1 2	Life Cycle Water Footprint of Hydrogenation-derived Renewable Diesel Production from Lignocellulosic Biomass
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6	Abstract
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10	

11 **1. Introduction**

Water is critical for humans. Water is consumed primarily through farming, industrial, and domestic uses (Rosegrant et al., 2002). 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 (Pereira et al., 2002; Krobel et al., 2014). Water sustains growth in dry boreal forest areas and could change the landscape from forest to grassland if availability drops low enough (Hogg, 1994). 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

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19 water use efficiency for biomass production (Kirkpatrick et al., 2006; Hsiao and Acevedo, 1974).
20 In addition to water consumption during plant growth, water is consumed in chemical processes
21 that convert biomass to usable energy sources (Dominguez-Faus et al., 2009). Therefore
22 investigating water requirements for different lignocellulosic biomass and various chemical
23 processes to convert biomass to energy sources is crucial in a water footprint study of biomass as
24 an energy source.

The production of biofuels not only depends on biomass but also the type of biofuels produced. 25 26 There are different types of biofuels available through current technology that can replace fossil-27 based diesel. Among these biofuels are biodiesel and hydrogenation-derived renewable diesel 28 (HDRD). The difference in biodiesel and HDRD is in their chemical composition and structure 29 (Natural Resources Canada, 2012). Biodiesel contains straight-chain fatty acid alkyl esters 30 produced from the transesterification process and HDRD contains alkanes, aromatic compounds, 31 and alkyl side chains produced from hydroprocessing (Knothe, 2010). The differences in 32 chemical composition and structure between biodiesel and HDRD result in different physical 33 properties, for example in cetane number and cloud point (Natural Resources Canada, 2012; 34 Knothe, 2010). A higher cetane number and ability to alter the isomerization process for better 35 cold flow properties make HDRD a better biofuel for use in colder climates than biodiesel 36 (Natural Resources Canada, 2012). The focus of this study is on HDRD because HDRD's 37 physical properties are suitable for both cold and warm climates, and so this study's results will 38 apply to both cold and warm climatic regions. To date, there has been limited research done on 39 the assessment of water footprints for the conversion of biomass feedstocks to HDRD.

40 The production of energy and fuels from biomass sources requires water both during the growth 41 of the biomass and during its conversion to fuels. Because water is an important resource, water 42 requirements are one of the factors to consider for the long-term sustainable production of 43 HDRD. The growing emphasis on renewable fuels emphasizes the need for a better 44 understanding of the water requirements of hydrogenation-derived renewable diesel from 45 renewable sources. To date there have been several studies on the water footprint of biofuel 46 production in general (Yang et al., 2011; Dominguez-Faus et al., 2009; King and Webber, 2009). 47 Singh et al. (2015) assessed the impact of producing biofuel in Alberta and concluded that 48 southern Alberta does not have enough water to meet the high irrigation water requirements due 49 to its dry climate. Singh et al.'s (2015) study highlighted that 860-1530 billion liters of water are 50 required to produce 4 billion liters of biofuel to partially meet the projected demand of biofuel in 51 Canada in the year 2025. Yang et al. (2011) examined the life cycle water footprint of biodiesel 52 production from microalgae and found that 3726 kg of water are required to produce 1 kg of 53 biodiesel if water is not recycled during biodiesel production. Dominguez-Faus et al. (2009) 54 looked into the water requirement for energy crops to produce ethanol and compared the water 55 footprint with that of existing power sources. Their results showed that when corn is irrigated for 56 ethanol production, 2.2-8.6 million liters of water are used, while biodiesel from soybean crops 57 requires 13.9-27.8 million liters for one MWh of energy produced. The study also revealed that the water requirement fluctuates depending on the type of biofuel produced and the geographical 58 59 location at which the biomass is grown; a higher precipitation area will reduce the water required 60 from irrigation (Dominguez-Faus et al., 2009). Singh and Kumar (2011) developed water 61 requirement factors for twelve biomass conversion pathways to ethanol and electricity. The 62 water requirement factors of ethanol production pathways of corn and wheat biomass range from

63 38.7-55.5 L H₂O /MJ of ethanol while the water requirement factors of electricity production 64 from corn stover and wheat straw range from 72.0-129.4 L H₂O /kWh of electricity (Singh and 65 Kumar, 2011). Differences in conversion pathways and water required for biomass production 66 due to geographical location resulted in a water requirement disparity between the values for the production of a unit of electricity calculated by Singh and Kumar and those of Dominguez-Faus 67 68 et al. King and Webber (2009) concluded that biofuels derived from soy and corn require more 69 water than fuels derived from fossil fuels, and soy requires less water than corn. King and 70 Webber (2009) also showed that irrigation plays a large part in water requirement; biomass 71 feedstock that requires irrigation uses 47-141 L H₂O/km (distance travelled by light duty vehicle 72 using the biofuel produced), a water consumption of 3 orders of magnitude higher than similar 73 feedstock that does not require irrigation (0.12-0.94 L H₂O/km). Singh et al. (2011) studied the 74 water requirement to produce biofuel from six different biomass feedstocks. In their study, corn 75 and wheat require 178 L H₂O /MJ of ethanol and 325 L H₂O /MJ of ethanol, respectively. With 76 little research done on the water requirements of HDRD production, especially in colder climatic 77 regions such as Canada, this study intends to fill the gap in knowledge on the life cycle water 78 requirements for converting the lignocellulosic biomass readily available in western Canada to 79 HDRD.

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

The 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:

8	• Pathway 1: Conversion of lignocellulosic biomass to bio-oil through fast pyrolysis
8	and further conversion of bio-oil to HDRD.
8	• Pathway 2: Conversion of lignocellulosic biomass to bio-crude through
8	8 hydrothermal liquefaction (HTL) and further conversion of bio-crude to HDRD.
8	• The study of the effects of the input parameters on the life cycle water footprint of HDRD
9) production from lignocellulosic biomass through sensitivity and uncertainty analyses.

91 The life cycle water footprint assessment methodology is explained in Section 2. Section 3 92 presents the water requirement inventory for each operation in the product life cycle and Section 93 4 develops several scenarios to examine the sensitivity of the selected model factors. Section 5 94 concludes the paper with the key findings and addresses future research on this topic.

95 **2. Methodology**

96 Water requirement considerations for the production of HDRD from lignocellulosic biomass 97 encompass the life cycle of lignocellulosic biomass from well to wheel. ISO 14040 suggests a 98 life cycle assessment framework with the following steps: goal and scope definition, life cycle 99 inventory analysis, impact assessment, and interpretation (International Organization for 100 Standardization, 2006). The goal and scope section defines the system boundary adopted for the 101 study and discusses how the results can benefit the intended industry and government. The life 102 cycle inventory is a compilation of the inputs required for computation and analysis and states 103 the assumptions for input values. The computation and analysis allow the environmental impact 104 to be assessed and interpreted for meaningful knowledge to be obtained from the study. This 105 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. The functional unit used
will measure the amount of water required to produce 1 MJ of HDRD on a well-to-wheel basis.
Scenarios were developed to examine how some important factors can affect the overall 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.

111 The process of lignocellulosic biomass production and conversion to HDRD by fast pyrolysis or 112 HTL and the subsequent hydroprocessing has several unit operations. The unit operations for the 113 conversion pathway via fast pyrolysis include: (1) production and harvesting of whole tree, forest 114 residues, and agricultural residues, (2) transportation of whole tree and forest residues in the 115 form of chips and agricultural residues in the form of bales to a fast pyrolysis plant, including 116 road construction, (3) bio-oil production via fast pyrolysis, (4) transportation of bio-oil to a 117 hydroprocessing plant, (5) bio-oil conversion to HDRD, and (6) transportation of HDRD to a 118 refinery for blending with fossil fuel-derived diesel and to the consumer. The conversion 119 pathway is illustrated in the system boundary diagram in Figure 1 with inputs and outputs 120 indicated. For the conversion of lignocellulosic biomass to HDRD via HTL, the unit operations 121 include: (1) production and harvesting of whole trees, forest residues, and agricultural residues, 122 (2) transportation of whole trees and forest residues in the form of chips and agricultural residues 123 in the form of bales to an HTL plant, (3) bio-crude production via HTL, (4) transportation of bio-124 crude to a hydroprocessing plant, (5) bio-crude conversion to HDRD, and (6) transportation of 125 HDRD to a refinery for blending with fossil fuel-derived diesel and to the consumer. This second 126 conversion pathway is illustrated in Figure 2.

127 This paper is based on the assumptions that, first, fast pyrolysis and HTL plants are located at 128 places with adequate biomass availability to meet the plant capacity of 2000 dry tonnes/day. 129 There is significant biomass potential in western Canada (Sultana and Kumar, 2012). Traveling 130 distances between harvesting locations, bio-oil production plants, HDRD production plants, and 131 the consumer are estimated based on the size of the plant. Second, road construction is assumed 132 to be required for whole tree biomass harvesting, but not for forest and agricultural residues, 133 because whole tree harvesting involves going into untapped forested areas. Third, it is considered 134 that soil nutrients removed due to the removal of the biomass feedstocks are returned through 135 fertilization and reforestation.

136

(Figure 1 here)

137

(Figure 2 here)

Water requirements in this study are 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 HDRD production. Forest residues refer to the chips produced from the branches and tops of the logged trees. In the current scenario in western Canada, forest residues are piled in the forest and burned to prevent forest fires (Kumar et al., 2003). Agricultural residues refer to the straw from wheat, oats and barley. In western Canada, most of these residues are left in the field to rot (Kumar et al., 2003).

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 (Czernik and Bridgwater, 2004; Lu et al.,

148 2009). To obtain a high heat transfer rate, the fast pyrolysis feed must have a moisture content of 149 less than 10% (Bridgwater et al., 1999). HTL is a thermal decomposition process that converts 150 biomass to bio-crude using super-critical state water as a medium (Elliott et al., 2015). In both 151 thermal decomposition processes, bio-gas and char are formed as co-products together with bio-152 oil/bio-crude (Zhu et al., 2013; Agblevor et al., 1995). The differences in fast pyrolysis and HTL 153 process conditions produce bio-oil and bio-crude of different properties. Bio-crude produced by 154 HTL has a lower oxygen content than bio-oil from fast pyrolysis (Toor et al., 2011; Mohan et al., 155 2006). Therefore, upgrading bio-crude to HDRD requires less hydrogen and energy input than 156 upgrading bio-oil produced by fast pyrolysis (Toor et al., 2011; Mohan et al., 2006). Detailed 157 descriptions for both processes are given in sections 3.5 and 3.6. These two biomass conversion 158 processes together with other unit operations, such as biomass production and hydroprocessing, 159 form entire conversion pathways from which data are collected and analyzed. A data-intensive 160 model is developed using site-specific data and operation conventions. With this model, 161 comparisons can be done between feedstocks and methods of bio-oil production to further 162 understand the factors affecting water use efficiency.

163 Water requirements in this study refer to both the direct and indirect use of water required to 164 produce biomass and convert it to HDRD (Singh and Kumar, 2011). The direct use of water is 165 defined as the water used throughout the entire biomass production period and the water required 166 for the chemical conversion of biomass to HDRD (i.e., cooling make-up water, steam generation, 167 etc.) (Singh and Kumar, 2011). The indirect use of water is defined as the water used to produce 168 fertilizers and that associated with the energy inputs (Singh and Kumar, 2011). In this study, the 169 indirect water use for infrastructure and equipment was not considered. For both direct and 170 indirect water use, the source is either surface or ground water (Singh and Kumar, 2011).

171 **3. Water requirement inventory**

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

174 **3.1.** Production of biomass

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

177 3.1.1. Forest biomass

178 Water use in the boreal forest is through evapotranspiration, the sum of transpiration and 179 evaporation (Spafford and Devito, 2013). Evapotranspiration can be separated into three parts, 180 canopy, understorey, and soil surface evaporation (Brown, 2010). Potential evapotranspiration is 181 the amount of evapotranspiration from the forest that would occur if there is sufficient water 182 (Spafford and Devito, 2013). In Alberta, a province in western Canada, water for boreal forest 183 growth comes in the form of precipitation, and the precipitation amount is known to be smaller 184 than the forest's potential evapotranspiration. The surface runoff is thus assumed to be negligible, 185 and the average annual precipitation is taken to be approximately equal to the actual 186 evapotranspiration (Spafford and Devito, 2013; Chasmer et al., 2010). The average rainfall of 187 Alberta's boreal plains forest is estimated to be 480 mm/yr (Downing and Pettapiece, 2006). 188 Harvestable yields of 84 dry tonnes/ha for whole tree (WT) and 0.247 dry tonnes/ha for forest 189 residues (FR) suggested by Kumar et al. (2003) are assumed to be the amount of biomass 190 produced with the average precipitation. However, not all precipitation should be allocated to the 191 biomass feedstock if only a portion is used for HDRD production. For example, forest residues

192 constitute 20% of the forest, and water allocation is conducted to allocate 20% of the 193 precipitation to forest residues. Using the average rainfall and the feedstock yield, the water use 194 for the production of WT and FR is computed (with Eq. 1) to be 5714.3 L H₂O/kg dry wood and 195 3886.6 L H₂O/kg dry wood, respectively.

196
$$WR_{wood\ production} = \frac{Avg.rainfall \times no.of\ years\ for\ tree\ growth \times \% allocation}{(Yield_{dry\ mass})}$$
 (1)

- 197 In this equation,
- 198 $WR_{wood production}$ = the water requirement for WT production, L H₂O/kg dry wood;

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

- 200 No. of years for tree growth = the number of years for tree growth before the next round of
- 201 harvest (FR is harvested on a yearly basis, while WT is harvested every 100 years), year;
- 202 %allocation = the allocation of water to the biomass of interest when it is produced along with

203 other biomass (FR has a 20% allocation, while WT has a 100% allocation);

- 204 Yield_{dry mass} = the yield of dry biomass harvest, dry kg/ha.
- In this article all equations are framed to illustrate the calculation principle. Unit conversion isnot included in the equations.

207 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 (McKenzie and Dunn, 2008). 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) (Sultana et al., 2010). 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).

217
$$Avg.water use/area = \frac{\sum_{crops}[water use(mm) \times area]}{\sum_{crops} area} \times \frac{mass of straw used as biomass}{mass of total straw+mass of grains}$$
 (2)

218
$$WR_{agricultural residues production} = \frac{Avg.water use/area}{net avg.yield of straw}$$
 (3)

- 219 In these equations,
- 220 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, $L H_2O/ha$;
- 223 WR_{agricultural residues production} = the water requirement for agricultural residues production, L H₂O/kg
- dry straw;
- 225 Net avg. yield of straw = the amount of dry straw used as biomass in a unit area, dry tonne/ha.

226 **3.2.** Harvest of biomass

227 This section introduces the harvesting process of whole trees, forest residues, and agricultural

- residues, and the water requirements associated with this operation.
- 229 *3.2.1.* Whole tree
- 230 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 an HTL plant for conversion to bio-oil or

232 bio-crude. These sub-unit operations use ultra-low sulphur diesel as energy. Felling operations 233 use 1.92 L diesel/dry tonne before the whole trees are skidded to the roadside at an energy use 234 rate of 2.14 L diesel/dry tonne (Kabir and Kumar, 2011). At the roadside, whole trees are 235 chipped at an energy use rate of 3.33 L diesel/dry tonne (Kabir and Kumar, 2011). Diesel inputs 236 contribute to the indirect water use of HDRD production, and the value of indirect water use can 237 be calculated by multiplying energy use/dry tonne wood by water use/energy unit; for example, 238 indirect water use for the felling sub-unit operation can be computed by multiplying 1.92 L 239 diesel/dry tonne wood by 2.2 L H₂O/L diesel. To produce wood chips, an indirect water use of 240 0.017 L H₂O/dry kg wood is required based on 2.2 L H₂O/L diesel water usage for diesel 241 production (King and Webber, 2009).

Operation	Value (Energy or mass/dry tonne wood)	Ref	Water use factor (L H ₂ O/Energy or mass)	Ref
Felling (L diesel)	1.92	(Kabir and Kumar, 2011)	2.2	(King and Webber, 2009)
Skidding (L diesel)	2.14	(Kabir and Kumar, 2011)	2.2	(King and Webber, 2009)
Chipping (L diesel)	3.33	(Kabir and Kumar, 2011)	2.2	(King and Webber, 2009)
Road construction (MJ diesel) ^a	0.073	(Stripple, 2001)	0.059	(King and Webber, 2009)
Road construction (kWh) ^a	0.018	(Stripple, 2001)	1.08	(Statistics Canada, 2014; Environment Canada, 2013)
Transportation (L diesel)	0.632	(Kabir and Kumar, 2012)	2.2	(King and Webber, 2009)

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

Fertilizer transport (MJ diesel)	12.41	(Binkley and Fisher, 2012)	0.059	(King and Webber, 2009)
Fertilizer spreading (MJ diesel)	0.60	(Binkley and Fisher, 2012)	0.059	(King and Webber, 2009)
Nitrogen replacement (kg N)	6.1	(Jones et al., 2009)	0.683	(Sheehan et al., 1998)

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

243

244 3.2.2. Forest residues

245 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 (Kumar et al., 2003). The harvesting processes 246 247 are the forwarding of the forest residues with a fuel use of 1.49 L diesel/dry tonne and the 248 chipping with a fuel use of 3.93 L diesel/dry tonne (Kabir and Kumar, 2011). The indirect water 249 requirement for diesel use is calculated to be 0.024 L H₂O/dry kg wood, when ultra-low sulphur 250 is used and the water use factor for diesel is 2.2 L H₂O/L diesel (King and Webber, 2009). Less water is required to harvest forest residues than whole trees because there are fewer sub-unit 251 252 operations in forest residues harvesting.

253 Table 2: Harvesting and fertilization water requirements (forest residues)

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	(Kabir and Kumar, 2011)	2.2	(King and Webber, 2009)
Chipping (L diesel)	3.93	(Kabir and Kumar, 2011)	2.2	(King and Webber, 2009)
Transportation (L	2.62	(Kabir and	2.2	(King and Webber,

diesel)		Kumar, 2012)		2009)
Fertilizer transport (MJ diesel)	14.68	(Binkley and Fisher, 2012)	0.059	(King and Webber, 2009)
Fertilizer spreading (MJ diesel)	202.43	(Binkley and Fisher, 2012)	0.059	(King and Webber, 2009)
Nitrogen replacement (kg N)	6.1	(Jones, et al., 2009)	0.683	(Sheehan et al., 1998)

254 3.2.3. Agricultural residues

255 There are more sub-unit operations for straw harvesting than for the harvesting of whole trees or 256 forest residues. The first sub-unit operation is raking to prepare the straw for baling; this uses 257 0.47 L diesel/dry tonne straw (Kabir and Kumar, 2011). The next 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 258 tonne straw, 0.83 L diesel/dry tonne straw, and 0.33 L diesel/dry tonne straw, respectively (Kabir 259 260 and Kumar, 2011). After totalling the field operations and multiplying the results by the water 261 use factor, we computed the indirect water use for harvesting and fertilization to be 0.047 L 262 H₂O/dry kg straw (see Table 3).

Table 3: Harvesting and fertilization water requirements (agricultural residues)

Operation	Value (Energy or mass/dry tonne straw)	Ref	Water use factor (L H ₂ O/Energy or mass)	Ref
Raking (L diesel)	0.47	(Kabir and Kumar, 2011)	2.2	(King and Webber, 2009)
Baling (L diesel)	2.9	(Kabir and Kumar, 2011)	2.2	(King and Webber, 2009)
Bale wrapper (L diesel)	0.128	(Kabir and Kumar, 2011)	2.2	(King and Webber, 2009)
Stacking (L diesel)	0.829	(Kabir and Kumar, 2011)	2.2	(King and Webber, 2009)
Bale loader (L diesel)	0.33	(Kabir and Kumar, 2011)	2.2	(King and Webber, 2009)
Transportation (L diesel)	2.798	(Kabir and Kumar, 2011)	2.2	(King and Webber, 2009)
Fertilizer transport (L diesel)	0.248	(Kabir and Kumar, 2011)	2.2	(King and Webber, 2009)
Fertilizer spreading (L diesel)	13.541	(Baquero, Esteban, Riba, Rius, & Puig, 2011)	2.2	(King and Webber, 2009)
Nitrogen replacement (kg N)	7.364	(Wang, 2011)	0.683	(Sheehan et al., 1998)
Phosphate replacement (kg P ₂ O ₅)	2.153	(Wang, 2011)	0.194	(Sheehan et al., 1998)
Potassium replacement (kg K ₂ O)	19.410	(Wang, 2011)	0.001	(Sheehan et al., 1998)
Sulphur replacement (kg S)	1.575	(Miller and Kumar, 2013)	0.683	(Singh and Kumar, 2011)

265 **3.3. Transportation of biomass**

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

268 3.3.1. Forest biomass

269 Fast pyrolysis and HTL plant locations are assumed to be at the centre of a circular biomass 270 harvest area. The average displacement of each point of the biomass harvest area to the centre of 271 a circular area was calculated to be 0.707r, where r is the radius of the circular area considered. 272 The boreal forest whole tree yield in Alberta is assumed to be 84 dry tonnes/ha (Kumar et al., 273 2003). The roads from the harvest site to the fast pyrolysis/HTL-based production plant are 274 usually not straight, so a tortuosity factor of 1.27 is used to estimate the average distance 275 required to transport biomass (Overend, 1982). To obtain 2000 dry tonnes/day with 84 dry 276 tonnes/ha vield, the average transportation distance (Equation 4) was worked out to be 19.4 km 277 after the tortuosity factor was factored in (Sarkar and Kumar, 2009). Chips are transported by 278 trailer trucks with a fuel economy of 0.33 L diesel/km with a full load of 17.5 tonnes. On the 279 return trip, in which it is assumed that the truck is empty, the fuel economy is better, at 0.24 L 280 diesel/km (Kabir & Kumar, 2012). The calculation is show here:

281
$$D_{avg,} = \sqrt{\frac{Plant\ capacity \times days_{operation}}{WT_{yield} \times \pi}} \times 0.707 \times 1.27$$
 (4)

where,

 D_{avg} = the average distance required to transport whole tree wood chips, km;

284 Plant capacity = the amount of biomass processed by a facility in a day, dry tonnes/day;

285 days_{operation} = the total number of operational days in the entire life of the plant, days;

286 WT_{yield} = the whole tree yield from forest, dry tonnes/ha.

287 Road construction is required for whole tree feedstock to transport wood chips to pyrolysis or an 288 HTL plant. No road construction is required, however, for forest residue feedstocks due to the 289 existing logging roads. Forest roads of six meters wide are classified as primary and secondary 290 roads; primary roads are long stretches of roads that can be used for transporting wood chips by 291 trailer trucks, and secondary roads can be used by fellers and skidders to fell and skid whole trees 292 over short distances at slow speeds to a roadside chipper for the chipping process. Because 293 primary roads are considerably longer than secondary roads, the construction of secondary roads 294 is assumed to have negligible impact compared to the construction of primary roads. For a 2000 295 dry tonnes/day biomass processing plant, we estimate that 700 km of primary roads will be built 296 over a period of 20 years (Kabir and Kumar, 2011). Water use in road construction is indirect 297 water use from energy production. Various forms of energy, amounting to 1731 GJ/km, are 298 required to provide materials and fuel for construction equipment (Stripple, 2001). A water use 299 factor of 0.0366 L H₂O/dry tonne wood is derived from the indirect water consumption of the 300 energy required in road construction.

The calculation for the transportation distance of whole tree feedstock is applied to forest residue feedstock. Forest residues yield 0.247 dry tonnes/ha (Kumar et al., 2003). 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. Forest residue wood chips have properties similar to whole tree wood chips. The fuel consumption of trailer trucks for transporting forest residue wood chips is assumed to be the same as for whole tree wood chips.

308 3.3.2. Agricultural biomass

309 Agricultural residues yield 0.517 dry tonnes/ha. A plant with a processing capacity of 2000 dry 310 tonnes a day will require a harvest area with an average transportation distance of 53.2 km after 311 tortuosity has been factored in (Sarkar and Kumar, 2010). Because of existing farm roads, no 312 road construction is required for the conversion pathway of agricultural biomass to HDRD. 313 Agricultural residues have different physical properties than forest wood. The main physical 314 property that affects transportation is density. Agricultural residues, moreover, are packed in 315 bales for transportation. The low density of agricultural residues means that the trailer truck is 316 limited by volume instead of mass. Hence 12.6 tonnes of agricultural residues are transported per 317 trip (Kabir and Kumar, 2012). The transportation fuel economy is taken to be 0.33 L diesel/km 318 for a full load and 0.24 L diesel/km for the return empty trip (Kabir and Kumar, 2012).

319 3.4. Fertilization

320 Nutrients are removed from the soil when biomass, in the form of trees or forest residues, are 321 harvested and used for the production of fuels. The forest needs to be fertilized to maintain long-322 term fertility (Borjesson, 2000). In this study, essential nutrients are considered. For the forest, 323 the return of ashes returns essential nutrients except nitrogen, which is not present in wood ash. 324 Nitrogen fertilizer, applied to encourage sapling growth in clear-cut plots, is included in this 325 study (Mahendrappa and Salonius, 1982); it assumed that 6.1 kg N/dry tonne wood removed is 326 required (Jones et al., 2009). The application of nitrogen includes transporting the fertilizer from 327 the fertilizer plant to the forest and spreading it. The distance from the fertilizer plant to the bio-328 oil/HTL plant is assumed to be 300 km, and the additional distance from the bio-oil/HTL plant to 329 the deforested plot of land is taken to be the same as the average biomass transportation distance.

330 The energy required to spread nitrogen is 0.60 MJ diesel/dry tonne wood (see Equation 5) for a 331 whole tree feedstock yield of 84 dry tonnes/ha (Binkley and Fisher, 2012). The transportation 332 energy required is 12.41 MJ diesel/dry tonne wood (Binkley and Fisher, 2012) (see Equation 6) 333 when the energy requirement for transport is 0.064 MJ diesel/kg N/km (Binkley and Fisher, 334 2012). For wood ash, similar parameters are used, but the transportation distance is reduced to 335 the distance between the bio-oil/HTL plant and the harvested area because the wood ash comes 336 from the bio-oil/HTL plant. Forest residues are harvested over a large area and therefore the 337 energy requirement for transportation and spreading is proportionally higher. The energy 338 requirement for ash and fertilizer spreading increases to 202.43 MJ diesel/dry tonne wood as the 339 harvesting area for FR is bigger than the harvesting area for WT (Binkley and Fisher, 2012). The 340 transportation energy requirement of ash and fertilizer remains at 0.064 MJ diesel/kg N/km for 341 FR, while the ash transportation distance is 80.3 km according to Equation 4, and the 342 transportation of fertilizer is 380.3 km with an additional 300 km of traveling from the fertilizer 343 plant to the bio-oil/HTL plant added to the distance from the bio-oil/HTL plant to the harvest 344 area.

345
$$Energy_{fertilizer spreading,dry tonne} = \frac{Energy_{fertilizer spreading,area}}{yield of biomass}$$
 (5)

346 $Energy_{fertilizer transport,dry tonne} = Energy_{transport} \times kg \ of \ N \times Distance$ (6)

347 In these equations,

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

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

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

353 Energy_{fertilizer transport, dry tonne} = the energy required to transport fertilizer per unit dry tonne of

354 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 with the removal of agricultural residues. The nutrients considered are nitrogen, phosphate, potassium, and sulphur. The soil's nutrient requirement is shown in Table 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 the fertilizer plant to the 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 (Baquero et al., 2011).

364 **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 (Czernik and Bridgwater, 2004; Lu et al., 2009). Feedstock size affects the heat transfer rate of fast pyrolysis, so the feedstock is ground to a size smaller than 2 mm before pyrolysis (Ringer et al., 2006). Water content in biomass feedstocks affects the water content of the bio-oil produced as well as the heat transfer efficiency of the feedstocks; hence, the feedstock must be dried to a moisture content range of 5-10 wt% (Bridgwater et al., 1999; Ringer et al., 372 2006). After being ground and dried, the feedstock undergoes fast pyrolysis typically at 500-550
373 °C, one atmospheric pressure, and 0.5 s residence time to produce a bio-oil yield of
374 approximately 59.9 wt% (dry basis) (Ringer et al., 2000). The operating conditions could vary
375 with variation in the processes.

376 In fast pyrolysis, water is directly used in the bio-oil cooling, bio-oil vapor cooling, ash 377 quenching, steam condensing, and steam producing processes. The used water is usually 378 recycled in the system to reduce water consumption; however, there is a fraction of water that is 379 not recycled. Water that is not recycled includes waste water and water lost through blowdown 380 and evaporation. Water losses through bio-oil and bio-oil vapor cooling are 0.027 L H₂O/kg bio-381 oil and 0.003 L H₂O/kg bio-oil, respectively (Ringer et al., 2006). Cooling water temperatures 382 are relatively low and reduce water losses. On the other hand, the steam condenser and steam 383 system, with higher temperatures than bio-oil cooling, use more water (1.077 L H₂O/kg bio-oil 384 and 0.026 L H₂O/kg bio-oil, respectively) (Ringer et al., 2006). Ash quenching requires water to 385 be sent to waste treatment after quenching and it contributes 0.203 L H₂O/kg bio-oil (Ringer et 386 al., 2006). Indirect water is the water consumed when electricity is used for pre-treatment and 387 pyrolysis processes. However, the combustion of char and gaseous products from the pyrolysis 388 process generates enough electricity to create surplus electricity. This surplus will result in 389 negative indirect water consumption as the electricity is assumed to be sent to the power grid. 390 Although whole tree and forest residues come from the same wood sources, the ash content of 391 wood chips from the two feedstocks differs. As a result, the outcomes of fast pyrolysis for whole 392 tree and forest residue feedstocks differ slightly. However, the impact from ash content is barely 393 noticeable among other heavier weighted factors in the computation of the water requirements of 394 the conversion pathways.

395 Table 4: Water requirements for pyrolysis (whole tree & forest residue)

Pyrolysis (whole tree &	Pyrolysis (whole tree & forest residue)					
Operation ^a	Value	Ref	Water use factor (L H ₂ O/ kWh)	Ref		
Bio-oil cooling (L $H_2O/kg \text{ bio-oil})^b$	0.027	(Ringer et al., 2006)	-			
Bio-oil vapor cooling (L H ₂ O/kg bio-oil) ^b	0.003	(Ringer et al., 2006)	-			
Steam condensing $(L H_2O/kg bio-oil)^b$	1.077	(Ringer et al., 2006)	-			
$\begin{array}{llllllllllllllllllllllllllllllllllll$	0.026	(Ringer et al., 2006)	-			
Ash quenching (L H_2O/kg bio-oil) (whole tree) ^b	0.203	(Ringer et al., 2006)	-			
Ash quenching (L H_2O/kg bio-oil) (forest residue) ^{b,c}	0.663	(Ringer et al., 2006)				
Recycle gas compression (kW)	10400	(Ringer et al., 2006)	1.08	(Statistics Canada, 2014; Environment Canada, 2013)		
Feedstock grinding (kW)	5600	(Ringer et al., 2006)	1.08	(Statistics Canada, 2014; Environment Canada, 2013)		
Other auxiliary (kW)	1248	(Ringer et al., 2006)	1.08	(Statistics Canada, 2014; Environment Canada, 2013)		
Electricity generated (kW)	19600	(Ringer et al., 2006)	1.08	(Statistics Canada, 2014; Environment Canada, 2013)		

^a Water requirement factors are derived based on a 2000 dry tonnes/day plant.

^b Values derived based on the flow rate of the processing plant.

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

396

397 Agricultural residues have a slightly different chemical composition than whole tree and forest

398 residues. Agricultural residues have more ash than wood and yield less bio-oil (Couhert et al.,

399 2009). Water use for pyrolysis is derived using mass and energy balances based on the process 400 requirements estimated by Ringer et al. (Ringer et al., 2006). Water use contributors for 401 agricultural residue pyrolysis are the same as those of the whole tree and forest residue pyrolysis 402 processes (when the same process is used), but more water is used for agricultural residue 403 pyrolysis due to the slightly lower projected bio-oil yield. Bio-oil cooling, bio-oil vapor cooling, 404 steam condensing, and steam producing processes for the pyrolysis of agricultural residues 405 require 0.027 L H₂O/kg bio-oil, 0.003 L H₂O/kg bio-oil, 1.08 L H₂O/kg bio-oil, and 0.026 L 406 H₂O/kg bio-oil, respectively. Agricultural residues have approximately 4 times more ash than 407 woody plants and hence the amount of water used for quenching is 0.89 L H₂O/kg bio-oil 408 (Sarkar and Kumar, 2010; Ringer et al., 2006).

410 **Table 5: Water requirements for pyrolysis (agricultural residue)**

Pyrolysis (agricultural r	Pyrolysis (agricultural residue)						
Operation ^a	Value	Ref	Water use factor (L H ₂ O/	Ref			
Bio-oil cooling (L H_2O/kg bio-oil) ^b	0.027	(Ringer et al., 2006)	kWh) -				
Bio-oil vapor cooling (L H ₂ O/kg bio-oil) ^b	0.003	(Ringer et al., 2006)	-				
$\begin{array}{llllllllllllllllllllllllllllllllllll$		(Ringer et al., 2006)	-				
$\begin{array}{llllllllllllllllllllllllllllllllllll$	0.026	(Ringer et al., 2006)	-				
Ash quenching $(L H_2O/kg bio-oil)^b$	0.890	(Ringer et al., 2006)	-				
Recycle gas compression (kW)	10400	(Ringer et al., 2006)	1.08	(Statistics Canada, 2014; Environment Canada, 2013)			
Feedstock grinding (kW)	5600	(Ringer et al., 2006)	1.08	(Statistics Canada, 2014; Environment Canada, 2013)			
Other auxiliary (kW)	1248	(Ringer et al., 2006)	1.08	(Statistics Canada, 2014; Environment Canada, 2013)			
Electricity generated (kW)	19600	(Ringer et al., 2006)	1.08	(Statistics Canada, 2014; Environment Canada, 2013)			

^a Water requirement factors are derived based on a 2000 dry tonnes/day plant. ^b Values derived based on the flow rate of the processing plant.

411 **3.6. Hydrothermal liquefaction**

HTL is a type of thermochemical liquefaction that converts biomass to bio-crude in presence of water (Zhu et al., 2013). 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 an HTL reactor (Elliott et al., 2015; Toor et al., 2011; Zhu et al., 2014; Xu and Lad, 2008). Inside the reactor, biomass undergoes a

417 reaction at 355 °C and is converted to oil, water, gas, and solid compounds containing char, ashes, 418 and unreacted biomass using water in a super-critical state as a solvent to catalyse the reaction 419 (Zhu et al., 2013; Zhu et al., 2014). After the reaction, effluents are filtered to remove solid 420 particles. Further down the process stream, the effluents are cooled, depressurized, and separated 421 into gaseous, aqueous, and oil phases. After the HTL process, the aqueous phase (containing 422 water) is separated from bio-crude, of which 80% is recycled and the rest is purged to waste 423 water treatment for anaerobic digestion (Zhu et al., 2014). Anaerobic digestion produces 424 methane-rich off-gas, which in turn can be used as an energy source in the HTL system (Zhu et 425 al., 2014).

426 Water use for the HTL of whole tree and forest residue feedstocks (see Table 6) includes indirect 427 water required for electricity used by the system and direct water by the biomass-water slurry 428 production. Although whole tree and forest residue feedstocks come from the same plant species, 429 there is a slight difference in their chemical composition, such as in the ash content, but the 430 difference in results from HTL between forest residues and whole tree is not significant 431 compared to other factors affecting the water requirements of forest residue and whole tree 432 biomass. HTL uses 12 MWe to keep the systems of a 2000 dry tonnes/day plant running (Zhu et 433 al., 2014). The operation does not include the generated electrical energy of 11 MWe coming 434 from combusting off-gas for a 2000 dry tonnes/day HTL plant (Zhu et al., 2014). Water use in 435 electrical energy generation is considered in this study as negative indirect water use. According 436 to Statistics Canada and Environment Canada, 1.08 L H₂O of water is required for every kWh 437 electrical energy produced (Statistics Canada, 2014; Environment Canada, 2013). This factor is 438 used to calculate the indirect water use for any electricity consumption or generation. A 20% 439 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.

443 Agricultural residues require a slightly different amount of water (see Table 7) than whole tree 444 and forest residues even when the HTL operations are the same. The energy inputs and their 445 corresponding indirect water uses for HTL process are derived from the bio-crude yield 446 estimates done by Akhtar and Amin, who established a relationship between lignin content and 447 bio-crude yield (Akhtar and Amin, 2011). A lignin content of 21.3 wt% for agriculture residues 448 and 24.3 wt% for wood (Toor et al., 2011) can produce an estimated bio-crude yield of 47.8% 449 from agricultural residues and 44.8% fromwoody biomass (Zhu et al., 2014; Akhtar and Amin, 450 2011; Zhu et al., 2011). This bio-crude yield affects the water use efficiency as it is based on the 451 functional unit. In terms of the operations of HTL, the electrical energy required for HTL 452 remains unchanged at approximately 12 MWe for a 2000 dry tonnes/day plant. Similarly, the 453 indirect water consumption for electricity production is assumed to be 1.08 L H₂O/kWh 454 (Statistics Canada, 2014; Environment Canada, 2013). With this conversion factor, the indirect 455 water requirement is estimated to be 0.35 L H_2O/kg dry straw. The amount of water recycled is 456 assumed to remain unchanged at 80% (Zhu et al., 2014); therefore, the direct water consumption 457 required from purging to waste water treatment is 1.17 L H₂O/kg dry straw.

HTL (whole tree and	HTL (whole tree and forest residue)						
Operation ^a	Value	Ref	Water use factor (L H ₂ O/kWh)	Ref 460			
Cooling water make- up (L H ₂ O/kg HDRD)	4.05	(Zhu et al., 2014)	-				
Boiler feed water make-up (L H ₂ O/kg HDRD)	0.67	(Zhu et al., 2014)	-				
Water purged / day (L H ₂ O/kg dry straw)	1.17	(Zhu et al., 2014)	-				
Natural gas flow rate (kg /hr)	1420	(Zhu et al., 2014)	0 L H ₂ O/kg	(King and Webber, 2009)			
Feed pre-treatment (MWe)	12.0	(Zhu et al., 2014)	1.08	(Statistics Canada, 2014; Environment Canada, 2013)			
Bio-crude production (MWe)	0.0	(Zhu et al., 2014)	1.08	(Statistics Canada, 2014; Environment Canada, 2013)			
Hydrotreating (MWe)	10.0	(Zhu et al., 2014)	1.08	(Statistics Canada, 2014; Environment Canada, 2013)			
Hydrocracking (MWe)	1.1	(Zhu et al., 2014)	1.08	(Statistics Canada, 2014; Environment Canada, 2013)			
Steam reforming (MWe)	3.4	(Zhu et al., 2014)	1.08	(Statistics Canada, 2014; Environment Canada, 2013)			
Other auxiliary (MWe)	0.3	(Zhu et al., 2014)	1.08	(Statistics Canada, 2014; Environment Canada, 2013)			
Electricity generation (MWe) ^b	11	(Zhu et al., 2014)	1.08	(Statistics Canada, 2014; Environment Canada, 2013)			

459 Table 6: Water requirement for HTL (whole tree and forest residue)

^a Water requirement factor and energy are based on a 2000 dry tonnes/day HTL plant capacity ^b Electricity is generated from the combustion of off-gas

461

463	Table 7: Water	requirement for HTL	(agricultural residue)

HTL (agricultural resi	due)			
Operation ^a	Value	Ref	Water use factor (L H ₂ O/kWh)	Ref
Cooling water make- up (L H ₂ O/kg HDRD) ^b	4.32	(Zhu et al 2014)	., -	
Boiler feed water make-up (L H ₂ O/kg HDRD) ^b	0.72	(Zhu et al 2014)	., -	
Water purged / day (L $H_2O/kg dry straw)^c$	1.17	(Zhu et al 2014)	., -	
Natural gas flow rate (kg /hr) ^d	1420	(Zhu et al 2014)		(King & Webber, 2009)
Feed pre-treatment (MWe) ^d	12.0	(Zhu et al 2014)	., 1.08	(Statistics Canada, 2014; Environment Canada, 2013)
Bio-crude production (MWe) ^d	0.0	(Zhu et al 2014)	., 1.08	(Statistics Canada, 2014; Environment Canada, 2013)
Hydrotreating (MWe) ^d	10.7	(Zhu et al 2014)	., 1.08	(Statistics Canada, 2014; Environment Canada, 2013)
Hydrocracking (MWe) ^d	1.2	(Zhu et al 2014)	., 1.08	(Statistics Canada, 2014; Environment Canada, 2013)
Steam reforming (MWe) ^d	3.6	(Zhu et al 2014)	., 1.08	(Statistics Canada, 2014; Environment Canada, 2013)
Other auxiliary (MWe) ^d	0.3	(Zhu et al 2014)	., 1.08	(Statistics Canada, 2014; Environment Canada, 2013)
Electricity generation (MWe) ^{d,e}	11	(Zhu et al 2014)	., 1.08	(Statistics Canada, 2014; Environment Canada, 2013)

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

^d Assumed energy required for HTL is only affected by process conditions ^e Electricity is generated from the combustion of off-gas

^b Assumed cooling water make-up and boiler feed water make-up are linearly proportional to the bio-oil
^c Assumed water produced through HTL is the same as for whole tree and forest

residues

464 **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 465 466 HDRD plant. There is no direct water use in the transportation of bio-oil/bio-crude, but the diesel 467 used contributes to indirect water use. The HDRD plant is assumed to be in an industrial area 468 with oil and gas processing facilities. Traveling distance is determined based on the distance 469 between the bio-oil/bio-crude production plants and the HDRD plant. Since the bio-oil/bio-crude 470 production plant locations are determined based on biomass availability, the distances between 471 bio-oil/bio-crude production plants and an HDRD plant are estimated to be 300 km for whole 472 trees and forest residues and 250 km for agricultural residues when the nearest areas of 473 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 474 475 diesel/km when not carrying a load (Miller and Kumar, 2013).

476 **3.8.** Upgrading bio-oil/bio-crude

477 Bio-oil/bio-crude must be upgraded in order for it to be converted into HDRD for use in diesel 478 engines. Upgrading takes place through hydrodeoxygenation, in which oxygen is removed from 479 the bio-oil/bio-crude to increase the stability and heating value of hydrocarbons using hydrogen 480 and a catalyst (Jones et al., 2009). Hydrogen, a reactant that is required for oxygen removal, is 481 produced by steam reforming using natural gas together with superheated steam (Jones et al., 482 2009; Zhu et al., 2014). Water input in the steam reforming process counts towards the total 483 water use in the production of HDRD from lignocellulosic biomass. Fast pyrolysis and HTL 484 have different process conditions, resulting in a difference in chemical structure and water use 485 for upgrading between bio-oil and bio-crude (Toor et al., 2011; Mohan et al., 2006).

486	The upgrading of pyrolysis bio-oil involves two hydrotreating steps followed by hydrocracking.
487	The first hydrotreating step is at a mild temperature of 270 °C and 140 bar to prevent phase
488	separation in the bio-oil (Jones et al., 2009). The second hydrotreating step operates at a higher
489	temperature of 350 °C and 140 bar and completes the hydrodeoxygenation process (Jones et al.,
490	2009). The heavy oil produced is hydrocracked into lighter hydrocarbons such as diesel and
491	gasoline to increase the HDRD yield. The direct water required in upgrading is used for cooling
492	tower make-up and the steam reforming boiler feed. These volumes of water amount to 0.09 L
493	H ₂ O/kg HDRD for cooling water and 0.83 L H ₂ O/kg HDRD for the steam reforming boiler feed.
494	For indirect water consumption, the electricity used for the plant is taken into account, and the
495	water required to produce the amount of electricity needed is computed to be 0.0103 L H ₂ O/MJ
496	HDRD. A breakdown of the hydroprocessing water requirement is shown in Table 8 and Table 9.

497 Table 8: Water requirement for hydroprocessing after pyrolysis (whole tree and forest
498 residue)

Hydroprocessing (whole tree and forest residue)					
Operation ^a	Value	Ref	Water use	Ref	
			factor (L		
			H ₂ O/kWh)		
Cooling water required (L	0.089	(Hsu,	-		
H ₂ O/kg HDRD)		2012)			
Boiler feed required (L	0.828	(Hsu,	-		
H ₂ O/kg HDRD)		2012)			
Natural gas (MJ/kg HDRD)	12.11	(Hsu,	0 L H ₂ O/kg	(King and Webber,	
		2012)		2009)	
Electricity (kWh/kg HDRD)	0.408	(Hsu,	1.08	(Statistics Canada,	
		2012)		2014; Environment	
				Canada, 2013)	

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

499

Hydroprocessing (agricultural residue)					
Operation ^a	Value	Ref	Water use	Ref	
			factor (L		
			H ₂ O/kWh)		
Cooling water required (L	0.089	(Hsu,	-		
H ₂ O/kg HDRD)		2012)			
Boiler feed required (L	0.828	(Hsu,	-		
H ₂ O/kg HDRD)		2012)			
Natural gas (MJ/kg HDRD)	12.18	(Hsu,	0 L H ₂ O/kg	(King and Webber,	
		2012)	_	2009)	
Electricity (kWh/kg HDRD)	0.410	(Hsu,	1.08	(Statistics Canada,	
		2012)		2014; Environment	
				Canada, 2013)	

501 **Table 9: 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

502

503 The upgrading of bio-crude from HTL also involves hydrotreating and hydrocracking. HTL 504 produces bio-crude with a lower oxygen content than bio-oil from fast pyrolysis (Baker and 505 Elliott, 1988). This lower oxygen content not only reduces the hydrotreating process from the 506 two stages required by the pyrolysis oil to a single stage but also reduces the amount of reactant 507 and energy required to carry out hydrotreating (Zhu et al., 2011). Bio-crude from HTL is first 508 hydrotreated using a fixed bed reactor at 400 °C with a supply of hydrogen. After hydrotreatment, 509 butane and lighter gas components are separated from the oil for stabilization. The heavier oil is 510 sent for hydrocracking that takes place at 400 °C and 80-150 bar with the addition of hydrogen 511 and in the presence of metal sulfide catalysts (Zhu et al., 2011). After hydrocracking, gasoline 512 and diesel are separated by distillation column. The energy and water required for hydrotreating 513 and hydrocracking HTL oil are shown in Table 6 and Table 7.

514 **3.9.** Transportation of HDRD

515 The transportation of HDRD from an HDRD production plant to consumers is considered in this 516 study because the use of energy in HDRD transportation involves water. Diesel consumption in 517 Alberta was 4.2 billion liters in 2013 (Government of Canada, 2014). With the province's 518 population residing mainly in Edmonton and Calgary (Government of Alberta - Municipal 519 Affairs, 2013), it is assumed in this study that the HDRD produced will be delivered to these two 520 cities for consumer use. The location of the HDRD plant is assumed to be in Redwater, Alberta, 521 and is 65 km and 380 km from Edmonton and Calgary, respectively. The average round trip 522 distance from Redwater to Edmonton and Calgary is 445 km. HDRD is transported by B-train 523 trucks with the same fuel economy as bio-oil/bio-crude transportation.

524 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.

532 4.1. Base case scenario

533 The base case scenario examines the individual unit operations of biomass production, 534 harvesting, bio-oil or bio-crude production (pyrolysis or HTL), hydroprocessing, and

- 535 transportation. Unit operation values are compiled in Table 10 and Table 11 for HDRD
- 536 production via fast pyrolysis and HTL, respectively.

Table 10: Water use efficiency for the conversion of lignocellulosic biomass to HDRD by fast pyrolysis

Unit operation (L					Agricu	ıltural	
H ₂ O/MJ HDRD)	Whole tree		Forest 1	residues	residues		
	Direct	Indirect	Direct	Indirect	Direct	Indirect	
	water use	water use	water use	water use	water use	water use	
Biomass production,							
harvesting and	497.79	0.002	338.58	0.003	83.55	0.004	
fertilization							
Fast pyrolysis	0.070	-0.011	0.093	-0.010	0.106	-0.011	
Hydroprocessing	0.021	0.010	0.021	0.010	0.022	0.010	
Transportation	-	0.001	-	0.001	-	0.001	
Total	497.88	0.002	338.69	0.004	83.68	0.004	

539

540 Table 11: Water use efficiency for the conversion of lignocellulosic biomass to HDRD by541 HTL

Unit operation (L					Agricu	ıltural
H ₂ O/MJ HDRD)	Whole tree		Forest r	residues	residues	
				Indirect		
	Direct	Indirect	Direct	water	Direct	Indirect
	water use	water use	water use	use	water use	water use
Biomass production,						
harvesting and	376.16	0.002	255.85	0.003	58.84	0.003
fertilization						
HTL	0.172	-	0.172	-	0.173	-
Hydroprocessing	0.016	0.013	0.016	0.013	0.017	0.013
Transportation	-	0.001	-	0.001	-	0.001
Total	376.35	0.016	256.04	0.017	59.03	0.017

The water use in biomass production constitutes more than 99.9% of all the water required to produce HDRD. This significant water use in the biomass production stage is consistent across conversion technologies (fast pyrolysis and HTL) and feedstocks (whole tree, forest residues, and agricultural residues). However, the total amount of water use per MJ of HDRD produced can also be greatly affected by the efficiency of conversion technologies. The higher yield of HDRD by HTL conversion makes HTL a more favorable conversion process than fast pyrolysis even when HTL uses more water than fast pyrolysis.

Water use is mainly for biomass production. Therefore, the choice of feedstock is critical in determining the overall water use to produce HDRD. In this study, we found that whole tree and forest residues require more water 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 harvests usually have a 100-year rotation (Kumar et al., 2003). A longer growing period increases the amount of water required.

Second, water requirements for whole tree growing and agriculture crop growing have been studied by various authors. However, in order to obtain the water requirements for forest residues (branches, leaves) and agriculture residues (straw), water allocations need to be made by the authors. In this study, we assume forest residues consumed 20% of the water requirement during tree growth and agriculture residues (used straw) consumed 10.9% of the water requirement for agricultural crop growth.

562 Conversion technologies affect the HDRD production efficiency, which then affects the water 563 use per MJ of HDRD produced. The results of our study showed that HDRD production via HTL 564 and hydroprocessing requires less water per MJ HDRD produced. The higher amount of HDRD 565 produced per kg of biomass for the HTL conversion pathway than for the fast pyrolysis 566 conversion pathway lowered the water required per unit MJ of HDRD. Water use efficiency is 567 measured by summing the water required for a unit MJ of HDRD produced. With a higher 568 HDRD output, HDRD production through HTL will result in a comparatively better water use 569 efficiency than HDRD through fast pyrolysis.

570 HTL uses more water than fast pyrolysis because of the higher water use in the cooling water 571 replacement and the 20% water sent to waste treatment. The water use difference between HTL 572 and fast pyrolysis is not restricted to bio-oil and bio-crude production. Bio-oil from pyrolysis and 573 bio-crude from HTL have different properties and so have different upgrading requirements. 574 Bio-crude from HTL has less oxygen than bio-oil from fast pyrolysis (Toor et al., 2011; Mohan 575 et al., 2006), and so the hydrogen and energy inputs for bio-oil upgrading are lower for bio-crude 576 from HTL than bio-oil from fast pyrolysis. Although less water is used in bio-crude upgrading 577 than bio-oil upgrading, the reduction in water use from the steam reformer is not sufficient to 578 compensate for the higher water use in cooling water losses and waste water generated in the 579 HTL process. On the other hand, fast pyrolysis decomposes biomass in a dry environment and 580 the water use contributed by bio-oil cooling is negligible when the losses are at 3% (Ringer et al., 581 2006). Even when the steam condenser and steam system lead to higher water consumption, 582 especially when more water is required for hydrogen production, fast pyrolysis requires lower 583 water consumption overall.

In the transportation unit operation, water use is the indirect water use not only from transporting material – fertilizers, biomass, bio-oil/bio-crude, and HDRD – but also from road construction. That said, transportation operations' contribution to water use is negligible compared to other 587 unit operations for all feedstocks. Hence differences in water use through road construction

588 whole trees and differences in transportation distance between feedstocks are not noticeable.

589 4.2. Other scenarios – Sensitivity analysis

- 590 The effects of the main inputs and contributing factors on the study results are analyzed by
- 591 introducing scenarios. Table 12 lists the scenarios.

592 Table 12: Scenarios for sensitivity analysis

	Scenarios
1	Decrease water from irrigation or precipitation by 10% 593
2	Increase water from irrigation or precipitation by 10%
3	Decrease biomass yield by 10%
4	Increase 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%
	Decrease transportation distance by 10% (without water use in biomass
11	production)
	Increase transportation distance by 10% (without water use in biomass
12	production)
	Decrease electricity usage by 10% (without water use in biomass
13	production)
	Increase electricity usage by 10% (without water use in biomass
14	production)
	Decrease harvesting energy usage by 10% (without water use in
15	biomass production)
	Increase harvesting energy usage by 10% (without water use in biomass
16	production)

594

595 The production of biomass is the main contributor to water use in producing HDRD from 596 lignocellulosic biomass (see Tables 10 and 11). Annual average rainfall usually varies by
approximately $\pm 10\%$ in Alberta (Alberta Environment and Sustainable Resource Development, 2014), and scenarios 1 and 2 investigate changes in water use by -10% and $\pm 10\%$ in the growing of biomass. The graphs in Figures 3 and 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 the production of biomass outweighs other contributors by a factor of more than 1000.

603

(Figure 3 here)

604

(Figure 4 here)

605 A sensitivity analysis is conducted on biomass yield in scenarios 3 and 4 for a fluctuation of 606 $\pm 10\%$. A range of $\pm 10\%$ is a good range based on the annual harvest fluctuations of agricultural 607 crops and the density of trees in Alberta's forests (Alberta Environment and Sustainable 608 Resource Development, 2014; Alberta Agriculture and Rural Development, 2014). Water use for 609 growth and biomass yield can have an almost equal but opposite effect on water use efficiency of 610 HDRD production for all feedstocks, as seen in Figures 3 and 4. Crop yield and forest cover can 611 vary over time, and a sensitivity analysis of scenarios 3 and 4 can show the impact of a change in 612 yield on water use efficiency. Biomass yield affects product output, and a lower yield has a lower 613 water use efficiency, unlike increases in precipitation and irrigation. This similar impact can be 614 explained by understanding the relationship of the water use factor in biomass production, 615 measured as L H₂O/kg biomass. In this relationship, an increase in irrigation or precipitation with 616 no increase in biomass yield is equivalent to decreasing biomass yield without an increase in 617 irrigation or precipitation. Scenario 4 shows a change that is less drastic than the one given in 618 scenario 3. The lower-magnitude results of scenario 4 compared to scenario 3 can be explained by the inverse relationship biomass yield has with water use efficiency, for a larger denominatorwill not decrease the final value by a constant factor.

621 Water use efficiency is measured by water input per unit of product output. After analyzing the 622 sensitivity of water use requirements with biomass production, we measured the sensitivity of 623 water use requirements towards product yields in scenarios 5 through 8. In scenarios 5 and 6, we 624 consider the impact of changing the intermediate product, bio-oil/bio-crude, while in scenarios 7 625 and 8, we consider the impact of changing the final product, HDRD, by $\pm 10\%$, taking the most 626 pessimistic and optimistic scenarios (Han et al., 2013; Kauffman et al., 2011; Choudhary and 627 Phillips, 2011). The sensitivity analysis results of scenarios 5 through 8 indicate an inverse 628 relationship of products and water use efficiency. When comparing scenarios 5 and 6 with 629 scenarios 7 and 8, we see that the impact of bio-oil/bio-crude yield on water use efficiency is the 630 same as HDRD yield because HDRD production comes from bio-oil/bio-crude output. A 631 reduction or an increase in bio-oil/bio-crude yield will create a similar magnitude of change in 632 HDRD yield due to the change in bio-oil/bio-crude input for hydroprocessing.

633 Scenarios 9 and 10 show the sensitivity of transportation distance on overall water requirements 634 of HDRD production. As transportation distance is likely to vary considerably based on the 635 terrain and change in harvesting plots, a sensitivity analysis needs to be conducted on 636 transportation distance. The negligible impact on overall water requirements when transportation 637 distance is changed is expected because most water use is from biomass production. To 638 understand how influential transportation distance and other factors are, scenarios 11 through 16 639 are conducted without the biomass production unit operation (see Figures 5 and 6). Scenarios 11 640 and 12 continue to test the sensitivity of changes in transportation distance on the results. A

641 change of 0.1% for all feedstocks showed that transportation distance is a small component of642 the entire conversion pathway.

643

(Figure 5 here)

644

(Figure 6 here)

High-efficient equipment consumes less electricity to process biomass through fast pyrolysis, HTL and hydroprocessing. Efficiency can increase due to the progress of technology and can also decrease due to the 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 trees require the least electricity consumption, followed by forest residues and agricultural residues.

Similarly, harvesting equipment is subject to changes in technology and the ill effects of inefficiency. Thus sensitivity analyses are conducted on harvesting energy use (scenarios 15 and 16). Agricultural residues are found to be the most sensitive towards changes in harvesting equipment efficiency, followed by forest residues and whole trees. The sensitivity in this case is caused by the number of unit operations for each feedstock. The agricultural residue feedstock pathway has more harvesting operations, so it is more affected by changes in harvesting efficiency than the other pathways.

659 4.3. Uncertainty analysis

660 An uncertainty analysis was conducted using a Monte Carlo simulation by creating a MATLAB 661 code capable of randomly picking values within the uncertainty ranges of all variables and 662 running 10 million iterations, which were translated into distribution curves (see Figures 7 and 8). 663 Due to uncertainty in published information, a triangular probability distribution was assumed 664 for all of the study's inputs. According to Huijbregts et al. (2001), uncertainty can be estimated 665 by classifying inputs and assigning a suitable uncertainty to each group under the classification 666 considered. In this study, inputs with known estimated uncertainty ranges such as biomass and 667 HDRD yields will have their uncertainty ranges used in the Monte Carlo analysis. Inputs with unknown uncertainty are estimated according to their impact on the final result. A 5% 668 669 uncertainty is assigned to variables with limited impact on the final result while inputs related to 670 transportation distance, biomass yields, and process have a 10% uncertainty assigned to them 671 due to both the greater uncertainty and greater impact on the final results (Huijbregts et al., 2001).

672 Table 13 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 673 674 whole tree feedstock to HDRD via pyrolysis are -11.6% and 13.2%, respectively. The percentage 675 deviations for the conversion pathway of whole tree feedstock to HDRD via HTL are smaller in magnitude than the pyrolysis case at -11.6% and 13.1% for the 10th and 90th percentiles, 676 677 respectively. Similar observations can be seen in Figures 7 and 8 with other feedstocks. The 678 distribution curves for HTL are narrower than those for fast pyrolysis because there are fewer 679 uncertainty inputs for HTL. When individual feedstocks curves are compared, we can see that 680 agricultural residues have the narrowest spread of values when the percentage deviations from

the median value at the 10th and 90th percentiles are -9.3% and 10.2%, respectively, for the fast 681 pyrolysis conversion pathway. The uncertainties of the variables used in the Monte Carlo 682 simulation resulted in the 50th percentile value, of all feedstocks, being always slightly higher 683 684 than the water requirements calculated in the base case. The calculations used in water 685 requirements resulted in the slight deviation from the value calculated in the base case. Based on 686 the distribution curves, the widest spread of results is still relatively concentrated near the 687 median value; therefore, the results of this study are fairly accurate given the uncertainties of 688 input variables.

	Water use efficiency of HDRD					
	production via fast pyrolysis and			Water use efficiency of HDRD		
	hydroprocessing			production via HTL and hydroprocessing		
	Whole	Forest	Agricultural	Whole	Forest	Agricultural
	tree	residue	residue	tree	residue	residue
Percentil	L H ₂ O/MJ	$L H_2O/MJ$	$L H_2O/MJ$	L H ₂ O/MJ	$L H_2O/MJ$	$L H_2O/MJ$
e	HDRD	HDRD	HDRD	HDRD	HDRD	HDRD
5%	424.89	268.55	74.01	322.31	203.61	52.44
10%	439.77	282.28	76.02	333.41	213.94	53.82
25%	466.18	307.51	79.58	353.16	232.96	56.28
50%	497.72	338.04	83.80	376.74	255.94	59.19
75%	531.36	370.43	88.24	401.99	280.32	62.29
90%	563.18	400.54	92.38	425.92	303.03	65.20
95%	582.75	418.86	94.91	440.69	316.82	66.98

689	Table 13:	Percentile valu	es of uncertainty	v distribution plots
007				

690

691

(Figure 7 here)

692

(Figure 8 here)

693 **5.** Conclusion

694 Water is a precious resource and a large part of water use is from industry. Making the right 695 decisions to reduce water dependency is important for industry to save both the cost and the need 696 to source for water while meeting the growing demand for diesel. This study looked into two 697 pathways to convert lignocellulosic biomass to HDRD and can be used to fill the current 698 research gap in this area. The results of this study show that biomass production is the main 699 determinant of water requirements in producing HDRD from lignocellulosic biomass. More than 700 99.9% of the water used in every conversion pathway and feedstock studied in this paper is used 701 for biomass production; water use in the other unit operations is negligible in comparison. High 702 water use at the biomass production stage shows that choosing biomass with low water demand 703 and better ability to cope in water stress conditions for HDRD production will reduce the impact 704 of water use on the environment. When water consumption is the consideration, agricultural 705 residue feedstock is a better option than the two woody biomass feedstocks studied due to the 706 faster growth rate of agricultural feedstock and overall lower water required for growth 707 compared to trees. When comparing conversion pathways, we find that HTL is more promising 708 with its slightly higher HDRD yield and water requirement savings of 24.4%, 24.4%, and 29.4% 709 for whole tree, forest residues, and agricultural residues, respectively, compared to fast pyrolysis. 710 Although cooling water losses and waste water generation in HTL are higher than those of the 711 fast pyrolysis process, HTL combined with hydroprocessing has a higher HDRD yield that 712 lowers the effective water consumption for HDRD production to a level below that of fast 713 pyrolysis. From this study, biomass production and HDRD yield are found to be crucial factors 714 when determining water use. In Singh and Kumar's (2011) study, water was not allocated in the

production of wheat straw. If it were, Singh and Kumar's water requirements for wheat straw production would give 934.4 L H₂O/dry kg of straw instead of 0L H₂O/dry kg of straw. This would bring the water requirement for ethanol production from wheat straw closer to the findings of water requirements for HDRD production from wheat straw. 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.

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- 880

Figure 1



Figure 1: System boundary of HDRD production via fast pyrolysis

Figure 2



Figure 2: System boundary of HDRD production via hydrothermal liquefaction



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



Figure 4: Sensitivity analysis for conversion to HDRD via HTL and hydroprocessing



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



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





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





Figure 8: Monte Carlo distribution conversion via HTL and hydroprocessing