07
Fertilizer transport (diesel)	6.4	kJ/kg N/km	[47]	45.25	MJ/L	[45]	2722	gCO _{2,eq} / L	[46]	0.033	1.99
Fertilizer spreading (diesel) ^c	50	MJ/h a	[47]	-	-	-	2727	gCO _{2,eq} /L	[46]	3.49E- 05	0.002
N ₂ O emission factor	0.01	N ₂ O/ N	[51]	-	-	-	-			-	1.07

Table 2-1: Harvesting and transportation of whole tree chips used for feedstock (functional unit: MJ HDRD)

^a Input quantities are calculated based on the productivity and fuel economy of the equipment.

^bLength of road constructed, energy coefficients, and emission coefficients are based on a 20-year pyrolysis plant life.

^c A tractor is assumed to be used for the spreading of fertilizer [47].

The agricultural residues considered refer to the straw that is available in Alberta. Straw is often left on the fields after grain harvesting. The sub-units involved to obtain straw as biomass begin with raking the straw into windrows that can be baled, with an energy consumption of 0.47 L ULSD/dry tonne [33]. The subsequent operations, using an identical grade of diesel, are baling, bale wrapping, stacking, loading, and trucking to a pyrolysis plant for bio-oil production with energy consumptions of 2.9 L diesel/dry tonne, 0.055 L diesel/bale, 0.83 L diesel/dry tonne, and 0.33 L diesel/km, respectively [33]. Because straw is less dense than wood chips, the truck carrying straw bales will be limited by volume rather than the weight limit of the truck. Because the agricultural residues are not returned to the soil after removal, essential nutrients are added to

maintain soil fertility. These are listed in Table 2-3 along with other input quantities for agricultural residues harvesting.

Table 2-2: Harvesting and transportation of forest residues chips used for feedstock (functional unit: MJ HDRD)

Forest residues											
Operation	Input quantity			Energy	Energy coefficient			Emission coefficient			Emissions
	Used value	Units	Ref	Used value	Units	Ref	Used value	Units	Ref	MJ/MJ	gCO _{2,eq} / MJ
Forwarding (diesel) ^a	0.52	L/m3	[33]	45.25	MJ/L	[45]	2727	gCO _{2,eq} /L	[46]	0.034	2.07
Chipping (diesel) ^a	3.93	L/dry tonne	[33]	45.25	MJ/L	[45]	2727	gCO _{2,eq} /L	[46]	0.010	0.63
Transportation of chips (diesel) ^a	0.24, 0.33	L/km	[48]	45.25	MJ/L	[45]	2722	gCO _{2,eq} /L	[46]	0.014	0.84
Nitrogen replacement	0.61	wt% N	[41]	49.45	MJ/k g	[50]	201.3	gCO _{2,eq} /kg	[50]	0.018	0.07
Fertilizer transport (diesel)	6.4	kJ/kg N/km	[47]	45.25	MJ/L	[45]	2722	gCO _{2,eq} /L	[46]	0.039	2.37
Fertilizer spreading (diesel) ^b	50	MJ/ha	[47]	-	-	-	2727	gCO _{2,eq} /L	[46]	0.012	0.72
N ₂ O emission factor	0.01	N ₂ O/ N	[51]	-	-	-	-	-	-	-	1.07

^a Input quantities are calculated based on productivity and fuel economy of the equipment.

^b A tractor is assumed to be used for the spreading of fertilizer [47].

Agricultural residues											
Operation	Input quantity			Energy coefficient			Emission coefficient			Energy input	Emissions
	Used value	Units	Ref	Used value	Units	Ref	Used value	Units	Ref	MJ/MJ	gCO _{2,eq} / MJ
Raking (diesel)	0.47	L/dry tonne	[33]	45.25	MJ/L	[45]	2727	gCO _{2,eq} /L	[46]	0.001	0.09
Baling (diesel) ^a	2.9	L/dry tonne	[33]	45.25	MJ/L	[45]	2727	gCO _{2,eq} /L	[46]	0.009	0.55
Bale wrapping (diesel) ^a	0.055	L/bale	[33]	45.25	MJ/L	[45]	2727	gCO _{2,eq} /L	[46]	3.99E-04	0.02
Bale stacking (diesel) ^a	0.83	L/dry tonne	[33]	45.25	MJ/L	[45]	2727	gCO _{2,eq} /L	[46]	0.003	0.16
Bale loading (diesel) ^a	0.33	L/dry tonne	[33]	45.25	MJ/L	[45]	2727	gCO _{2,eq} /L	[46]	0.001	0.06
Transportation of bales (diesel) ^a	0.24, 0.33	L/km	[48]	45.25	MJ/L	[45]	2722	gCO _{2,eq} /L	[46]	0.009	0.53
Nitrogen replacement ^b	6	kg N/tonne	[52]	49.45	MJ/kg	[50]	201.3	gCO _{2,eq} /kg	[50]	0.023	0.09
Phosphate replacement ^b	1.85	kg P ₂ O ₅ /tonne	[52]	14.13	MJ/kg	[50]	439.8	gCO _{2,eq} /kg	[50]	0.002	0.06
Potassium replacement ^b	15	kg K ₂ O /tonne	[52]	8.84	MJ/kg	[50]	568.9	gCO _{2,eq} /kg	[50]	0.010	0.65
Sulphur replacement ^b	1.4	kg S /tonne	[52]	11.26	MJ/kg	[53]	17.73	gCO _{2,eq} /kg	[50]	0.001	0.002
Fertilizer transport (diesel) ^c	0.24, 0.33	L/km	[48]	45.25	MJ/L	[45]	2722	gCO _{2,eq} /L	[46]	1.69E-04	0.01
Fertilizer spreading (diesel) ^c	7	L/ha	[54]	45.25	MJ/L	[45]	2727	gCO _{2,eq} /L	[46]	0.016	0.95
N ₂ O emission factor	0.01	N ₂ O/N	[51]	-	-		-	-	-	-	1.37

Table 2-3 Harvesting and transportation of agricultural residues used for feedstock (functional unit: MJ HDRD)

^a Input quantities are calculated based on productivity and fuel economy of the equipment.

^bNutrient replacement is estimated based on average nutrient content in straw.

^c The truck for fertilizer transport is assumed to be the same as the truck for bale transport.

^d A tractor is assumed to be used for the spreading of fertilizer [54].

2.3.3 Transportation of forest woodchips and agricultural residues to a pyrolysis plant

After whole trees are chipped, the chips are transported by trailer trucks to a pyrolysis plant where they are converted to bio-oil. The collection area for forest biomass is assumed to be circular, with the pyrolysis plant located at the center. Based on this geometry, the average transportation displacement of the biomass collection area is found to be 0.707 r by equating the area of the outer ring (from r to r_{avg}) to the area of the inner circle with the radius r_{avg} , where r is the length of the radius of the circular area and r_{avg} is the average transportation displacement. The actual hauling distance is not a straight road to the pyrolysis plant. The actual distance can be estimated using a tortuosity factor, which is defined as the ratio of the actual distance over displacement. In this assessment, a tortuosity factor of 1.27 is used to account for the non-linear transportation distance [55], and a mean transportation distance of 19.5 km is derived. The truck capacity is 17.5 tonnes with an efficiency of 0.33 L of diesel per kilometer. For the return trip, it is assumed that the trucks are empty and therefore the efficiency improves to 0.24 L of diesel per kilometer [56]. Road construction for whole tree feedstock is required to transport wood chips to a pyrolysis plant located at an average distance of 19.5 km away. This, however, is not necessary for forest and agricultural residues feedstocks due to the existing roads available from logging and farming operations. Road infrastructure of 6 meters wide for chip transport involves primary and secondary roads; primary roads are used for trailer trucks to transport chips to a pyrolysis plant and the secondary roads are used by skidders and fellers. Secondary roads are significantly shorter than primary roads, and secondary roads do not need to be of the same quality as primary roads due to the slow-moving equipment using secondary roads; therefore, emissions and energy input associated with secondary road construction are negligible. When considering a pyrolysis plant life of 20 years, an estimated 700 km of primary roads are required, and these primary roads are constructed with an emission factor of 403,845 kg CO_{2,eq}/km and an energy factor of 1731 GJ/km [33, 49].

Forest residue chips are also transported by trailer trucks. Similarly, a transportation displacement of 0.707 r and a tortuosity factor of 1.27 are applied to calculate the transportation distance [55]. If we consider that 15-25% of the whole tree are forest residues – approximately 24.7 dry tonnes/harvested hectare – the forest residues available for collection over a 100-year

period is 0.247 dry tonnes/ha [40]. A mean transportation distance of 80.3 km for trailer trucks to transport forest residues chips to a 2000 dry tonnes/day pyrolysis plant is derived. Forest residue biomass is scarcer than whole tree biomass; as a result, a longer transportation distance is required for forest residue collection than for whole trees. The truck capacity and fuel economy for the transportation of forest residue chips are identical to those for whole tree chip transportation.

It is assumed that agricultural farmlands are square and that a pyrolysis plant is located in the centre of the square. The transportation distance of agricultural residues is calculated by taking the average distance of every point within a square plot to the center of the plot and multiplying it by a tortuosity factor of 1.27 [55]. Assuming a yield of 0.517 dry tonnes/ha straw biomass for a square plot of agricultural farmland, we derived an average transportation distance of 53.2 km for agricultural residues to the pyrolysis plant. Appendix A shows the methodology for calculating transportation distances for all feedstocks and also the associated assumptions.

2.3.4 Fast pyrolysis

Fast pyrolysis, the thermal decomposition of biomass in the absence of oxygen, is used to produce bio-oil in the form of vapors, charcoal, and non-condensable gas [57]. To meet the short residence time of fast pyrolysis, fast pyrolysis requires efficient heat transfer during the conversion of wood biomass to bio-oil; thus, the feedstock must be <6 mm to achieve a surface-to-volume ratio sufficient for efficient heat transfer [41]. For whole tree and forest residues, after wood chips are ground to 2-6 mm, they are reduced to less than 10% moisture content by a direct contact dryer using the heat energy from the hot combustion exhaust from the fast pyrolysis combustor before that exhaust is released to the atmosphere. A circulating fluidized bed reactor is then run at 500 °C and atmospheric pressure with a vapor residence time of 1 s to yield 72% bio-oil, 12% gases, and 16% char [15]. Bio-chars are separated by a series of cyclones while the vapor is condensed to recover bio-oil before the vapor is further broken down under the catalytic effects of bio-char and ashes [58, 59, 60]. To provide heat energy for fast pyrolysis, some bio-char and all the non-condensable gases are combusted. The bio-oil separated from bio-char and gases is delivered to a hydro-processing plant for HDRD production.

Whole tree											
Operation	Input quantity			Energy coefficient			Emission coefficient			Energy input	Emissions
	Used value	Units	Ref	Used value	Units	Ref	Used value	Units	Ref	MJ/MJ	gCO _{2,eq} /MJ
Grinding & drying	388.8	Wh/kg biofuel	[15]	9.89	MJ/k Wh	[45]	840	gCO _{2,eq} /kWh	[61]	0.083	7.082
Natural gas start up	1.58	kJ/kg biofuel	[15]	-	-		56.58	gCO _{2,eq} /MJ	[50]	3.43E -5	0.002
Pyrolysis	313.5	Wh/kg	[15]	9.89	MJ/k Wh	[45]	840	gCO _{2,eq} /kWh	[61]	0.067	5.711
Transportation of ash to forest (diesel) ^a	0.24, 0.33	L/km	[48]	45.25	MJ/L	[45]	2722	gCO _{2,eq} /L	[46]	1.94E -5	0.001
Spreading of ash (diesel) ^b	50	MJ/ha		-	-		2727	gCO _{2,eq} /L	[46]	3.49E -5	0.002
Transportation of bio-oil (diesel)	0.31, 0.50	L/km	[62]	45.25	MJ/L	[45]	2722	gCO _{2,eq} /L	[46]	0.008	0.479

Table 2-4: Fast pyrolysis of whole tree feedstock (functional unit: MJ HDRD)

^a The truck for ash transportation is assumed to be the same as the truck used for transporting wood chips.

^bAsh spreading method for the forest land is assumed to be the same as the method used for fertilizer spreading.

Forest residues											
Operation	Input quantity			Energy coefficient			Emission coefficient			Energy input	Emissions
	Used value	Units	Ref	Used value	Units	Ref	Used value	Units	Ref	MJ/MJ	gCO _{2,eq} / MJ
Grinding & drying	388.8	Wh/kg biofuel	[15]	9.89	MJ/kWh	[45]	840	gCO _{2,eq} /kWh	[61]	0.083	7.082
Natural gas start up	1.58	kJ/kg biofuel	[15]				56.58	gCO _{2,eq} /MJ	[50]	3.43E-5	0.002
Pyrolysis	313.5	Wh/kg biofuel	[15]	9.89	MJ/kWh	[45]	840	gCO _{2,eq} /kWh	[61]	0.067	5.711
Transportation of ash to forest (diesel) ^a	0.24, 0.33	L/km	[48]	45.25	MJ/L	[45]	2722	gCO _{2,eq} /L	[46]	8.01E-5	0.005
Spreading of ash (diesel) ^b	50	MJ/ha					2727	gCO _{2,eq} /L	[46]	0.012	0.715
Transportation of bio-oil (diesel)	0.31, 0.50	L/km	[62]	45.25	MJ/L	[45]	2722	gCO _{2,eq} /L	[46]	0.008	0.479

Table 2-5: Fast pyrolysis of forest residue feedstock (functional unit: MJ HDRD)

^a The truck for transportation of ash is assumed to be the same as the truck used for transporting wood chips.

^b Ash spreading method for the forest land is assumed to be the same as the method used for fertilizer spreading.

Similar to whole tree and forest residues feedstocks, agricultural residue straw must be approximately 3.2 mm for fast pyrolysis; the straw is reduced with a hammer mill [63]. The straw is dried with the heat from combustion exhaust until its moisture is reduced to 7%. The agricultural residues' fast pyrolysis parameters of 500 °C operating temperature, atmospheric pressure, and a vapor residence time of 1 s, similar to those of whole tree and forest residues, correspond to a yield of 71.6% bio-oil (including water content), 16.4% bio-char, and 12.0% gases [64]. Using the cyclone separator, bio-oil is separated from the other co-products before its delivery to a hydro-processing plant. For agricultural residues, all char and gases are combusted to provide energy for the fast pyrolysis process. Details of the energy inputs and GHG emissions for the fast pyrolysis process are shown in Table 2-4 through Table 2-6.

Agricultural residues											
Operation	Input quantity			Energy coefficient			Emission coefficient			Energy Emissions input	
	Used value	Units	Ref	Used value	Units	Ref	Used value	Units	Ref	MJ/MJ	gCO _{2,eq} /MJ
Grinding	24.66	kWh/dry tonne	[63]	9.89	MJ/kWh	[45]	840	gCO _{2,eq} /kWh	[61]	0.020	1.681
Drying	234.5	Wh/dry kg	[65]	9.89	MJ/kWh	[45]	840	gCO _{2,eq} / kWh	[61]	0.160	13.589
Pyrolysis	487.3	Wh/kg bio-oil	[65]	9.89	MJ/kWh	[45]	840	gCO _{2,eq} /kWh	[61]	0.258	21.885
Combustion of char ^a										- 0.372	-29.85
Transportation of ash to forest (diesel) ^b	0.24, 0.33	L/km	[48]	45.25	MJ/L	[45]	2722	gCO _{2,eq} /L	[46]	2.76E-4	0.017
Spreading of ash (diesel) ^c	7	L/ha	[54]	45.25	MJ/L	[45]	2727	gCO _{2,eq} /L	[46]	0.042	2.547
Transportation of bio-oil (diesel)	0.31, 0.50	L/km	[62]	45.25	MJ/L	[45]	2722	gCO _{2,eq} /L	[46]	0.007	0.409

Table 2-6: Fast pyrolysis of agricultural residue feedstock (functional unit: MJ HDRD)

^a Combustion of char provided credits for energy input and GHG emissions due to the allocating of GHG emissions and energy input to bio-char by energy allocation.

^b The truck for transportation of ash is assumed to be the same as the truck used for transporting agricultural residues.

^c Ash spreading method for the agricultural land is assumed to be the same as the method used for fertilizer spreading.

Process conditions affect the products produced; fast pyrolysis parameters favor the production of bio-oil, which is what we are seeking as an intermediate product [66]. However, due to the instability of bio-oil, phase-separation tends to occur both during the pyrolysis process, and during the aging process of bio-oil [67]. Given the unstable nature of bio-oil, bio-oil has to be converted to other forms of fuel within 4 weeks to maintain the quality required for HDRD conversion [64]; thus, we assume that the transportation and storage time of bio-oil is less than 4 weeks.

2.3.5 Transportation of bio-oil from a pyrolysis plant to an HDRD plant

Bio-oil is transported to an HDRD plant by super-B train truck with a capacity of 60 m³ [62]. It is assumed that the super-B train trucks are fully loaded with bio-oil when traveling to an HDRD plant and empty on the return trip and that they have a fuel consumption of 0.50 L/km when fully loaded and 0.31 L/km when empty [62]. Due to the availability of oil and gas facilities in the Redwater area, Alberta, we have assumed an HDRD plant location in Redwater. Based on this assumption, the distances from the pyrolysis plants to the HDRD plant are estimated to be 300 km for whole trees and forest residues and 250 km for agricultural residues.

2.3.6 Upgrading of bio-oil

Bio-oil is stabilized and converted to HDRD by the removal of oxygen through the hydrodeoxygenation process [41]. Bio-oil is hydrotreated at 140 bar and 270 oC using Co-Mo as a catalyst in the presence of H2 [15]. This first step of hydrotreating maintains the stability of the bio-oil by exposing it to a mild hydrodeoxygenation process before the second step, which involves higher temperature and pressure [68]. With some of the oxygen removed in the form of water, the bio-oil then goes through a second hydrotreating at 140 bar and 350 oC using Co-Mo as a catalyst in the presence of H2 to remove the remaining oxygen in the partially deoxygenated oil [15]. After oxygen removal, distillation takes place to separate heavier hydrocarbons for cracking. A second round of distillation then separates gasoline and diesel as products. The hydrogen used in hydrotreating is provided by steam reforming with water as input and energy supplied from natural gas, off-gas, and electricity [15]. All fossil fuel energy inputs for each

chemical process are shown in Table 2-7 through Table 2-9. These energy inputs include electricity for equipment (i.e., for pumps and compressors) and natural gas for heating.

Whole tree											
Operation	Input quantity			Energy coefficient			Emission coefficient			Energy input	Emissions
	Used value	Unit	Ref	Used value	Unit	Ref	Used value	Unit	Ref	MJ/MJ	gCO _{2,eq} / MJ
Hydrotreating	33.64	Wh/kg biofuel	[15]	9.89	MJ/k Wh	[45]	840	gCO _{2,eq} /kWh	[61]	0.008	0.650
Hydrocracking/ distillation	47.10	Wh/kg biofuel	[15]	9.89	MJ/k Wh	[45]	840	gCO _{2,eq} /kWh	[61]	0.011	0.910
Steam reforming	53.82	Wh/kg biofuel	[15]	9.89	MJ/k Wh	[45]	840	gCO _{2,eq} /kWh	[61]	0.012	1.040
Natural gas used	256.9 5	g/kg biofuel	[15]	52.23	MJ/k g	[50]	56.58	gCO _{2,eq} /kg	[50]	0.309	17.463
Transportation of bio-oil (diesel) ^a	0.31, 0.50	L/km	[62]	45.25	MJ/L	[45]	2722	gCO _{2,eq} /L	[46]	0.008	0.490

Table 2-7: Hydro-processing of bio-oil for whole tree feedstock (functional unit: MJ HDRD)

^a The super B-train trucks used for bio-oil transportation is assumed to be used to transport HDRD.

Forest residues											
Operation	Input quantity			Energy coefficient			Emission coefficient			Energy input	Emissions
	Used value	Unit	Ref	Used value	Unit	Ref	Used value	Unit	Ref	MJ/MJ	gCO _{2,eq} /M J
Hydrotreating	33.64	Wh/kg biofuel	[15]	9.89	MJ/ kWh	[45]	840	gCO _{2,eq} /kWh	[61]	0.008	0.650
Hydrocracking / distillation	47.10	Wh/kg biofuel	[15]	9.89	MJ/ kWh	[45]	840	gCO _{2,eq} /kWh	[61]	0.011	0.910
Steam reforming	53.82	Wh/kg biofuel	[15]	9.89	MJ/ kWh	[45]	840	gCO _{2,eq} /kWh	[61]	0.012	1.040
Natural gas used	256.95	g/kg biofuel	[15]	52.23	MJ/ kg	[50]	56.58	gCO _{2,eq} /kg	[50]	0.309	17.463
Transportation of bio-oil (diesel) ^a	0.31, 0.50	L/km	[62]	45.25	MJ/ L	[45]	2722	gCO _{2,eq} /L	[46]	0.008	0.490

Table 2-8: Hydro-processing of bio-oil for forest residue feedstock (functional unit: MJ HDRD)

^a The super B-train trucks used for bio-oil transportation is assumed to be used to transport HDRD.
Agricultural re	sidues										
Operation	Input quantity		Energy	Energy coefficient		Emissi	Emission coefficient			Emissions	
	Used value	Unit	Ref	Used value	Unit	Ref	Used value	Unit	Ref	MJ/MJ	gCO _{2,eq} / MJ
Hydrotreating ^a	58.2	Wh/kg HDRD	[65]	9.89	MJ/k Wh	[45]	840	gCO _{2,eq} /kWh	[61]	0.013	1.137
Hydrocracking / distillation ^a	81.5	Wh/kg HDRD	[65]	9.89	MJ/k Wh	[45]	840	gCO _{2,eq} /kWh	[61]	0.019	1.592
Steam reforming ^a	93.1	Wh/kg HDRD	[65]	9.89	MJ/k Wh	[45]	840	gCO _{2,eq} /kWh	[61]	0.021	1.819
Natural gas used	236	g/kg HDRD	[65]	52.23	MJ/k g	[50]	56.58	gCO _{2,eq} /kg	[50]	0.286	16.208
Transportation of bio-oil (diesel) ^b	0.31, 0.50	L/km	[62]	45.25	MJ/L	[45]	2722	gCO _{2,eq} /L	[46]	0.008	0.488

Table 2-9: Hydro-processing of bio-oil for agricultural residue feedstock (functional unit: MJ HDRD)

^a Electrical energy consumption of hydroprocessing bio-oil derived from agricultural residues is assumed to follow the electrical energy consumption distribution of hydroprocessing bio-oil derived from whole tree and forest residues, where the electrical energy distribution is 25%, 30%, and 40% for hydrotreating, hydrocracking and distillation, and steam reforming, respectively.

^b The super B-train trucks used for bio-oil transportation are assumed to be used to transport HDRD.

2.3.7 Transportation of HDRD

4.2 billion liters of diesel were consumed in Alberta in 2013 [5]. 76.8% of Albertans reside in urban areas; hence we assume that all of the HDRD produced (approximately 243 million L/year) is below the demand from all urban areas combined [69]. Alberta's two main cities are 65 km and 380 km, respectively, from Redwater, the site of the proposed HDRD plant. The average distance to transport HDRD to the two cities is approximately 445 km (round trip). Similar to bio-oil transportation, super B-train trucks would be used for HDRD transportation.

2.3.8 N₂O emissions and land use change

N₂O is released from the soil after nitrogen fertilizer is applied, contributing to global warming with a global warming potential 298 times greater than CO₂ [51]. Nitrogen fertilizer is required to ensure that the sapling growth rate in the boreal forest does not slow down following the loss

of nitrogen [70], but the corresponding N₂O emissions will also be present from forest lands due to the nitrification and denitrification processes in the soil [51]. Although nitrogen can be returned to the soil by atmospheric deposition, only 5% of the nitrogen from the combustion of logging residues can be returned to the forest in the form of NO_x [71]. Therefore, the fertilization of forest soils with nitrogen is still required. Other nutrients can be returned to the forest by returning the wood ash, which contains essential nutrients except nitrogen, thereby both returning nutrients to the soil and making ash disposal unnecessary. Furthermore, wood ash can have a neutralizing effect on the soil by reducing the natural acidity caused by tree growth [71]. It is assumed that forest growth remains unchanged after the removal of whole tree biomass and forest residues as long as nutrients are replaced through wood ash deposition and nitrogen fertilization [72]. In addition, the forests in Alberta are still first generation forests, hence the forest companies do not fertilize the forest [40]. As shown in Table 2-1 energy requirements to transport and spread nitrogen fertilizer are 6.4 kJ/kg N/km and 50 MJ/ha [47].

The application of nitrogen fertilizer to a field after the field loses nitrogen through the removal of agricultural residues will result in the release of N_2O by nitrification and denitrification in the soil. Nevertheless, to ensure there is no negative impact on future crop yield, fertilization of nitrogen and other nutrients will be carried out. The decrease in crop yield ranges from 0.05-0.15 dry tonnes/ha when there is a net decrease in N content of 1.5-4.5 kg N/tonnes straw harvested [73]. Besides nitrogen, removing agricultural residues from the field removes the carbon that would otherwise be returned to the soil, but the effects of removal are inconclusive because other influential factors affect crop yields simultaneously [74, 75]. In this study, we assume that there is no reduction of carbon in the soil over time [76].

Land use change can contribute a large amount of GHG emissions. This is because soil carbon content is often high, and it is estimated that soil carbon content reduction has contributed 158 Gtonnes C since 1850 through land use change, compared to 330 Gtonnes C from combustion during the same period [77]. Therefore slight changes to carbon concentration can lead to significant changes in GHG emissions. For forest and field, carbon is stored in three types of natural pools: vegetation, litter, and soil. With land use change, the equilibrium of the carbon stored in these pools will change and therefore the carbon concentration in the soil will change

over time [73] with the carbon lost through the emission of CO_2 to the atmosphere [78]. In this study, we do not consider the conversion of existing forest and agricultural land for other land uses, and thus it is assumed that the carbon content of soil does not change due to changes in land use.

2.4 Results and discussion

A life cycle assessment is sensitive to allocation methods, assumptions, and system boundary. In this study, allocation methods, assumptions, and system boundary are defined and the corresponding GHG emissions and NER of the LCA across three feedstocks are shown in graphs for comparison. Pyrolysis yields vary slightly in the literature depending on the pyrolysis conditions and feedstocks. For example, Peters et al. reported bio-oil yields of 68.8%, while Ringer et al. reported bio-oil yields of 73% [30, 79]. To determine how bio-oil yield affects the results of the LCA, sensitivity analyses are conducted on bio-oil yield along with other factors that might have an impact on the LCA to make this study more comprehensive.

2.4.1 Base case scenario

The base case for whole tree feedstock, in terms of GHG emissions and energy, is 39.7 gCO_{2,eq}/MJ HDRD with an NER of 1.71 MJ/MJ. The corresponding base case results for forest residues are 42.3 gCO_{2,eq}/MJ HDRD with an NER of 1.55 MJ/MJ and 35.4 gCO_{2,eq}/MJ HDRD with an NER of 1.90 MJ/MJ for agricultural residues. A higher NER likely relates to lower GHG emissions, but N₂O emissions and using more electricity instead of natural gas can shift the relationship between NER and GHG emissions. This study showed that harvesting biomass feedstock from agricultural residues is more efficient than harvesting biomass feedstock from whole tree or forest residues due to the better productivity of the field equipment. The better productivity is likely related to terrain differences and the moisture content of feedstock (refer to Figure 2-2). Canada's forest industry carries out first cut operations in the forest. Because of the initial high concentration of nutrients in the intact forest, logging operators currently do not replace nutrients. If it is assumed in this study that forest lands are not fertilized after the harvesting, GHG emissions of whole tree feedstock will be 37.6 gCO_{2,eq}/MJ HDRD with an

NER of 1.87 MJ/MJ. For the forest residues, GHG emissions will be 37.3 gCO_{2,eq}/MJ HDRD with an NER of 1.77 MJ/MJ if nutrient return is not carried out. With most of the fossil fuel consumption occurring in the hydro-processing stage followed by fast pyrolysis, the GHG emissions factor and NER do not differ much even though the percentage difference in fossil fuel demand for harvesting the three feedstocks differs significantly (refer to Figure 2-3). When we compare our study's GHG emissions with fossil-based diesel emissions at 90.8 gCO_{2,eq}/MJ diesel [73, 80], the percentage reductions in GHGs for using HDRD in its pure form are 56.3%, 53.4%, and 61.1% for whole tree, forest residues, and agricultural residues, respectively. The reason for GHG emissions savings when using HDRD is that GHG emissions from HDRD combustion are not reflected in Figure 2-3 as they are accounted for by the absorption of CO₂ during the growth stage of biomass.



Figure 2-2: Base case energy input for various feedstocks



× Harvesting

Transportation

Pyrolysis III Hydro-processing

Fossil diesel emissions

Figure 2-3: Base case GHG emissions for various feedstocks

2.4.2 Other scenarios - Sensitivity analysis

As indicated in Table 2-10, the scenarios in this study focus on how changes in the main contributors to GHG emissions and NER affect the overall results. The base case considered the return of ashes to the harvested soil to minimize nutrient loss and to reduce the need to landfill the ashes. In scenario 1, we investigated the use of trailer trucks on their return journey to send the ashes back to the forest or farm, i.e., transportation resource use was maximized and ash transportation was studied. In scenario 2, we studied the impact of sending ashes to an existing landfill if return of ashes to the soil is not welcomed by stakeholders. The energy input and GHG emissions of ash transportation to the landfill, assumed to be 50 km away from the pyrolysis plant, are looked into for scenario 2. As for biomass transportation, trucks of the same carrying capacity and fuel economy are used for ash transportation. Because it is assumed in the study that existing landfills will be used, energy and emissions from landfill construction are not considered. The productivity of fast pyrolysis and hydroprocessing greatly affect the GHG emissions and NER. To understand the impact on the emissions and NER, scenarios 3 to 6 were set up to study a 10% increase and decrease in yield. N₂O has a GWP of 298 times that of CO₂,

and this high GWP can cause an impact on the overall GHG emissions of HDRD production. For scenarios 7 and 8 we studied the impact of N₂O emissions factor ranges suggested by the IPCC to understand changes in emissions factor on the total emissions of HDRD production. For scenario 9, we considered forest residues and agricultural residues as by-products to facilitate comparison with studies that treat these residues as by-products or when soil fertilization is not required after residue removal. Bio-oil can replace natural gas to produce hydrogen in the steam reforming process to reduce the reliance on fossil fuel. In scenario 10, the use of bio-oil to produce hydrogen for hydrotreating instead of natural gas was considered. This scenario tested the benefits of HDRD production with reduced fossil fuel dependency by using the intermediate product generated in the production process. Transportation distance can fluctuate depending on the terrain and location of facilities. Scenarios 11 and 12 investigated how sensitive the results are toward changes in transportation distance when there is a change in transportation distance of $\pm 10\%$.

In scenario 1, ash sent back to the forest or field by return trailer trucks was investigated. The difference in the GHG emissions and NER between the base case and scenario 1 is negligible for all three feedstocks. This is mainly due to the low energy requirement for the delivery of ashes. In scenario 2, ashes were not returned, and this resulted in a lower GHG emissions and a higher NER. In this scenario, ashes were treated as waste and sent to an existing landfill. Ash spreading over the land contributes more to energy use and GHG emissions than the transportation of ashes to the field. Therefore, whole tree feedstock with a smaller harvest area than the other two feedstocks shows little change in energy use and GHG emissions between the base case, scenario 1, and scenario 2 due to minimal ash spreading over a small harvest area. On the other hand, forest residue and agricultural residue feedstocks, with larger harvest areas than whole tree feedstock, showed more significant differences in energy input and GHG emissions between scenario 2 and the base case.

For scenarios 3-6, sensitivity tests were conducted on product yields. All sub-unit operations are affected by the yields from fast pyrolysis and hydro-processing unit operations. A 10% change in bio-oil and HDRD yields was studied to see its effect on the NER and GHG emissions. Based on the understanding that efficiency is the amount of product output from a unit of input, a change

in yield will be analogous to a change in the efficiency of pyrolysis and hydro-processing. All energy inputs are based on 1 MJ of HDRD produced; as a result, a drop in bio-oil output during pyrolysis or a drop in HDRD output in hydroprocessing causes more energy input and GHG emissions in the harvesting and transportation stages to obtain 1 MJ of HDRD as a final product. Scenarios 3-6 support the use of fast pyrolysis over other forms of bio-oil production methods to obtain the most bio-oil for HDRD production, for higher bio-oil yield translates to lower energy inputs and GHG emissions in the harvesting and transportation stages.

Scenarios 7-8 show the limits of N₂O emissions factors according to the IPCC-stated uncertainty range of 0.003 to 0.03 [51]. Emissions from N₂O affect overall GHG emissions values because N₂O's GWP is 298 times that of CO₂, and nitrogen replacement is considered in all our feedstocks. With more nitrogen fertilizer used for agricultural residues than the other two feedstocks studied, agricultural residues are most sensitive to N₂O emissions, ranging from -2.7% to 7.7% followed by whole tree and forest residues, ranging from -1.9% to 5.4% and -1.8% to 5.0%, respectively. Changes in emissions factors of N₂O, however, do not have any impact on energy input or NER across all feedstocks.

In scenario 9, residues were treated as a by-product, which means that GHG emissions and energy required for fertilization are counted towards the harvesting of logs and grains but not of residues. Without the need for fertilization, the amount of GHG emissions drops significantly and falls below those of whole tree feedstock, especially those of agricultural residues. Compared to the base case, a lack of fertilization resulted in an 18.2% increase in the NER and a 14.1% reduction in GHG emissions for agricultural residues, and a 14.3% increase in the NER and an 11.7% reduction in GHG emissions for forest residues.

Scenario 10 suggested the use of bio-oil to produce hydrogen instead of using a non-renewable fuel, natural gas. Figure 2-4 shows that for all feedstocks, this scenario led to higher GHG emissions than the base case; on the other hand, the NER (see Figure 2-5) showed a mix of results, with whole tree achieving the same NER as the base case while forest residues experienced a lower NER in scenario 10 and agricultural residues NER increased from 1.90 to 1.94 MJ/MJ. There are several factors affecting the NER and GHG emissions in scenario 10.

First, the use of bio-oil to produce hydrogen reduces the emissions and energy input from natural gas, but the amount of bio-oil available for HDRD conversion is reduced, leading to a net reduction of HDRD produced. This reduction in yield increases the GHG emissions per unit MJ of HDRD and also decreases the NER, given that NER is measured by the energy content of HDRD produced per unit of non-renewable energy input. Second, with the reduction in yield, there is an increase in electrical energy used per unit MJ of HDRD produced when natural gas is not used for the steam reformer. This increase in electrical energy use is also amplified by the high emissions associated with electricity generation in Alberta due to fossil-fuel based electricity production. The breakdown of the GHG emissions and energy input of the unit operations of the three feedstocks is shown in Table 2-11 and Table 2-12.

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Scenarios	
Base case	Ashes are returned to the soil to replace minerals
1	Ashes are sent back to the soil by return chip and bale trucks
2	Ashes are sent to a landfill for disposal
3	Decrease bio-oil yield by 10%
4	Increase bio-oil yield by 10%
5	Decrease HDRD yield by 10%
6	Increase HDRD yield by 10%
7	Decrease N ₂ O emissions factor to 0.003
8	Increase N ₂ O emissions factor to 0.03
9	Forest residues and agricultural straw are treated as by-products and there is no need for
	fertilization when they are removed
10	Hydrogen production from bio-oil instead of natural gas in steam reformer
11	Decrease transportation distance by 10%
12	Increase transportation distance by 10%

The difference between scenarios 11 and 12 is barely noticeable. This shows that transportation distance does not have as much impact on GHG emissions and NER as compared to other factors. The changes in GHG emissions are 0.8%, 1%, and 0.5% for whole tree, forest residues, and agricultural residues, respectively. For the NER, percentage changes of 0.8%, 1%, and 0.4% are observed for whole tree, forest residues, and agricultural residues, respectively. The low impact on the GHG emissions and NER is because much higher GHG emissions and fossil energy input are observed in fast pyrolysis and hydroprocessing, thus reducing the impact caused by transportation distance.



Figure 2-4: GHG emissions of base case and considered scenarios



Figure 2-5: NER of base case and considered scenarios

Scenario 10: GHG emissions of unit operations for each feedstock (gCO _{2,eq} /MJ HDRD)						
Operations	Whole tree	Forest residues	Agricultural residues			
Harvesting	5.67	9.11	4.33			
Transportation	3.14	2.22	1.73			
Pyrolysis	16.82	17.76	15.00			
Hydro-processing	22.28	22.27	20.52			
Total	47.91	51.36	41.58			

Table 2-11: GHG emissions of unit operations for each feedstock (g CO_{2,eq}/MJ HDRD)

Table 2-12: Non-renewable energy	y input o	of unit ope	erations for e	each feedstock	(MJ/MJ HDRD)
	,,				(1110/1110/110/100)

Scenario 10: Non-renewable energy input of unit operations for each feedstock (MJ/MJ HDRD)						
Operations	Whole tree	Forest residues	Agricultural residues			
Harvesting	0.093	0.150	0.070			
Transportation	0.030	0.037	0.029			
Pyrolysis	0.198	0.213	0.171			
Hydro-processing	0.262	0.262	0.245			
Total	0.583	0.662	0.515			

2.4.3 Discussion of results

The values of the base case scenario for the three feedstocks range from 35.4 to 42.3 gCO_{2,eq}/MJ HDRD and 1.55 to 1.90 MJ/MJ for GHG emissions and NER, respectively. Hsu [16] arrived at figures of 39 gCO_{2,eq}/MJ HDRD and 1.56 MJ/MJ NER. Hsu's NER and GHG values are very close to the values found in this study. From the use of different feedstocks, we know that different varieties of biomass feedstock will result in different sub-unit operations such as harvesting methods and transportation distance. The chemical composition of biomass can also change the yield of the pyrolysis and hydroprocessing. Any minor difference in GHG emissions between Hsu's results and the forest residues studied in this paper can be attributed to the differences in the emissions of sub-unit operations and the assumptions taken.

HDRD can be produced with other feedstocks. Miller and Kumar reported GHG emissions of 38 and 48 gCO_{2,eq}/MJ HDRD and NER values of 2.0 and 1.7 MJ/MJ for camelina and canola feedstocks, respectively [62]. Comparing the NER values from their study with those from this study shows that lignocellulosic biomass requires approximately 0.03 to 0.15 MJ of fossil fuel

input more than camelina and canola for every 1 MJ of HDRD produced. However, the emissions amount is relatively similar among camelina, canola, and lignocellulosic biomass in their HDRD conversion pathways. One of the reasons for the difference in GHG emissions and energy input is the use of mass allocation, rather than energy allocation as used in this study. In Miller and Kumar's work, the allocation of GHG emissions and energy input to oilseed meal reduced the emissions and energy input allocated to HDRD. In addition, the oil extraction method studied by Miller and Kumar is not as energy intensive as pyrolysis, hence the difference in energy requirement. Moreover, feedstock type determines the calorific value and harvesting requirements and thus has an impact on the feasibility of producing HDRD from it. Compared to the feedstock from canola and camelina, the feedstocks chosen for this study are suitable for efficient HDRD conversion.

Some researchers have studied other types of renewable fuel such as biodiesel. Cherubini et al. reported a GHG emission range of 32.6 to 57.1 gCO_{2,eq}/MJ HDRD and an NER of 1.4 to 2.5 MJ/MJ for biodiesel derived from rapeseed, soy, and sunflower [73]. The results from of lignocellulosic biomass conversion to HDRD fall into the NER range of biodiesel production, making HDRD conversion from the three feedstocks studied favorable when compared to biodiesel in terms of net energy production. GHG emissions from the lignocellulosic biomass conversion for fast pyrolysis, hydrotreating, and hydrocracking, also lie in the lower half of the range found by Cherubini and his colleagues, suggesting that the environmental sustainability of HDRD is relatively similar to biodiesel.

2.4.4 Uncertainty analysis

Uncertainty analyses are calculated by assigning an uncertainty value for each input followed by a Monte Carlo simulation with 10 million iterations to obtain an accurate uncertainty on the GHG emissions and NER. An uncertainty analysis was conducted for the three feedstocks considered in this study. A framework by Huijbregts et al. was adopted to classify data and assign adequate uncertainty [81]. The assigned uncertainty for harvesting, fertilizing, and collection is 5%, while the transportation distance, bio-oil yield, and HDRD yield are assigned an uncertainty of 10% due to the possible ranges suggested by other studies and their impact on the results [31, 82, 83]. Without sufficient information to determine the distribution of probability of each input, a triangular distribution is assumed. The Monte Carlo simulation results are given in Figure 2-6 for the GHG emissions and Figure 2-7 for the NER.



Figure 2-6: Uncertainty results of GHG emissions for three feedstocks using Monte Carlo distribution

Based on the uncertainty analysis, the largest value of the 95th percentile across all feedstocks for GHG emissions is below 45 gCO_{2,eq}/MJ HDRD (see Figure 2-6), indicating that it is much more environmentally friendly to adopt the use of HDRD than fossil fuels. For the NER, the spread across all feedstocks is well above 1, suggesting that the biomass conversion process is viable in producing more output energy than the input energy required to produce HDRD. By taking the range from the 10th to the 90th percentiles, it is found that the percentage deviations for whole tree GHG emissions range from -3.7% to +3.9% and for forest residues and agricultural residues from -4.0% to +4.5% and -15.0% to +19.0%, respectively. For the NER, similar observations are noticed for the whole tree case -3.7% to +3.9% - while those for forest residues and agricultural residues range from -4.5% to +4.4% and -13.8% to +14.6%, respectively. The larger variation is found for agricultural residues because they have more input variables than the other two feedstocks.



Figure 2-7: Uncertainty results of NER for three feedstocks using Monte Carlo distribution

	NER			GHG		
						Agricultural
				Whole tree	Forest residue	residue
	Whole	Forest		GHG	GHG	GHG
	tree	residue	Agricultural	emissions	emissions	emissions
	NER	NER	residue	g CO _{2,eq} /MJ	g CO _{2,eq} /MJ	g CO _{2,eq} /MJ
Percentile	value	value	NER value	HDRD	HDRD	HDRD
5%	1.624	1.457	1.575	37.903	40.251	28.926
10%	1.641	1.476	1.638	38.288	40.691	30.108
25%	1.670	1.509	1.759	38.964	41.472	32.443
50%	1.704	1.545	1.901	39.752	42.399	35.428
75%	1.739	1.581	2.047	40.569	43.383	38.818
90%	1.771	1.613	2.179	41.321	44.306	42.166
95%	1.789	1.632	2.254	41.775	44.866	44.107

Table 2-13: Percentile values of uncertainty distribution plots

2.5 Conclusion

In the absence of environmental impact assessments on biomass to biodiesel and HDRD conversion to assist industry and government in future commercialization of HDRD production plants in Alberta, a life cycle assessment was conducted on the lignocellulosic biomass available

in Canada for conversion to HDRD. The results show that GHG emissions can be 39-47% of those of petroleum diesel alternatives, indicating that renewable diesel can mitigate GHG emissions to a certain extent. In terms of energy production, the NER for all three feedstocks is at least 1.55 MJ/MJ, proving that HDRD is more sustainable than fossil fuel diesel.

The major energy consumers and GHG emitters from the HDRD conversion process unit operations are fast pyrolysis and hydroprocessing. The energy-intensive processes of producing hydrogen used in hydroprocessing and drying feedstock for pyrolysis contribute to the high energy consumption and GHG emissions of the entire conversion pathway from biomass to HDRD. HDRD can be made a more attractive alternative to fossil fuel dependency if hydroprocessing efficiency is further improved.

When deciding which feedstock to use in order to reduce emissions and energy consumption, one should note that emissions can be reduced considerably during harvesting, and harvesting greatly depends on the availability of biomass within a unit area. Among the three feedstocks considered in this study, whole tree biomass has the advantage when it comes to biomass collection due to its shorter transportation distance. However, agricultural feedstock has a higher harvesting efficiency than whole tree harvesting, and the existing road infrastructure in farmland leads to overall lower energy use and GHG emissions for the harvesting and transporting of biomass compared to whole tree feedstock. Furthermore, if residues were considered by-products of tree-felling and grain harvesting, the fertilization of forest and fields would not be required and this would make residues biomass more favorable than whole tree biomass.

Chapter 3: Development of water requirement factors for lignocellulosic biomass to renewable diesel conversion pathways²

Chapter 3 looks at the water requirements to produce HDRD from whole tree, forest residues, and agricultural residues following the LCA adopted in chapter 2. An additional conversion pathway that replaces fast pyrolysis by HTL is added to the study for a more comprehensive study result.

3.1 Introduction

Water is critical for humans. Water is consumed primarily through farming, industrial, and domestic uses [84]. Canada's semi-arid prairies have limited water availability, a consideration for crop growth, and depend on irrigation to compensate for the lack of water from precipitation [13, 14]. Water sustains growth in dry boreal forest areas and could even change the landscape from forest to grassland if availability drops low enough [85]. The speed of plant growth and water demand varies with plant species. These differences can affect the amount of dry mass produced per unit of water used and water use efficiency for biomass production [86, 87]. Therefore investigating water requirements for different lignocellulosic biomass becomes crucial in biomass selection.

The production of biofuels not only depends on biomass but also the type of biofuels to be produced. There are different types of biofuels available with our current technology to replace fossil-based diesel. Among these biofuels are biodiesel and hydrogenation-derived renewable diesel (HDRD). The difference in biodiesel and HDRD comes from their chemical composition and structure [8]. Biodiesel contains straight-chain fatty acid alkyl esters produced from the transesterification process and HDRD contains alkanes, aromatic compounds, and alkyl side

² Wong A., Zhang H., Kumar A. Development of water requirement factors for lignocellulosic biomass to renewable diesel conversion pathways. Bioresource Technology, 2015 (to be submitted).

chains produced from hydroprocessing [28]. The differences in chemical composition and structure between biodiesel and HDRD result in different physical properties, such as cetane number and cloud point [8, 28]. The higher cetane number and ability to alter the isomerization process for better cold flow properties make HDRD a better biofuel to be adopted for use in colder climates than biodiesel [8]. The focus of this study is on HDRD because HDRD's physical properties are suitable for both cold and warm climates, and so this study's results will apply to both cold and warm climatic regions. Currently, there has been very limited research done on the assessment of water footprints for the conversion of biomass feedstocks to HDRD.

The production of energy and fuels from biomass sources requires water both during the growth of the biomass as well as during its conversion to fuels. Because water is an important resource, water requirements will be one of the factors to consider for the long-term sustainable production of HDRD. The growing emphasis on renewable fuels emphasizes the need for a better understanding of the water requirements of hydrogenation-derived renewable diesel from renewable sources. To date there have been several studies on the water footprint of biofuel production in general [20, 21, 88]. Singh et al. assessed the impact of producing biofuel in Alberta and concluded that southern Alberta does not have enough water to meet the high irrigation water requirements due to the dry climate [89]. Singh et al.'s study highlighted that 860-1530 billion liters of water are required to produce 4 billion liters of biofuels to meet a partial projected demand of biofuels in Canada in the year 2025 [89]. Yang et al. examined the life cycle water footprint of biodiesel production from microalgae and found that 3726 kg of water is required to produce 1 kg of biodiesel if water is not recycled during biodiesel production [88]. Dominguez-Faus et al. looked into the water requirement for energy crops to produce ethanol and compared the water footprint with that of existing power sources [20]. Their results showed that when corn is irrigated for ethanol production, 2.2-8.6 million liters of water are used, while biodiesel from soybean crops requires 13.9-27.8 million liters for one MWh of energy produced [20]. The study also revealed that the water requirement fluctuates depending on the type of biofuel produced and the geographical location at which the biomass is grown; a higher precipitation area will reduce the water required from irrigation [20]. Singh and Kumar developed water requirement factors for twelve biomass conversion pathways to ethanol and

electricity [90]. The water requirement factors of ethanol production pathways of corn and wheat biomass range from 38.7-55.5 L H₂O/MJ of ethanol while the water requirement factors of electricity production from corn stover and wheat straw range from 72.0-129.4 L H₂O/kWh of electricity [90]. Differences in the conversion pathway and water required for biomass production due to geographical location resulted in a water requirement disparity between the values calculated by Singh and Kumar for the production of a unit of electricity and the values of Dominguez-Faus et al. King and Webber concluded that biofuels derived from soy and corn require more water than fuels derived from fossil fuels, and soy requires less water than corn [21]. King and Webber also showed that irrigation plays a large part in water requirement; biomass feedstock that requires irrigation has, 47-141 L H₂O/km (distance travelled by light duty vehicle using the biofuel produced), a water consumption of 3 orders of magnitude higher than similar feedstock that does not require irrigation (0.12-0.94 L H_2O/km) [21]. Singh et al. have studied the water requirement to produce biofuel from six different biomass feedstocks. In their study, corn and wheat requires 178 L H₂O/MJ of ethanol and 325 L H₂O/MJ of ethanol, respectively [91]. With little research done on the water requirements of HDRD production, especially in colder climatic regions such as Canada, this thesis intends to fill the gap in knowledge on the life cycle water requirements for converting the lignocellulosic biomass readily available in western Canada to HDRD.

The overall objective of this study is to assess the life cycle water footprint of HDRD production from biomass feedstocks. The specific objectives include:

- Development of a framework to assess the water footprint for all stages of HDRD production from lignocellulosic biomass for two conversion pathways. These two pathways are:
 - Pathway 1: Conversion of lignocellulosic biomass to pyrolysis through fast pyrolysis and further conversion of bio-oil to HDRD.
 - Pathway 2: Conversion of lignocellulosic biomass to bio-crude through hydrothermal liquefaction (HTL) and further conversion of bio-crude to HDRD.

• Study the variation of the input parameters on the life cycle water footprint of HDRD production from lignocellulosic biomass through sensitivity and uncertainty analysis.

3.2 Methodology

The water requirement for the production of HDRD from lignocellulosic biomass encompasses the life cycle of lignocellulosic biomass from well-to-wheel. ISO 14040 suggested a life cycle assessment framework with the following steps: goal and scope definition, life cycle inventory analysis, impact assessment, and interpretation [32]. The goal and scope section defines the system boundary adopted for the study and discusses how the results can benefit the intended industry and government. The life cycle inventory is a compilation of the inputs required for computation and analysis and states the assumptions for input values. The computation and analysis allow the environmental impact to be assessed and interpreted for meaningful knowledge to be obtained from the study. This study uses an energy functional unit of 1 MJ of HDRD as the basis of analysis; accordingly, the inputs are converted to L H₂O/MJ HDRD to compile water use results. An uncertainty analysis using a Monte Carlo simulation is also included to find out how the distribution of the results is affected by the uncertainty of inputs.

This paper is based on the assumption that first, pyrolysis and HTL plants are located at places with adequate biomass availability to meet the plant capacity of 2000 dry tonnes/day. There is a significant potential of biomass in western Canada [92]. Traveling distances between harvesting locations, bio-oil production plants, HDRD production plants, and consumer are estimated based on the size of the plant. Second, it is also considered that soil nutrients removed due to removal of the biomass feedstocks are returned back through the fertilization and reforestation.

Water requirement in this study is estimated for three feedstock types: whole tree, forest residues, and agricultural residues. In the whole tree case, trees are chipped into chips which will be used as a feedstock for production of HDRD. Forest residues refer to the chips produced from branches and tops of the logging residues. In the current scenario in western Canada, forest residues are piled and burned in the forest to prevent forest fires [40]. Agricultural residues refer

to the straws from wheat and barley. In western Canada, most of these residues are left in the field to rot [40].

The study includes two methods of converting biomass to bio-oil or bio-crude: fast pyrolysis and HTL. Fast pyrolysis is a thermal decomposition process that uses a high heat transfer rate in the absence of oxygen to obtain high yields of bio-oil [93, 94]. To obtain a high heat transfer rate, the fast pyrolysis feed must have a moisture content of less than 10% [57]. HTL is a thermal decomposition process that converts biomass to bio-crude using super-critical state water to act as a medium [95]. In both thermal decomposition processes, bio-gas and char are formed as coproducts together with bio-oil/bio-crude [96, 97]. The difference in fast pyrolysis and HTL process conditions produces bio-oil and bio-crude of different properties. Bio-crude produced by HTL has a lower oxygen content than bio-oil from fast pyrolysis [82, 98]. Therefore, upgrading bio-crude to HDRD requires less hydrogen and energy input compared to upgrading bio-oil produced by fast pyrolysis [82, 98]. Detailed descriptions for both processes are given in sections 3.3.5 and 3.3.6. These two biomass conversion processes together with other unit operations, such as biomass production and hydroprocessing, form entire conversion pathways for data to be collected from and analyzed. A data-intensive model is developed using site-specific data and operation conventions. With this model, comparisons can be done between feedstocks and methods of bio-oil production to further understand the factors affecting water use efficiency.

The process of lignocellulosic biomass production and conversion to HDRD by fast pyrolysis or HTL and the subsequent hydroprocessing has several unit operations. The unit operations for the conversion pathway via fast pyrolysis include: (1) production and harvesting of whole tree, forest residues, and agricultural residues, (2) transportation of whole tree and forest residues in the form of chips and agricultural residues in the form of bales to a fast pyrolysis plant, (3) bio-oil production via fast pyrolysis, (4) transportation of bio-oil to a hydroprocessing plant, (5) bio-oil conversion to HDRD, and (6) transportation of HDRD to a refinery for blending with fossil fuel-derived diesel and to consumer. This pathway is illustrated in the system boundary diagram in Figure 3-1 with inputs and outputs indicated. For the conversion of lignocellulosic biomass to HDRD via HTL, the unit operations include: (1) production and harvesting of whole tree, forest residues, and agricultural residues, (2) transportation of whole tree and forest residues in the figure 3-1 with inputs and outputs indicated. For the conversion of lignocellulosic biomass to HDRD via HTL, the unit operations include: (1) production and harvesting of whole tree, forest residues, and agricultural residues, (2) transportation of whole tree and forest residues in the

form of chips and agricultural residues in the form of bales to an HTL plant, (3) bio-crude production via HTL, (4) transportation of bio-crude to a hydroprocessing plant, (5) bio-crude conversion to HDRD, and (6) transportation of HDRD to a refinery for blending with fossil fuel-derived diesel and to consumer. This second conversion method is illustrated in Figure 3-2.



Figure 3-1: System boundary of HDRD production via fast pyrolysis



Figure 3-2: System boundary of HDRD production via hydrothermal liquefaction

Water requirements in this study refer to both the direct and indirect water required to produce biomass and convert it to HDRD [90]. The direct use of water is defined as the water used throughout the entire biomass production period and the water required for the chemical conversion of biomass to HDRD (i.e., cooling make-up water, steam generation, etc.) [90]. The

indirect use of water is defined as the water used to produce fertilizers and that associated with the energy inputs [90]. For both direct and indirect water use, the source is either surface or ground water [90].

3.3 Water requirement inventory

Water requirements computed in this inventory are categorized based on the unit operations that make up the entire conversion pathway of lignocellulosic biomass to HDRD.

3.3.1 Production of biomass

This section introduces the water use in the production phase of forest biomass and agriculture biomass.

3.3.1.1 Forest biomass

Water use in boreal forest is through evapotranspiration, the sum of transpiration and evaporation [99]. Evapotranspiration can be separated into three parts, canopy, understorey, and soil surface evaporation [100]. Potential evapotranspiration is the amount of evapotranspiration from the forest that would occur if there is sufficient water [99]. In Alberta, which is one of the western Canadian Provinces, water for the boreal forest growth comes in the form of precipitation, and the precipitation amount is known to be smaller than the forest's potential evapotranspiration. The surface runoff is thus assumed to be negligible, and the average annual precipitation is taken to be approximately equal to the actual evapotranspiration [99, 101]. The average rainfall of Alberta's boreal plains forest is estimated to be 480 mm/yr [102]. Harvestable yields of 84 dry tonnes/ha for whole tree (WT) and 0.247 dry tonnes/ha for forest residues (FR) suggested by Kumar et al. are assumed to be the amount of biomass produced with the average precipitation [40]. However, not all precipitation should be allocated to the biomass feedstock if only a portion is used for HDRD production. For example, forest residues constitute 20% of the forest [40], and water allocation is conducted to allocate 20% of the precipitation to forest residues. Using the average rainfall and the feedstock yield, the water use for the production of WT and FR is

computed (with Eq. 1) to be 5714.3 L H_2O/kg dry wood and 3886.6 L H_2O/kg dry wood, respectively (see Appendix B for detailed calculations).

$$WR_{wood \ production} = \frac{Avg.rainfall \times no.of \ years \ for \ tree \ growth \times \% allocation}{(Yield_{dry \ mass})}$$
(1)

where,

WR_{wood production} – the water requirement for WT production, L H₂O/kg dry wood;

Avg. rainfall – the average rainfall over a year, mm/year;

No. of years for tree growth – the number of years for tree growth before the next round of harvest (FR is harvested on a yearly basis, while WT is harvested every 100 years), year;

%allocation – the allocation of water to the biomass of interest when it is produced along with other biomass (FR has a 20% allocation, while WT has a 100% allocation);

Yield_{dry mass} – the yield of dry biomass harvest, dry kg/ha.

3.3.1.2 Agricultural biomass

Agricultural residues are obtained from farmland after grains are removed. The water requirement for Alberta crops is computed based on the water required for crop growth. The water use to grow wheat, barley, and oats is 460 mm, 445 mm, and 430 mm precipitation equivalent, respectively [103]. The water required to grow crops is weighted based on mass to obtain an average water use. For biomass yield, the amount of straw yield per unit area is also weighted based on the production mass of residues over a period of 12 years (1997-2008) [43]. The net average yield of straw is computed to be 0.517 dry tonne/ha. Water use per unit kg of dry straw can be derived from these values to give 953.8 L H₂O/dry kg straw (Equations 2 and 3).

$$Avg. water use/area = \frac{\sum_{crops} [water use(mm) \times area]}{\sum_{crops} area} \times \frac{mass \ of \ straw \ used \ as \ biomass}{mass \ of \ total \ straw+mass \ of \ grains}$$
(2)

$$WR_{agricultural residues production} = \frac{Avg.water use/area}{net avg.yield of straw}$$
(3)

where,

Water use – the recommended water requirement for crop growth, mm;

Area – the area used to grow a certain type of crop, ha;

Avg. water use/area – the average water usage to grow crops per unit area, L H₂O/ha;

WR_{agricultural residues production} – the water requirement for agricultural residues production, L H₂O/kg dry wood;

Net avg. yield of straw – the amount of dry straw used as biomass in a unit area, dry tonne/ha.

In Singh and Kumar's study [90], water was not allocated in the production of wheat straw. If water were allocated to wheat straw, Singh and Kumar's water requirements for wheat straw production will give 934.4 L H₂O/dry kg of straw instead of 0 L H₂O/dry kg of straw [90].

3.3.2 Harvest of biomass

This section introduces the harvesting process of whole tree, forest residues, and agricultural residues, and the water requirements associated to these operations.

3.3.2.1 Whole tree

Whole tree harvesting involves the sub-unit operations of felling, skidding, and chipping before the trees are transported as chips to a pyrolysis plant or a HTL plant for conversion to bio-oil or bio-crude. These sub-unit operations use ultra-low sulphur diesel as energy. Felling operations use 1.92 L diesel/dry tonne before the whole trees are skidded to roadside at an energy use rate of 2.14 L diesel/dry tonne [33]. At the roadside, whole trees are chipped at an energy use of 3.33 L diesel/dry tonne [33]. Diesel inputs contribute to the indirect water use of HDRD production, and the value of indirect water use can be calculated by multiplying energy use/dry tonne wood by water use/energy unit; for example, indirect water use for the felling sub-unit operation can be computed by multiplying 1.92 L diesel/dry tonne wood by 2.2 L H₂O/L diesel. To produce wood chips, an indirect water use of 0.017 L H₂O/dry kg wood is required based on 2.2 L H₂O/L diesel water usage for diesel production [21].

Harvesting and fertilization (whole tree)							
Operation	Value (Energy or mass/dry	Ref	Water use factor (L H ₂ O/Energy	Ref			
.	tonne wood)	[22]	or mass)	[21]			
Felling (L diesel)	1.92	[33]	2.2	[21]			
Skidding (L diesel)	2.14	[33]	2.2	[21]			
Chipping (L diesel)	3.33	[33]	2.2	[21]			
Road construction (MJ diesel) ^a	0.073	[49]	0.059	[21]			
Road construction (kWh) ^a	0.018	[49]	1.08	[104, 105]			
Transportation (L diesel)	0.632	[48]	2.2	[21]			
Fertilizer transport (MJ diesel)	12.41	[47]	0.059	[21]			
Fertilizer spreading (MJ diesel)	0.60	[47]	0.059	[21]			
Nitrogen replacement (kg N)	6.1	[106]	0.683	[107]			

Table 3-1: Harvesting and fertilization water requirements (whole tree)

^a road construction is based on a 2000 dry tonnes/day and 20 year plant life

3.3.2.2 Forest residues

Branches and tree tops that are left along the sides of logging roads after trees are delimbed by logging operations are known as forest residues [40]. The harvesting processes are the forwarding of the forest residues with a fuel use of 1.49 L diesel/dry tonne and chipping with a fuel use of 3.93 L diesel/dry tonne [33]. The indirect water requirement for diesel use is calculated to be 0.024 L H₂O/dry kg wood, when ultra-low sulphur is used and water use factor for diesel is 2.2 L H₂O/L diesel [21]. Less water is required to harvest forest residues than whole trees because of fewer sub-unit operations in forest residues harvesting.

Harvesting and fertilization (forest residue)							
Operation	Value (Energy or mass/dry tonne wood)	Ref	Water use factor (L H ₂ O/Energy or mass)	Ref			
Forwarding (L diesel)	1.49	[33]	2.2	[21]			
Chipping (L diesel)	3.93	[33]	2.2	[21]			
Transportation (L diesel)	2.62	[48]	2.2	[21]			
Fertilizer transport (MJ diesel)	14.68	[47]	0.059	[21]			
Fertilizer spreading (MJ diesel)	202.43	[47]	0.059	[21]			
Nitrogen replacement (kg N)	6.1	[106]	0.683	[107]			

Table 3-2: Harvesting and fertilization water requirements (forest residue)

Table 3-3: Harvesting and fertilization water requirements (agricultural residue)

Harvesting and fertilization (agricultural residue)						
	Value (Energy		Water use factor			
Operation	or mass/dry	Ref	(L H ₂ O/Energy	Ref		
	tonne straw)		or mass)			
Raking (L diesel)	0.47	[33]	2.2	[21]		
Baling (L diesel)	2.9	[33]	2.2	[21]		
Bale wrapper (L diesel)	0.128	[33]	2.2	[21]		
Stacking (L diesel)	0.829	[33]	2.2	[21]		
Bale loader (L diesel)	0.33	[33]	2.2	[21]		
Transportation (L	2.798	Г <i>4</i> 0 1	2.2	[21]		
diesel)	2.198	[48]	2.2	[21]		
Fertilizer transport (L	0.248	[48]	2.2	[21]		
diesel)	0.240		2.2			
Fertilizer spreading (L	13.541	[54]	2.2	[21]		
diesel)	13.341	[34]	2.2			
Nitrogen replacement	7.364	[50]	0.683	[107]		
(kg N)	,	[20]	0.002			
Phosphate replacement	2.153	[50]	0.194	[107]		
$(\text{kg P}_2\text{O}_5)$		[0 0]		[10,]		
Potassium replacement	19.410	[50]	0.001	[107]		
$(\text{kg K}_2\text{O})$		[]		[]		
Sulphur replacement	1.575	[62]	0.683	[90]		
(kg S)		L]				

3.3.2.3 Agricultural residues

There are more sub-unit operations for straw harvesting than for whole tree or forest residues. The first sub-unit operation is raking to prepare the straw for baling; this uses 0.47 L diesel/dry tonne straw [33]. The next few steps are baling, bale wrapping, bale stacking, and bale loading with fuel uses of 2.9 L diesel/dry tonne straw, 0.13 L diesel/dry tonne straw, 0.83 L diesel/dry tonne straw, and 0.33 L diesel/dry tonne straw, respectively [33]. After totalling the field operations and multiplying the results by the water use factor, the indirect water use for harvesting and fertilization is computed to be 0.047 L H₂O/dry kg straw (see Table 3-3).

3.3.3 Transportation of biomass

This section introduces the transportation phase of whole tree, forest residues, and agricultural residues, and the water requirements associated to transportation.

3.3.3.1 Forest biomass

Fast Pyrolysis and hydrothermal liquefaction plant locations are assumed to be at the centre of a circular biomass harvest area. The average displacement of each point of the biomass harvest area to the centre of a circular area was calculated to be 0.707r, where r is the radius of the circular area considered. The boreal forest whole tree yield in Alberta is assumed to be 84 dry tonnes/ha [40]. The roads from the harvest site to the fast pyrolysis/HTL-based production plant are usually not straight, so a tortuosity factor of 1.27 is used to estimate the average distance required to transport biomass [55]. To obtain 2000 dry tonnes a day with 84 dry tonnes/ha yield, the average transportation distance (Equation 4) was worked out to be 19.4 km after the tortuosity factor was factored in [108]. Chips are transported by trailer trucks with a fuel economy of 0.33 L diesel/km with a full load of 17.5 tonnes. On the return trip, in which it is assumed that the truck is empty, the fuel economy is better, at 0.24 L diesel/km [48]. The calculation is show here:

$$D_{avg,} = \sqrt{\frac{Plant\ capacity \times days_{operation}}{WT_{yield} \times \pi}} \times 0.707 \times 1.27 \tag{4}$$

where,

 D_{avg} – the average distance required to transport whole tree wood chips, km; Plant capacity – the amount of biomass processed by a facility in a day, dry tonnes/day; days_{operation} – the total number of operational days in the entire life of the plant, days; WT_{yield} – the whole tree yield from forest, dry tonnes/ha.

Road construction is required for whole tree feedstock to transport wood chips to pyrolysis or an HTL plant. No road construction is required, however, for forest residues feedstocks due to the existing logging roads. Forest roads of six meters wide are classified as primary and secondary roads; primary roads are long stretches of roads that can be used for transporting wood chips by trailer trucks, and secondary roads can be used by fellers and skidders to fell and skid whole trees over short distances at slow speeds to a roadside chipper for the chipping process. Because primary roads are considerably longer than secondary roads, the construction of secondary roads is assumed to have negligible impact compared to the construction of primary roads. For a 2000 dry tonnes/day biomass processing plant, we estimate that 700 km of primary roads will be built over a period of 20 years [33]. Water use in road construction is indirect water use from energy production. Various forms of energy, amounting to 1731 GJ/km, are required to provide materials and fuel for construction equipment [49]. A water use factor of 0.0366 L H₂O/dry tonne wood is derived from the indirect water consumption of the energy required in road construction.

The calculation for the transportation distance of whole tree feedstock is applied to forest residues feedstock. The availability of forest residues has a yield of 0.247 dry tonnes/ha [40]. Based on this yield, 2000 dry tonnes of forest residues per day can be collected from a circular forest area with an average collection radius of 80.3 km after the tortuosity factor has been factored in. The wood chips from forest residues have similar properties as whole tree wood chips. The fuel consumption of trailer trucks for transporting forest residues wood chips is assumed to be the same as for whole tree feedstock.

3.3.3.2 Agricultural biomass

Agricultural residues have a yield of 0.517 dry tonnes/ha. A plant with a processing capacity of 2000 dry tonnes a day will require a harvest area with an average transportation distance of 53.2 km after tortuosity has been factored in [109]. These 53.2 km of roads are available in the form of existing farm roads; as a result, there is no road construction required for the conversion pathway of agricultural biomass to HDRD. Agricultural residues have different physical properties than forest wood. The main physical property that affects transportation is density. Agricultural residues, moreover, are packed in bales for transportation. The low density of agricultural residues means that the trailer truck is limited by volume instead of mass. Hence 12.6 tonnes of agricultural residues are transported per trip [48]. The transportation fuel economy is taken to be 0.33 L diesel/km for a full load and 0.24 L diesel/km for the return empty trip [48].

3.3.4 Fertilization

Nutrients are removed from the soil when biomass, in the form of trees or forest residues are harvested and used for production of fuels. Forest needs to be fertilized to maintain long-term fertility [71]. In this study, essential nutrients are considered. For forest, the return of ashes returns essential nutrients except nitrogen, which is not present in wood ashes. Nitrogen fertilizer, applied to encourage sapling growth in clear-cut plots, is included in this study [70]. This is required in the amount of 6.1 kg N/dry tonne wood removed [106]. The application of nitrogen includes spreading the fertilizer and transporting it from the fertilizer plant to the forest. The distance from the fertilizer plant to the bio-oil/HTL plant is assumed to be 300 km, and the additional distance from the bio-oil/HTL plant to the deforested plot of land is taken to be the same as the average biomass transportation distance. The energy required to spread nitrogen is 0.60 MJ diesel/dry tonne wood (see equation 5) for a whole tree feedstock yield of 84 dry tonnes/ha [47]. The transportation energy required is 12.41 MJ diesel/dry tonne wood [47] (see equation 6) when the energy requirement for transport is 0.064 MJ diesel/kg N/km [47]. For wood ash, similar parameters are used, but the transportation distance is reduced to the distance between the bio-oil/HTL plant and the harvested area because the wood ash comes from the biooil/HTL plant. Forest residues are harvested over a large area and therefore the energy requirement for transportation and spreading is proportionally higher. The energy requirement of

ash and fertilizer spreading increased to 202.43 MJ diesel/dry tonne wood as the harvesting area for FR is bigger than the harvesting area for WT [47]. The transportation energy requirement of ash and fertilizer remains at 0.064 MJ diesel/kg N/km for the FR case, while the ash transportation distance is 80.3 km according to equation 4, and the transportation of fertilizer is 380.3 km with an additional 300 km of traveling from the fertilizer plant to the bio-oil/HTL plant added to the distance from the bio-oil/HTL plant to harvest area.

$$Energy_{fertilizer spreading,dry tonne} = \frac{Energy_{fertilizer spreading,area}}{yield of biomass}$$
(5)

 $Energy_{fertilizer\ transport, dry\ tonne} = Energy_{transport} \times kg\ of\ N \times Distance$ (6)

where,

Energy_{fertilizer spreading, dry tonne} – the energy required to spread fertilizers over land based on per unit dry tonne biomass removed from land, MJ/dry tonne;

Energy_{fertilizer spreading, area} – the energy required to spread fertilizers over land based on per unit land area, MJ/ha;

Yield of biomass – the amount of biomass harvested in a unit area, dry tonnes/ha;

Energy_{fertilizer} transport, dry tonne – the energy required to transport fertilizer per unit dry tonne of biomass harvested from land, MJ/dry tonne;

Energy_{transport} – the energy required to transport one kg of nitrogen over a distance of 1 km, MJ/kg N/km.

Agricultural farmland requires additional fertilization after the nutrients are removed due to removal of agricultural residues for biofuel production purposes. The nutrients considered are nitrogen, phosphate, potassium, and sulphur. The land's nutrient requirement is shown in Table 3-3. The fertilization process is made up of the delivery and spreading of fertilizer. Farmlands are more accessible than forests; thus, a distance of 250 km is assumed from fertilizer plant to farmland. Spreading the fertilizer across the field requires less energy than spreading across the forest due to the more level ground surface and requires 7 L diesel/ha of field [54].

3.3.5 Fast pyrolysis

Fast pyrolysis is a direct way to convert biomass to bio-oil. Fast pyrolysis, a thermal decomposition process, uses a high heat transfer rate in the absence of oxygen to obtain high yields of bio-oil [93, 94]. Feedstock size affects the heat transfer rate of fast pyrolysis, so the feedstock is ground to a size smaller than 2 mm before pyrolysis [79]. Water content in biomass feedstocks affects the water content of the bio-oil produced as well as the heat transfer efficiency to the feedstocks; hence, feedstock must be dried to a moisture content range of 5-10 wt% [57, 79]. After the pre-treatment of feedstock by grinding and drying, the feedstock undergoes fast pyrolysis typically at 500-550 °C, one atmospheric pressure, and 0.5 s residence time to produce a bio-oil yield of approximately 59.9 wt% (dry basis) [60, 79]. The operating conditions could vary with the variation in the processes.

Pyrolysis (whole tree)				
Operation ^a	Value	Ref	Water use factor	Ref
			$(L H_2O/kWh)$	
Bio-oil cooling (L H ₂ O/kg bio-oil) ^b	0.027	[79]	-	
Bio-oil vapor cooling (L H ₂ O/kg bio-	0.003	[79]	-	
oil) ^b				
Steam condensing (L H ₂ O/kg bio-oil) ^b	1.077	[79]	-	
Steam system (L H ₂ O/kg bio-oil) ^b	0.026	[79]	-	
Ash quenching (L H ₂ O/kg bio-oil) ^b	0.203	[79]	-	
Recycle gas compression (kW)	10400	[79]	1.08	[104, 105]
Feedstock grinding (kW)	5600	[79]	1.08	[104, 105]
Other auxiliary (kW)	1248	[79]	1.08	[104, 105]
Electricity generated (kW)	19600	[79]	1.08	[104, 105]

Table 3-4: Water requirements for pyrolysis (whole tree)

^a Water requirement factors are derived based on a 550 dry tons/day plant for a 2000 dry tonnes/day plant. The 550 dry tons/day plant is assumed to be scalable linearly to 2000 dry tonnes/day plant.

^b Values derived based on flowrate of process plant.

Pyrolysis (forest residues)				
Operation ^a	Value	Ref	Water use factor (L H ₂ O/ kWh)	Ref
Bio-oil cooling (L H ₂ O/kg bio-oil) ^b	0.027	[79]	-	
Bio-oil vapor cooling (L H ₂ O/kg bio-oil) ^b	0.003	[79]	-	
Steam condensing (L H ₂ O/kg bio-oil) ^b	1.077	[79]	-	
Steam system (LH ₂ O/kg bio-oil) ^b	0.026	[79]	-	
Ash quenching (L H ₂ O/kg bio-oil) ^{b,c}	0.663	[79]	-	
Recycle gas compression (kW)	10400	[79]	1.08	[104, 105]
Feedstock grinding (kW)	5600	[79]	1.08	[104, 105]
Other auxiliary (kW)	1248	[79]	1.08	[104, 105]
Electricity generated (kW)	19600	[79]	1.08	[104, 105]

Table 3-5: Water requirements for pyrolysis (forest residue)

^a Water requirement factors are derived based on a 550 dry tons/day plant for a 2000 dry tonnes/day plant. The 550 dry tons/day plant is assumed to be scalable linearly to 2000 dry tonnes/day plant.

^b Values derived based on flowrate of process plant.

^c Ash quenching water requirement is derived based on ash content of forest residues.

In fast pyrolysis, mostly water is directly used in bio-oil cooling, bio-oil vapor cooling, ash quenching, steam condensing, and steam producing processes. The used water is usually recycled within the system to reduce water consumption; however, there is a fraction of water that is not recycled. Three streams of water that are not recycled are waste water, blowdown losses, and evaporative losses. Water losses through bio-oil and bio-oil vapor cooling are 0.027 L H_2O/kg bio-oil and 0.003 L H_2O/kg bio-oil, respectively [79]. Cooling water temperatures are relatively low, and water losses are reduced. On the other hand, steam condenser and steam system with higher temperatures compared to bio-oil cooling have a higher water use (1.077 L H_2O/kg bio-oil and 0.026 L H_2O/kg bio-oil, respectively) [79]. Ash quenching requires water to be sent to waste treatment after quenching and it contributes 0.203 L H_2O/kg bio-oil [79]. Indirect water is consumed when electricity is used for pre-treatment and pyrolysis processes generates enough electricity to create surplus electricity. This surplus will result in negative indirect water

consumption as the electricity is assumed to be sent to the power grid. Although whole tree and forest residues come from the same wood sources, the ash content of wood chips from the two feedstocks are different. As a result, the outcomes of fast pyrolysis for whole tree and forest residues feedstocks differ slightly. However, the impact from ash content is barely noticeable among other heavier weighted factors in the computation of the water requirements of the conversion pathways.

Pyrolysis (agricultural residues)				
Operation ^a	Value	Ref	Water use factor (L H ₂ O/ kWh)	Ref
Bio-oil cooling (L H ₂ O/kg bio-oil) ^b	0.027	[79]	-	
Bio-oil vapor cooling (L H_2O/kg bio-oil) ^b	0.003	[79]	-	
Steam condensing (L H ₂ O/kg bio-oil) ^b	1.083	[79]	-	
Steam system (L H ₂ O/kg bio-oil) ^b	0.026	[79]	-	
Ash quenching (L H ₂ O/kg bio-oil) ^b	0.890	[79]	-	
Recycle gas compression (kW)	10400	[79]	1.08	[104, 105]
Feedstock grinding (kW)	5600	[79]	1.08	[104, 105]
Other auxiliary (kW)	1248	[79]	1.08	[104, 105]
Electricity generated (kW)	19600	[79]	1.08	[104, 105]

Table 3-6: Water requirements for pyrolysis (agricultural residue)

^a Water requirement factors are derived based on a 550 dry tons/day plant for a 2000 dry tonnes/day plant. The 550 dry tons/day plant is assumed to be scalable linearly to 2000 dry tonnes/day plant.

^b Values derived based on flowrate of process plant.

Agricultural residues have a slightly different chemical composition than whole tree and forest residues. Agricultural residues have more ash than wood and yield less bio-oil [59]. Water use for pyrolysis is derived using mass and energy balances based on the process requirements estimated by Ringer et al. [79]. Water use contributors for agricultural residues pyrolysis are the same as those of whole tree and forest residues pyrolysis processes (when the same process is used), but the quantity of water used for agricultural residues pyrolysis is slightly higher due to the slightly lower projected bio-oil yield. Bio-oil cooling, bio-oil vapor cooling, steam

condensing, and steam producing processes for the pyrolysis of agricultural residues require $0.027 \text{ L H}_2\text{O}/\text{kg}$ bio-oil, $0.003 \text{ L H}_2\text{O}/\text{kg}$ bio-oil, $1.08 \text{ L H}_2\text{O}/\text{kg}$ bio-oil, and $0.026 \text{ L H}_2\text{O}/\text{kg}$ bio-oil, respectively. Agricultural residues have approximately 4 times more ash than woody plants and hence the amount of water used for quenching is $0.89 \text{ L H}_2\text{O}/\text{kg}$ bio-oil [109, 79].

3.3.6 Hydrothermal liquefaction

HTL is a type of thermochemical liquefaction that converts biomass in bio-crude in presence of water [96]. A biomass-water slurry with a 15% dry biomass content is used as a feed to HTL. This slurry is pumped to a pressure of 0.6 MPa and further increased to a pressure of 20.4 MPa with preheating to 327 °C before it is sent to a HTL reactor [95, 98, 110, 111]. Inside the reactor, biomass undergoes a reaction at 355 °C and is converted to oil, water, gas, and solid compounds containing char, ashes, and unreacted biomass using water in a super-critical state as a solvent to catalyse the reaction [96, 110]. After the reaction, effluents are filtered to remove solid particles. Further down the process stream, the effluents are cooled, depressurized, and separated into gaseous, aqueous, and oil phases. After the HTL process, the aqueous phase (containing water) is separated from bio-crude, of which 80% is recycled and the rest is purged to waste water treatment for anaerobic digestion [110]. Anaerobic digestion produces methane rich off-gas, which in turn can be used as an energy source in the hydrothermal liquefaction system [110].

Water use for the HTL of whole tree and forest residues feedstocks includes indirect water required for electricity used by the system and direct water by the biomass-water slurry production. Although whole tree and forest residue feedstocks come from the same species of plants there is a slight difference in their chemical composition, such as the ash content, but the difference in results from HTL between forest residues and whole tree is not significant compared to other factors affecting the water requirements of forest residues and whole trees. Hydrothermal liquefaction uses 12 MWe to keep the systems of a 2000 dry tonnes/day plant running [110]. The operation does not include the generated electrical energy of 11 MWe coming from combusting off gas for a 2000 dry tonnes/day HTL plant [110]. Water use in electrical energy generation is considered in this study as negative indirect water use. According to Statistics Canada and Environment Canada, 1.08 L H₂O of water is required for every kWh

electrical energy produced [104, 105]. This factor is used to calculate the indirect water use for any electricity consumption or generation. A 20% water make-up is accounted as direct water use when 80% of the water from the HTL process flow is recycled to produce a biomass-water slurry. The remaining 20% of water from the HTL process flow is sent to waste water treatment for off-gas production. This contributes to a water loss of 1.17 L H₂O/kg dry wood.

Hydrothermal liquefaction (whole tree and forest residue)								
Operation ^a	Value	Ref	Water use factor	Ref				
			(LH ₂ O/kWh)					
Cooling water make-up (L H ₂ O/kg	4.05	[110]	-					
HDRD)	4.03							
Boiler feed water make-up (L	0.67	[110]	-					
H ₂ O/kg HDRD)	0.07							
Water purged / day (L H ₂ O/kg dry	1.17	[110]	-					
straw)	1.1/							
Natural gas flow rate (kg /hr)	1420	[110]	0 L H ₂ O/kg	[21]				
Feed pre-treatment (MWe)	12.0	[110]	1.08	[104, 105]				
HBio-crude production (MWe)	0.0	[110]	1.08	[104, 105]				
Hydrotreating (MWe)	10.0	[110]	1.08	[104, 105]				
Hydrocracking (MWe)	1.1	[110]	1.08	[104, 105]				
Steam reforming (MWe)	3.4	[110]	1.08	[104, 105]				
Other auxiliary (MWe)	0.3	[110]	1.08	[104, 105]				
Electricity generation (MWe) ^b	11	[110]	1.08	[104, 105]				

Table 3-7: Water requirement for hydrothermal liquefaction (whole tree and forest residue)

^a Water requirement factor and energy are based on 2000 dry tonnes/day HTL plant capacity

^b Electricity is generated from the combustion of off-gas

Agricultural residues require a slightly different amount of water than whole tree and forest residues even when the hydrothermal liquefaction operations are the same. The energy inputs and their corresponding indirect water uses for hydrothermal liquefaction process are derived from the bio-crude yield estimates done by Akhtar and Amin [112]. Akhtar and Amin established a relationship between the amount of lignin and bio-crude yield [112]. Based on a lignin content of 21.3 wt% for agriculture residues and 24.3 wt% for wood [98], the bio-crude

yield from agricultural residues is estimated to be 47.8% when woody biomass produces a biocrude yield of 44.8% [110, 112, 113]. This bio-crude yield will then affect the water use efficiency as it is based on the functional unit. In terms of the operations of hydrothermal liquefaction, the electrical energy required for hydrothermal liquefaction remains unchanged at approximately 12 MWe for a 2000 dry tonnes/day plant. Similarly, the indirect water consumption for electricity production is assumed to be 1.08 L H₂O/kWh [104, 105]. With this conversion factor, the indirect water requirement is estimated to be 0.35 L H₂O/kg dry straw. The amount of water recycled is assumed to remain unchanged at 80% [110]; therefore the direct water consumption required from purging to waste water treatment is 1.17 L H₂O/kg dry straw.

Hydrothermal liquefaction (agricultural residue)							
Operation ^a	Value	Ref	Water use factor	Ref			
			$(L H_2O/kWh)$				
Cooling water make-up (L H ₂ O/kg	4.32	[110]	-				
HDRD) ^b							
Boiler feed water make-up (L H ₂ O/kg	0.72	[110]	-				
HDRD) ^b							
Water purged / day (L H ₂ O/kg dry	1.17	[110]	-				
straw) ^c							
Natural gas flow rate (kg /hr) ^d	1420	[110]	0 L H ₂ O/kg	[21]			
Feed pre-treatment (MWe) ^d	12.0	[110]	1.08	[104, 105]			
HBio-crude production (MWe) ^d	0.0	[110]	11.08	[104, 105]			
Hydrotreating (MWe) ^d	10.7	[110]	11.08	[104, 105]			
Hydrocracking (MWe) ^d	1.2	[110]	11.08	[104, 105]			
Steam reforming (MWe) ^d	3.6	[110]	11.08	[104, 105]			
Other auxiliary (MWe) ^d	0.3	[110]	11.08	[104, 105]			
Electricity generation (MWe) ^{d,e}	11	[110]	11.08	[104, 105]			

Table 3-8: Water requirement for hydrothermal liquefaction (agricultural residue)

^a Water requirement factor and energy are based on 2000 dry tonnes/day HTL plant capacity

^b Assumed Cooling water make-up and boiler feed water make-up is linearly proportional to the bio-oil produced

^c Assumed water produced through HTL is the same as whole tree and forest residues

^d Assumed energy required for HTL is only affected by process conditions

^e Electricity is generated from the combustion of off-gas
3.3.7 Transportation of bio-oil/bio-crude

B-train trucks are used to transport bio-oil or bio-crude from pyrolysis or HTL plants to an HDRD plant. There is no direct water use in the transportation of bio-oil/bio-crude, but the diesel used contributes to indirect water use. The HDRD plant is assumed to be an industrial area with oil and gas processing facilities. Traveling distance is determined based on the distance between the bio-oil/bio-crude production plants and the HDRD plant. Since the bio-oil/bio-crude production plant locations are determined based on availability of biomass, the distances between bio-oil/bio-crude production plants and an HDRD plant are estimated to be 300 km for whole trees and forest residues and 250 km for agricultural residues when the nearest areas of harvestable forest and farm are chosen. The other trucking component is fuel economy. B-train trucks are able to carry 60 m³ of bio-oil/bio-crude at 0.5 L diesel/km; the trucks consume 0.31 L diesel/km when not carrying a load [62].

3.3.8 Upgrading of bio-oil/bio-crude

Bio-oil/bio-crude must be upgraded in order for it to be converted into HDRD for use in diesel engines. Upgrading takes place through hydrodeoxygenation, in which oxygen is removed from the bio-oil/bio-crude to increase stability and heating value of hydrocarbons using hydrogen and a catalyst [106]. Hydrogen, a reactant that is required for oxygen removal, is produced by steam reforming using natural gas together with superheated steam [106, 110]. Water input in the steam reforming process counts towards the total water use in the production of HDRD from lignocellulosic biomass. Fast pyrolysis and HTL have different process conditions, resulting in a difference in chemical structure and water use for upgrading between bio-oil and bio-crude [82, 98].

The upgrading of pyrolysis bio-oil involves two hydrotreating steps followed by hydrocracking. The first hydrotreating step is at a mild temperature of 270 °C and 140 bar to prevent phase separation in the bio-oil [106]. The second hydrotreating step operates at a higher temperature of 350 °C and 140 bar and completes the hydrodeoxygenation process [106]. The heavy oil produced is hydrocracked into lighter hydrocarbons such as diesel and gasoline to increase the

HDRD yield. The direct water required in upgrading is used for cooling tower make-up and the steam reforming boiler feed. These volumes of water amount to 0.09 L H₂O/kg HDRD for cooling water and 0.83 L H₂O/kg HDRD for the steam reforming boiler feed. For indirect water consumption, the electricity used for the plant is taken into account, and the water required to produce the amount of electricity needed is computed to be 0.0103 L H₂O/MJ HDRD. A breakdown of the hydroprocessing water requirement is shown in Table 3-9 and Table 3-10.

Hydroprocessing (whole tree and forest residue)						
Operation ^a	Value	Ref	Water use factor	Ref		
			$(L H_2O/kWh)$			
Cooling water required (L H ₂ O/kg	0.089	[16]	-			
HDRD)						
Boiler feed required (L H ₂ O/kg	0.828	[16]	-			
HDRD)						
Natural gas (MJ/kg HDRD)	12.11	[16]	0 L H ₂ O/kg	[21]		
Electricity (kWh/kg HDRD)	0.408	[16]	1.08	[104, 105]		

Table 3-9: Water requirement for hydroprocessing after pyrolysis (whole tree and forest residue)

^a Derived based on the information given for a 2000 dry tonnes/ day plant

Hydroprocessing (agricultural residue)						
Operation ^a	Value	Ref	Water use factor	Ref		
			(LH ₂ O/kWh)			
Cooling water required (L H ₂ O/kg	0.089	[16]	-			
HDRD)						
Boiler feed required (L H2O/kg	0.828	[16]	-			
HDRD)						
Natural gas (MJ/kg HDRD)	12.18	[16]	0 L H ₂ O/kg	[21]		
Electricity (kWh/kg HDRD)	0.410	[16]	1.08	[104, 105]		

Table 3-10: Water requirement for hydroprocessing after pyrolysis (agricultural residue)

^a Derived based on the information given for a 2000 dry tonnes/ day plant and mass and energy balance The upgrading of bio-crude from HTL also involves hydrotreating and hydrocracking. HTL produces bio-crude with lower oxygen content than bio-oil from fast pyrolysis [114]. This lower oxygen content not only reduces the hydrotreating process from the two stages required by the pyrolysis oil to a single stage but also reduces the amount of reactant and the energy required to carry out hydrotreating [113]. Bio-crude from HTL is first hydrotreated using a fixed bed reactor at 400 °C with a supply of hydrogen. After hydrotreatment, butane and lighter gas components are separated from the oil for stabilization. The heavier oil is sent for hydrocracking that takes place at 400 °C and 80-150 bar with the addition of hydrogen and in the presence of metal sulfide catalysts [113]. After hydrocracking, gasoline and diesel are separated by distillation column. The energy and water required for hydrotreating and hydrocracking hydrothermal liquefaction oil are shown in Table 3-7 and Table 3-8.

3.3.9 Transportation of HDRD

The transportation of HDRD from an HDRD production plant to consumers is considered in this study because the use of energy in HDRD transportation involves water. Diesel consumption in Alberta was 4.2 billion liters in 2013 [5]. With the province's population residing mainly in Edmonton and Calgary [69], it is assumed in this study that the HDRD produced will be delivered to these two cities for consumer use. The location of the HDRD plant is assumed to be in Redwater, Alberta, and is 65 km and 380 km from Edmonton and Calgary, respectively. The average round trip distance from Redwater to Edmonton and Calgary is 445 km. HDRD will be transported by B-train trucks with the same fuel economy as bio-oil/bio-crude transportation. This can be further adopted in other jurisdiction with changes to the distance to the plants and population.

3.4 Results and discussion

A base case scenario is set up to understand the water requirements for each feedstock and conversion pathway. Comparisons and analyses are done between feedstocks and conversion pathways on water requirements for sub-unit operations, unit operations, and the final water requirement for the base case scenario. Then, the results are shared and the other scenarios are

discussed to understand how other factors can affect the overall water requirement of HDRD production. Last, an uncertainty analysis is conducted using a Monte Carlo simulation to address how the results are affected by the uncertainty of the inputs used in this study.

3.4.1 Base case scenario

The base case scenario examines the individual unit operations of biomass production, harvesting, bio-oil or bio-crude production (pyrolysis or HTL), hydroprocessing, and transportation. Unit operation values are compiled in Table 3-11 and Table 3-12 for HDRD production via fast pyrolysis and HTL, respectively.

Whole tree and forest residues as feedstocks for HDRD production have higher water requirements than agricultural residues. There are two reasons for this. First, plant growth rates vary. Agricultural crops take less than one year to grow while tree harvesting usually adopts a 100-year rotation [40]. A longer growing period increases the amount of water required. This difference in growth rates means that agricultural residues use only a fraction of the water per kg dry biomass that whole tree and forest residues do.

Unit operation (L H2O/MJ HDRD)	Whole tree	Forest residue	Agricultural residue
Biomass production	497.79	338.58	83.55
Biomass harvesting and fertilization	0.002	0.003	0.004
Fast pyrolysis	0.059	0.083	0.097
Hydroprocessing	0.032	0.032	0.035
Transportation	0.001	0.001	0.001
Total	497.88	338.69	83.69

Table 3-11: Water use efficiency for the conversion of lignocellulosic biomass to HDRD by fast pyrolysis

Unit operation (L H ₂ O/MJ HDRD)	Whole tree	Forest residue	Agricultural
			residue
Biomass production	376.16	255.85	58.84
Biomass harvesting and fertilization	0.002	0.003	0.003
Hydrothermal liquefaction	0.172	0.172	0.173
Hydroprocessing	0.029	0.029	0.03
Transportation	0.001	0.001	0.001
Total	376.36	256.06	59.05

Table 3-12: Water use efficiency for the conversion of lignocellulosic biomass to HDRD by hydrothermal liquefaction

Second, water allocation is done for agricultural residues because grains are sold as a food source. This allocation of water use in agricultural crop growth means that water use in agricultural crop growth is divided between grains and residues. There is no allocation for whole tree because biomass from these feedstocks is solely used for HDRD production; thus, the full amount of precipitation contributes toward the water use for whole trees production. For forest residues, 20% of total precipitation is allocated, resulting in a lower water requirement compared to whole tree. However, the lower yield of the forest residues relative to whole tree increases the water use per unit dry forest residues to give a value higher than 20% of water use for whole tree feedstock. For agricultural residues, 10.9% of total precipitation is allocated to grains and unused straw. This results in a lower water requirement for agricultural residues relative to whole tree and forest residues.

Whole tree harvesting and fertilizing unit operations proved to have the lowest water requirement of the feedstocks studied. The whole tree harvest area is significantly smaller than that of the other two feedstocks due to the difference in biomass yield, and this reduces the indirect water use from biomass transportation. In addition, the fertilizing process is related to the harvest area; therefore, forest residues and agricultural residues incur a higher indirect water use from the use of diesel to spread the fertilizers. In this study, it is assumed that the fertilization process for agricultural residues feedstock does not include the return of ashes to replenish nutrient loss, and the indirect water use for fertilizer production is included in this unit operation, reflecting a higher water use than forest residues.

HDRD production via HTL and hydroprocessing requires less water per unit HDRD produced. The higher amount of HDRD produced per kg of biomass for the HTL conversion pathway than the fast pyrolysis conversion pathway lowered the water required per unit MJ of HDRD. The measurement of water efficiency is done by summing the water required for a unit MJ of HDRD produced. With a higher HDRD output, HDRD production through HTL will comparatively get a better water use efficiency than HDRD through fast pyrolysis.

The HTL uses more water than the fast pyrolysis from the higher water use in cooling water replacement and the 20% water sent to waste treatment. The water use difference between HTL and fast pyrolysis is not just restricted to the production of bio-oil or bio-crude. Bio-oil from pyrolysis and bio-crude from HTL have different properties, resulting in a difference in bio-oil upgrading requirements. Bio-crude from hydrothermal liquefaction has a lower oxygen content than bio-oil from fast pyrolysis [82, 98]; as a result, hydrogen and energy inputs for bio-oil upgrading are lower for bio-crude from HTL than bio-oil from fast pyrolysis as well. Although less water is used in bio-crude upgrading than bio-oil upgrading, the reduction in water use from the steam reformer is not sufficient to compensate for the higher water use in cooling water losses and waste water generated in the HTL process. On the other hand, fast pyrolysis decomposes biomass in a dry environment and the water use contributed by bio-oil cooling is negligible when the losses are at 3% [79]. Even when the steam condenser and steam system led to higher water consumption, especially when more water is required for hydrogen production, fast pyrolysis requires lower water consumption overall.

In the transportation unit operation, water use are the indirect water use that not only comes from transporting of materials, such as fertilizers, biomass, bio-oil/bio-crude, and HDRD, but also road construction. Transportation operations' contribution to water use is negligible compared to other unit operations for all feedstocks. With this low amount of water use for transportation as a whole, differences in water use caused by road construction for the case of whole tree and differences in transportation distance between feedstocks are not noticeable.

3.4.2 Other scenarios – Sensitivity analysis

The effects of the main inputs and contributing factors on the study results are analyzed by introducing scenarios. Table 3-13 lists the scenarios.

The production of biomass is the main contributor to water use in producing HDRD from lignocellulosic biomass. Annual average rainfall usually varies by approximately $\pm 10\%$ in Alberta [115], and scenarios 1 and 2 investigate changes in water use by -10% and +10% in the growing of biomass. The graphs in Figure 3-3 and Figure 3-4 show that water use in biomass production is almost directly proportional to the total water use of HDRD production for all three feedstocks and both conversion pathways. The directly proportional relationship is observed because water use in production of biomass outweighs other contributors by a factor of more than 1000.

Table 3-13:	Scenarios	for sensitivity	analysis

Scer	narios
1	Decrease in water from irrigation or precipitation by 10%
2	Increase in water from irrigation or precipitation by 10%
3	Decrease in biomass yield by 10%
4	Increase in biomass yield by 10%
5	Decrease bio-oil/bio-crude yield by 10%
6	Increase bio-oil/bio-crude yield by 10%
7	Decrease HDRD yield by 10%
8	Increase HDRD yield by 10%
9	Decrease transportation distance by 10%
10	Increase transportation distance by 10%
11	Decrease transportation distance by 10% (without water use in biomass production)
12	Increase transportation distance by 10% (without water use in biomass production)
13	Decrease electricity usage by 10% (without water use in biomass production)
14	Increase electricity usage by 10% (without water use in biomass production)
15	Decrease harvesting energy usage by 10% (without water use in biomass production)
16	Increase harvesting energy usage by 10% (without water use in biomass production)



Figure 3-3: Sensitivity analysis for conversion to HDRD via fast pyrolysis and hydroprocessing



Figure 3-4: Sensitivity analysis for conversion to HDRD via hydrothermal liquefaction and hydroprocessing



Figure 3-5: Sensitivity analysis for conversion to HDRD via fast pyrolysis and hydroprocessing (without considering water use in biomass production)



Figure 3-6: Sensitivity analysis for conversion to HDRD via hydrothermal liquefaction and hydroprocessing (without considering water use in biomass production)

A sensitivity analysis is conducted on biomass yield in scenarios 3 and 4 for a fluctuation of $\pm 10\%$. A range of $\pm 10\%$ is a good range based on the annual harvest fluctuations of agricultural crops and density of trees in Alberta's forests [12, 116]. Water use for growth and biomass yield can have an almost equal but opposite effect on water use efficiency of HDRD production for all feedstocks, as seen in Figure 3-3 and Figure 3-4. Crop yield and forest cover can vary over time, and a sensitivity analysis of scenarios 3 and 4 can assess the impact of a change in yield on water use efficiency.

Biomass yield affects product output, and a lower yield has a similar impact on water use efficiency compared to an increase in precipitation and irrigation. This similar impact can be explained by understanding the relationship of the water use factor in biomass production, L H_2O/kg biomass. In this relationship, an increase in irrigation or precipitation with no increase in biomass yield is equivalent to decreasing biomass yield without an increase in irrigation or precipitation. Scenario 4 shows a change that is less drastic than scenario 3. This observation can be explained by the inverse relationship biomass yield has with water use efficiency, for a larger denominator will not decrease the final value by a constant factor.

Water use efficiency is measured by water input per unit of product output. After analyzing the sensitivity of water use requirements with biomass production, the sensitivity of water use requirements towards product yields is measured in scenarios 5 through 8. In scenarios 5 and 6, we consider the impact of changing the intermediate product, bio-oil/bio-crude, while in scenarios 7 and 8, we consider the impact of changing the final product, HDRD, by $\pm 10\%$, taking the most pessimistic and optimistic scenarios [17, 31, 83]. The sensitivity analysis results of scenarios 5 through 8 indicate an inverse relationship of products and water use efficiency. When comparing scenarios 5 and 6 with scenarios 7 and 8, the impact of bio-oil/bio-crude yield on water use efficiency is the same as HDRD yield because HDRD production comes from bio-oil/bio-crude output. A reduction or an increase in bio-oil/bio-crude yield will create a similar magnitude of change in HDRD yield due to the change in bio-oil/bio-crude input for hydroprocessing.

Scenarios 9 and 10 investigate the sensitivity of transportation distance on overall water requirements of HDRD production. As transportation distance is likely to vary considerably based on the terrain and change in harvesting plots, a sensitivity analysis needs to be conducted on transportation distance. The negligible impact on overall water requirements when transportation distance is changed is expected because most water use is from biomass production. To understand how influential transportation distance and other factors are, scenarios 11 through 16 are conducted without the biomass production unit operation (see Figure 3-5 and Figure 3-6). Scenarios 11 and 12 continue to test the sensitivity of changes in transportation distance on the results. The percentage change of 0.1% for all feedstocks showed that transportation distance is a small component of the entire conversion pathway.

Electricity consumption of fast pyrolysis, HTL, and hydroprocessing indicates the efficiency of equipment. Efficiency can increase over time due to the progress of technology and can also decrease due to aging of equipment. A sensitivity test on electricity consumption is conducted in scenarios 13 and 14. Whole tree feedstock has the lowest water requirement for the conversion of biomass to HDRD among all feedstocks. This lower water requirement suggests that whole tree is the most sensitive towards a change in electricity consumption followed by forest residues and agricultural residues.

Similarly, harvesting equipment is also subject to changes in technology and the ill effects of inefficiency. To address this, a sensitivity analysis is conducted on harvesting energy use in scenarios 15 and 16. Agricultural residues are shown to be the most sensitive towards changing of efficiency in harvesting equipment followed by forest residues and whole tree. The sensitivity in this case is caused by the number of unit operations for each individual feedstock. Agricultural residue has more harvesting operations, so it is more affected by the change in harvesting efficiency.

3.4.3 Uncertainty analysis

An uncertainty analysis is conducted using a Monte Carlo simulation with 10 million iterations. This simulation is conducted by creating a MATLAB code capable of randomly picking values

within the uncertainty ranges of all variables and computing them for 10 million iterations. The results from these iterations were then translated into distribution curves shown in Figure 3-7 and Figure 3-8. Due to uncertainty in published information, a triangular probability distribution is assumed for all of the study's inputs. According to Huijbregts et al. (2001), uncertainty can be estimated by classifying inputs and assigning a suitable uncertainty to each group under the classification considered [81]. In this study, inputs with known estimated uncertainty ranges such as biomass and HDRD yields will have their uncertainty ranges used in the Monte Carlo analysis. Inputs with unknown uncertainty ranges will have their ranges estimated according to their impact on the final result. A 5% uncertainty is assigned to variables with limited impact on the final result while inputs related to transportation distance, biomass yields, and process inputs have a 10% uncertainty assigned to them due to the greater uncertainty and greater impact on the final result of study [81]. Table 3-14 shows the value of water use efficiency at various percentiles. The percentage deviations from the median value at the 10th and 90th percentiles for the conversion pathway of whole tree feedstock to HDRD via pyrolysis are -11.6% and 13.2%, respectively. The percentage deviation for the conversion pathway of whole tree feedstock to HDRD via HTL is smaller in magnitude than the pyrolysis case at -11.5% and 13.1% for the 10th and 90th percentiles, respectively. Similar observations can be seen with other feedstocks in Figure 3-7 and Figure 3-8. The distribution curves in Figure 3-8 are narrower than those in Figure 3-7 because there are fewer uncertainty inputs for HTL. When individual feedstocks curves are compared, we can see that agricultural residues have the narrowest spread of values when the percentage deviation from the median value at the 10th and 90th percentiles is -9.3% and 10.2%, respectively, for the fast pyrolysis conversion pathway. The uncertainties of the variables used in the Monte Carlo simulation resulted in the 50th percentile value, of all feedstocks, to be always slightly higher than the water requirements calculated in the base case. The calculations used in water requirements resulted in the slight deviation from the value calculated in the base case. Based on the distribution curves, the widest spread of results is still relatively concentrated near the median value; therefore, the results of this study are fairly accurate given the uncertainties of input variables.

	C C				Water use efficiency of HDRD production via hydrothermal					
	hy	hydroprocessing					liquefaction and hydroprocessing			
			Fo	rest	Ag	ricultural		Forest	Agricultural	
	W	hole tree	res	sidue	res	idue	Whole tree	residue	rest	idue
	L	H_2O/MJ	L	H_2O/MJ	L	H_2O/MJ	$L H_2O/MJ$	$L H_2O/MJ$	L	H ₂ O/MJ
Percentile	HI	ORD	HI	ORD	ΗI	DRD	HDRD	HDRD	HD	RD
5%	42	4.89	26	8.55	74	.01	322.31	203.61	52.	44
10%	43	9.77	28	2.28	76	.02	333.41	213.94	53.	82
25%	46	6.18	30	7.51	79.	.58	353.16	232.96	56.	28
50%	49	7.72	33	8.04	83.	.80	376.74	255.94	59.	19
75%	53	1.36	37	0.43	88.	.24	401.99	280.32	62.	29
90%	56	3.18	40	0.54	92.	.38	425.92	303.03	65.	20
95%	58	2.75	41	8.86	94.	.91	440.69	316.82	66.	98

Table 3-14: Percentile values of uncertainty distribution plots



Figure 3-7: Monte Carlo distribution for conversion via fast pyrolysis and hydroprocessing



Figure 3-8: Monte Carlo distribution conversion via hydrothermal liquefaction and hydroprocessing

3.5 Conclusion

Water is a precious resource and a large part of water use is from industry. Making the right decisions to reduce water dependency is important for industry to save both the cost and the need to source for water while meeting the growing demand for diesel. This study looked into two pathways to convert lignocellulosic biomass to HDRD and can be used to fill the current gap in this area. The results of this study show that biomass production is the main determinant of water requirement in producing HDRD from lignocellulosic biomass. More than 99.9% of the water used in every conversion pathway and feedstock studied in this paper is used for biomass production; water use in the other unit operations is negligible in comparison. High water use at the biomass production stage shows that a choice of biomass with low water demand and better ability to cope in water stress conditions for HDRD production will reduce water use impact on the environment. When water consumption is the consideration, agricultural residues feedstock is a better option than the other two woody biomass feedstocks studied due to the faster growth rate of agricultural feedstock and its overall lower water required for growth compared to trees.

When comparing conversion pathways, we find that HTL is more promising with its slightly higher HDRD yield and water requirement savings of 24.4%, 24.4%, and 29.4% for whole tree, forest residues, and agricultural residues, respectively, compared to fast pyrolysis. Although cooling water losses and waste water generation in HTL are higher than those of the fast pyrolysis process, HTL combined with hydroprocessing has a higher HDRD yield that lowers the effective water consumption for HDRD production to a level below that of the process using fast pyrolysis. From this study, biomass production and HDRD yield are found to be crucial factors when determining water use. Future research should be extended to more types of lignocellulosic biomass feedstocks to understand how different plants handle water stress during dry years, so biomass production can be achieved with less dependency on water availability.

Chapter 4: Conclusions and Recommendations for Future Work

GHG emissions from combustion of fossil fuels are one of the concerns government is trying to address. This is shown in the implementation of renewable fuels regulations in Canada and RFS in Alberta. A minimum of 25% fewer GHG emissions stated in RFS calls for a need to measure the amount of GHG emissions from renewable fuel. There is a need to conduct an LCA on renewable fuel for the quantification of GHG emissions. Environmental sustainability encompasses more than just GHG emissions, and factors such as fossil fuel derived energy and water use requirements form part of environmental impact assessments of an LCA. The purpose of this research is to estimate the amount of GHG emissions, net-energy ratio (a metric for estimation of energy output to fossil fuel energy input) and water use required to produce HDRD from lignocellulosic biomass. In this research, a detailed LCA is conducted with a focus on western Canada.

4.1 GHG emissions and net energy ratio

In this study, GHG emissions and the NER of producing HDRD was estimated through development of a data-intensive model based on 2000 dry tonnes per day capacity for whole tree, forest residues, and agricultural residues. This developed model allows Alberta-based data inputs to be used for greater accuracy and impact of variables on final result to be examined in different scenarios. To standardize the form of measurement, all inputs are measured by a functional unit of 1 MJ of HDRD produced. This model can further be used for other jurisdictions with different data set as appropriate.

The GHG emissions and NER of base case scenario of feedstocks studied varies from $35.4 - 42.3 \text{ gCO}_{2,eq}/\text{MJ}$ HDRD and 1.55 - 1.90 MJ/MJ, with the agricultural residues having the lowest GHG emissions and highest NER. The efficiency of harvesting and transportation of biomass unit operations contributed to most of the difference in GHG emissions and NER between feedstocks. Since the main differences between feedstocks are harvesting and transportation unit

operations, the choice of feedstock to reduce GHG emissions and energy use should be based on the amount of fertilization required, biomass yield, and transportation distance of biomass.

The main contributing factors of the GHG emissions and NER are analyzed further through a sensitivity analysis. The scenarios studied in the sensitivity analysis are the return of ash to forest and farm, ash dumping at a landfill site, bio-oil yield, HDRD yield, the N₂O emission factor, fertilization of forest and farm, production of hydrogen gas using bio-oil, and total transportation distance. The scenarios looking at the ash return to the forest, farm, or landfill site and transportation distance do not show significant contributing factors to GHG emissions and fossil energy usage. Similar findings are also observed in scenarios 11 and 12 where overall transportation distance is considered. The importance of fertilization is reflected in scenario 9 where residues are treated as by-products of logging and grain harvesting operations. Without the need for fertilization, residues are a more attractive option compared to whole tree biomass especially when whole tree biomass requires an additional component of road construction that increases the GHG emissions and energy use. From the sensitivity analysis, yields are found to be important and affect the GHG emissions per unit MJ HDRD produced and NER more than the other factors in scenarios 3 through 6. In scenario 10, the effect of reduction in HDRD yield on GHG emissions and NER outweighs the effect of reduction in GHG emissions and fossil fuel energy by using bio-oil to produce hydrogen through steam reforming in the hydro-processing unit operation.

4.2 Water use requirements

In this study, water use requirements are studied for three feedstocks, whole tree, forest residues, agricultural residues, with the inclusion of additional conversion pathway that utilizes HTL instead of fast pyrolysis to produce intermediate product, bio-oil. A data-intensive model is built based on 2000 dry tonnes per day capacity with data inputs converted to a reference functional unit 1 MJ of HDRD produced.

Total water use requirements for the conversion pathway of lignocellulosic biomass to HDRD through fast pyrolysis are 497.88 L H₂O/MJ HDRD, 338.69 L H₂O/MJ HDRD, 83.69 L H₂O/MJ

HDRD for whole tree, forest residues, and agricultural residues, respectively. The biomass production unit operation contributes more than 99.9% of the total water use requirements. As a consequence of this substantial water contribution, the water allocations conducted on feedstocks are the main factors contributing to differences in water use for HDRD production between feedstocks. Apart from water allocation, the feedstock yield played a role in determining the water use per unit of biomass harvested. For the conversion pathway of lignocellulosic biomass to HDRD through HTL, water use requirements are found to be 376.36 L H₂O/MJ HDRD, 256.06 L H₂O/MJ HDRD, 59.05 L H₂O/MJ HDRD for whole tree, forest residues, and agricultural residues, respectively. The higher HDRD yield from HTL followed by hydroprocessing compared to the conversion pathway of fast pyrolysis followed by hydroprocessing leads to a lower water use requirement per unit MJ of HDRD. These water use savings range from 24.4% to 29.4% for the three feedstocks studied and show that the adoption of HTL instead of fast pyrolysis reduces the input required to produce a unit output. Agricultural residue feedstock requires less water to produce and convert to HDRD compared to the other feedstocks in the study. The understanding that total water use depends heavily on water use in biomass production leads to the conclusion that water use can be reduced by changing the feedstock. A feedstock that can manage water stress and does not require much water during the entire growth period will be a better choice of biomass to produce HDRD.

4.3 **Recommendations for Future work**

This study focuses on the GHG emissions, fossil fuel energy inputs, and water use requirements of producing HDRD from lignocellulosic biomass that is available in Alberta. Hydroprocessing of bio-oil is a relatively new technology with few commercial implementation. Life cycle of HDRD production is thus able to benefit in accuracy of results from further research and data gathering in hydroprocessing. Further research work can be done to provide a more comprehensive study, and the followings are recommended:

• Experiments on measuring effects on HDRD yield by varying the hydrotreating process parameters such as pressure, temperature, and catalyst can prove to be useful in providing

more data for LCA. Process conditions are factors that affect energy consumption and production yield and in turn the final result of study; hence, it will be useful to have experimental data inputs to validate the results of LCA and reduce the level of uncertainty of this theoretical approach;

- A more specific study should be conducted on plant species and compare the difference between plant species available in the forest and agricultural industry of Alberta. Different lignocellulosic biomass has different amount of lignin, cellulose, and hemicellulose. Difference in properties can affect HDRD output when bio-oil production is dependent on the chemical properties of biomass feedstock. The physical properties of biomass can also make a difference in GHG emissions of HDRD production by changing the energy consumption of pre-treatment and transportation, for grinding and drying of biomass makes up the majority of energy consumption in pyrolysis and density affects transportation efficiency;
- Extend LCA research of HDRD production to hydrothermal liquefaction. Hydrothermal liquefaction is an alternative to fast pyrolysis and produces bio-oil of lower acidity and lower oxygen content than bio-oil from fast pyrolysis; the lower oxygen content reduces the amount of hydrogen required for hydrotreating, too. As shown in chapter 3, increase in final product will decrease the amount of input required per unit output. With an increase in HDRD yield, the amount of GHG emissions that comes from the use of fossil fuel energy for every unit of HDRD produced will decrease.
- Water use in biomass production is the main component of water use requirements for HDRD production from lignocellulosic biomass. This means that accuracy of data of water use in producing biomass for HDRD production plays a major role in improving the accuracy of the study. Site-specific measuring techniques such as eddy-covariance or other precipitation and irrigation measurements can be performed to increase the accuracy of water use requirements of HDRD production.

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Appendix A. Biomass transportation distance calculations

For a circular plot of land (for whole tree and forest residues) with the processing plant in the middle of it represented by a "**star**", the average distance is calculated by equating area of the circle, " A_1 ", with the area of the ring, A_2 ".

In the diagram, " \mathbf{R}_1 " is the radius of the inner circle (representing the average displacement from centre of circular plot) while " \mathbf{R}_2 " is the radius of the entire circular plot of land of concerned.

$$A_{1} = A_{2}$$

$$\pi R_{1}^{2} = \pi R_{2}^{2} - \pi R_{1}^{2}$$

$$\pi R_{2}^{2} = 2\pi R_{1}^{2}$$

$$R_{2}^{2} = 2R_{1}^{2}$$

$$R_{1} = \frac{1}{\sqrt{2}}R_{2}$$

$$R_{1} \approx 0.707R_{2}$$

The average distance, "R1", is 0.707 of "R2".



A square plot of land is assumed for agricultural land. The "**star**" in the middle of a square plot of agricultural land shows the assumed plant of concern.

In this square plot of land, "L" is the length of the side of the square agricultural plot of land, and "d" is the distance of an arbitrary point within the agricultural plot of land to the **star**.

To obtain the theoretical average distance from the middle of the square to any point within the plot of land, an integration has to be done. The calculations below show the method of calculating the average distance (D_{avg}).

Looking at the 4 equal squares within the square plot of land (shown in the diagram above), the average distance to the **star** in any of the 4 smaller squares is the same. Therefore computing the average distance within a small square to **star**, the average distance within the agricultural plot of land to the **star** can be obtained.

Double integration gives us a volumetric unit. When the solution of double integration is divided by the area $L^2/8$, the average distance of all the points within the small square to the **star** is obtained. This is why there is a factor of $8/L^2$ in the formula.

$$D_{avg} = \int_0^{L/2} \int_0^x \sqrt{x^2 + y^2} \, dy \, dx \, \frac{8}{L^2}$$

To facilitate the integration, w is substituted in the formula, where w=y/x,

$$D_{avg} = \int_0^{L/2} \int_0^1 x^2 \sqrt{1 + w^2} \, dw \, dx \, \frac{8}{L^2}$$
$$D_{avg} = \int_0^1 \sqrt{1 + w^2} \, dw \int_0^{L/2} x^2 \, dx \, \frac{8}{L^2}$$
$$D_{avg} = \int_0^1 \sqrt{1 + w^2} \, dw \, \frac{1}{3} \left(\frac{L}{2}\right)^3 \, \frac{8}{L^2}$$

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$$D_{avg} = \frac{L}{6} \left(\sqrt{2} + \ln(1 + \sqrt{2}) \right)$$

$$D_{avg} = 0.541L$$



Appendix B. Water requirement for biomass production calculations

	Whole tree	Forest residues	Agricultural residues
Yield	84 dry tonnes/ha	0.247 dry tonnes/ha	0.517 dry tonnes/ha
Number of years per cycle	100 years	1 year	1 year
Amount of precipitation / irrigation	480 mm/year	480 mm/year	452 mm/year
Amount of water / year / ha	0.48 m/year × 10000 m ² /ha = 4800 m ³ /year/ha = 4,800,000 L/year/ha	0.48 m/year × 10000 m ² /ha = 4800 m ³ /year/ha = 4,800,000 L/year/ha	0.452 m/year × 10000 m ² /ha = 4519.06 m ³ /year/ha = 4,519,056 L/year/ha
Amount of water in 100 years	480,000,000 L/(100year)/ha	-	-
% allocation to feedstock	100%	20% (Forest residues constitutes 20% of whole tree biomass)	10.9% (with 50.9% allocation to grains an 38.2% allocation to unutilized straw)
Water / dry tonne	48000000 L/(100year)/ha ÷ 84 dry tonnes/ha = 5,714,286 L/dry tonne	4800000 L/year/ha × 20% ÷ 0.247 dry tonnes/ha = 3,886,640 L/dry tonne	4519056 L/year/ha × 10.9% ÷ 0.517 dry tonnes/ha = 953,789 L/dry tonn
Water / dry kg biomass	5714.3 L/dry kg	3886.6 L/dry kg	953.8 L/dry kg
Water / kg bio- oil	5714.3 L/dry kg ÷ 0.599 (59.9% bio-oil yield) = 9,539 L/kg bio-oil	3886.6 L/dry kg ÷ 0.599 <i>(59.9% bio-oil</i> <i>yield)</i> = 6,488.5 L/kg bio-oil	953.8 L/dry kg ÷ 0.596 (59.6% bio-oil yield) =1,601.3 L/kg bio-oil
Water / MJ HDRD	9539 L/kg bio-oil ÷ (0.253 × 42.79 MJ/kg	6488.5 L/kg bio-oil ÷ (0.253 × 42.79 MJ/kg	1601.3 L/kg bio-oil ÷ (0.253 × 42.79 MJ/kg

	HDRD + $0.188 \times$	HDRD + $0.188 \times$	$HDRD + 0.188 \times 44.40$
(18.8% gasoline,	44.40 MJ/kg bio-	44.40 MJ/kg bio-	MJ/kg bio-gasoline)
25.3% HDRD	gasoline)	gasoline)	
yields) (based on	= 497.79 L/MJ	= 338.57 L/MJ	= 83.55 L/MJ HDRD
energy	HDRD	HDRD	
allocation)			