SUPPLEMENTARY MATERIAL 1: Goal and scope definition

This section presents the detailed information on goal and scope definition of the study.

As mentioned by the UNEP/SETAC guidelines for LCSA, each of the three tools has different aim, but still a consistent goal and scope is recommended when applying the three techniques of LCSA [1].

1. Goal

The goal of this study is to assess the sustainability performance (environmental, economic and social impacts) of HDPE life cycle by Dow Chemical Canada facility in Alberta, Canada. The assessment is based on the application of the three techniques: LCA, LCC and S-LCA. The common goal is to improve the sustainability performance of the product system. Therefore, in this study, each of these tools is applied while considering an integrated approach in mind. The impact results for the three dimensions are identified. Then, an integrated/combined analysis is conducted to analyze the synergies and tradeoffs between the three dimensions' impact results and propose recommendations of sustainability improvements for the case study product.

2. Functional unit

For the current study, the functional unit considered is the production of 1,000 kg of HDPE at Dow Chemical Canada facility. While the results of LCA and LCC are linked to the functional unit, the results of S-LCA conducted by Hannouf and Assefa [2] represented the social performance of the companies responsible for the different processes of the production of HDPE along its life cycle. Relating the S-LCA results to the functional unit could be done by using the working hours. However, as this method was criticized by its relevance to the workers' stakeholder group only and not other groups [3], it was not used by Hannouf and Assefa [2].

3. Reference flow

The reference flow is the amount of raw natural gas (kg), crude oil (kg), processed natural gas (kg), refined petroleum products (kg) and amount of ethylene (kg) required for the production of 1,000 kg of HDPE.

4. System boundaries

Even though differences between the way the techniques handle the actual system do exist [4]. In this study, a similar system boundary for the three techniques has been chosen. The same scope considered in the S-LCA part by Hannouf and Assefa [2] is considered for the other two tools of LCSA which is from cradle-to-gate taking into account extraction and processing of natural gas, extraction and refining of petroleum products, transportation, ethylene production and HDPE manufacture (Please see Figure 1 below). Therefore, the cradle-to-gate life cycle of HDPE is divided into seven phases as shown in Figure 1.

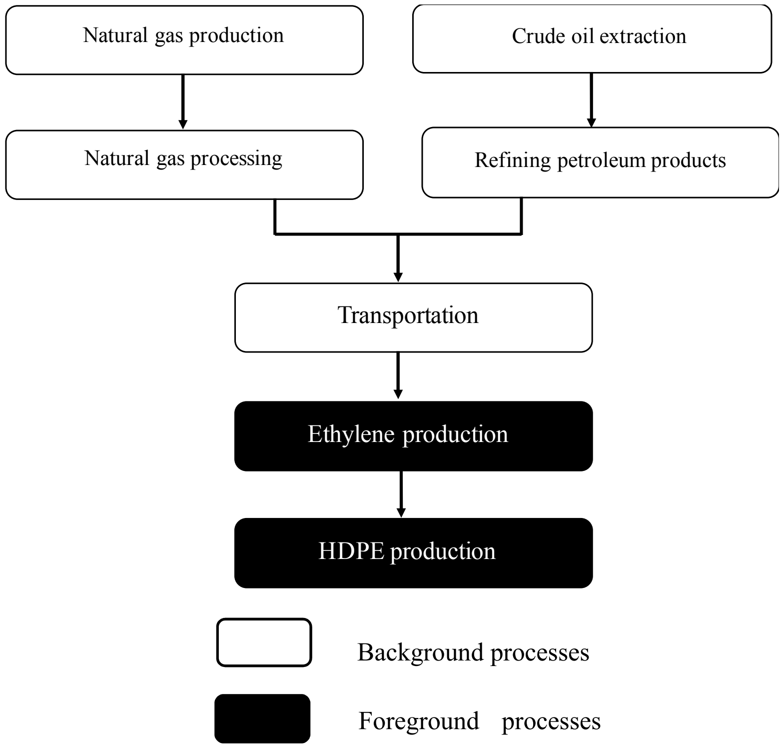

Figure 1. Dividing the production processes of HDPE between foreground and background processes (Based on Hannouf and Assefa [2] and Franklin Associates report, Franklin Associates [5])

Foreground and background processes have been determined. The foreground system includes the operations within the company and in the supply chain for which the company has some level of control. The background system includes the operations outside the control of the company. These were identified specifically for Dow Chemical Canada by using secondary sources such as Dow chemical Canada's website and reports.

HDPE in Alberta is manufactured by steam cracking ethane to produce ethylene mainly from natural gas [6,7]. However, due to data availability issue, it is assumed here that HDPE is produced using natural gas and petroleum products as raw materials.

5. Impact categories

For LCA, the climate change is the only impact category considered in this study as the goal of this research is to guide one of the large GHG emitters in Alberta, Canada "Dow Chemical Canada facility" to develop sustainability improvements along their product life cycle that can reduce GHG emissions while achieving sustainability goals.

For LCC, three types of cost categories are considered: raw materials costs, energy costs and labor costs. Due to data availability issues, all other internal costs such as financial costs, research and development costs, maintenance costs etc. and revenues are not considered.

For S-LCA, all stakeholders and subcategories were considered by Hannouf and Assefa [2] by applying the UNEP/SETAC S-LCA guidelines. However, due to data availability issues at the different levels of data collection for foreground and background processes, evaluation of some subcategories such as working hours, feedback mechanisms and supplier relations was not possible [2].

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SUPPLEMENTARY MATERIAL 2: LCA inventory analysis

This section presents some detailed information on the LCA inventory analysis and transportation calculations.

The environmental life cycle inventory (LCI) of HDPE production is developed taking into account the inputs (e.g. natural gas, crude oil) and outputs (e.g. carbon dioxide (CO2), methane (CH4) and (N2O)) of the stages of HDPE production.

Every effort has been done to search for specific data for Alberta and Canada. Foreground data is collected from a detailed LCI report on types of polyethylene published by Franklin Associates. This report was based on primary data (specifically on polyethylene production and ethylene production) from chemical manufacturers in North America including our case study company here "Dow Chemical". According to the report, the data provided is representative for the majority of North American production [26]. Background data is collected from the US LCI database for Canada and US except the transportation emissions data for petroleum products collected from the Ecoinvent unit processes database due to non available data in the US LCI database.

Based on the report by Franklin Associates, it has been determined that 990 kg ethylene are required for the production of 1,000 kg HDPE. 212.1 kg refined petroleum products and 949 kg processed natural gas are needed for the production of 1,000 kg ethylene.

Adding to this, 1,005 kg raw natural gas are required for the production of 1,000 kg processed natural gas; 1,018 kg crude oil are needed for the production of 1,000 kg refined petroleum products [1].

Using this information, it was calculated that 939.5 kg (rounded to 940 kg) processed natural and 210.4 kg (rounded to 210 kg) refined petroleum products are required for the production of 990 kg ethylene. In addition, it has been determined that about 945 kg raw natural gas can produce 940 kg processed natural gas. About 214 kg crude oil are required for the production of 210 kg refined petroleum products (see Figure 1 below).

Figure 1 presents the flow diagram of the materials inputs for the production of 1,000 kg HDPE.

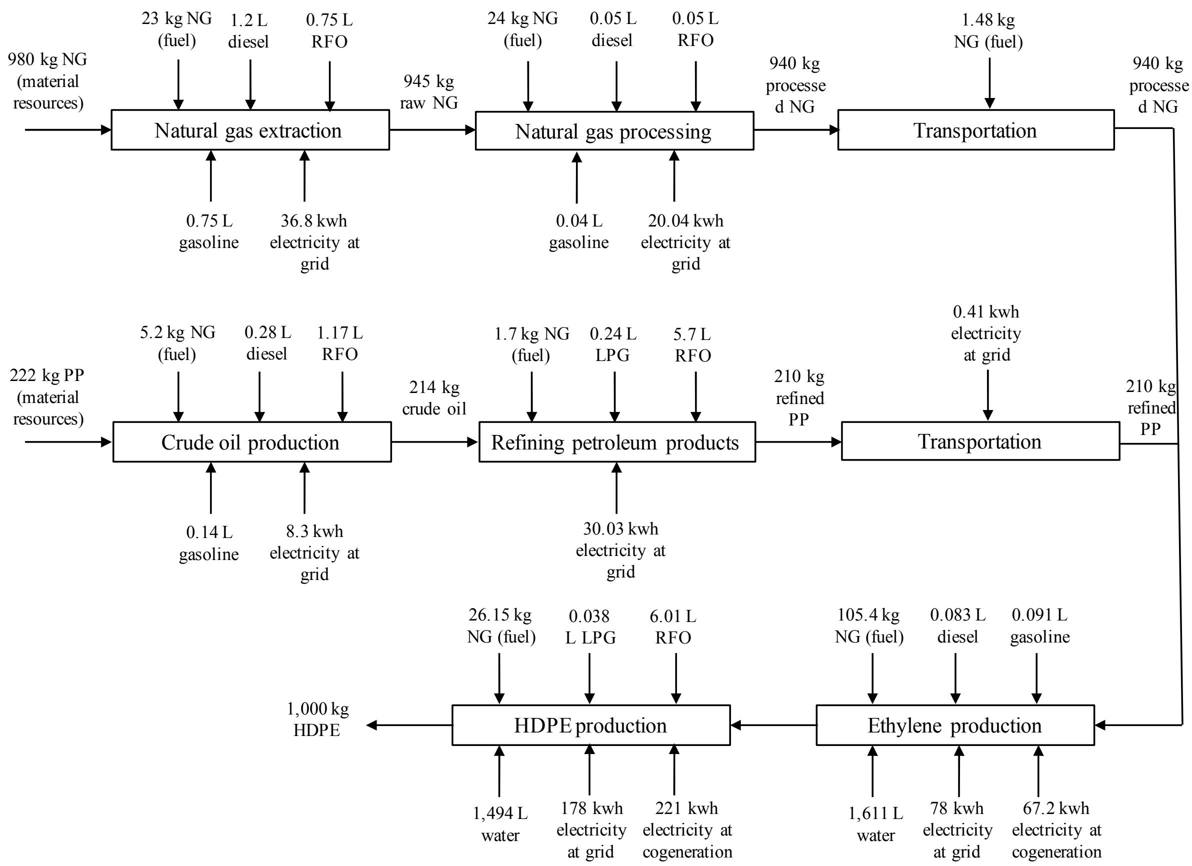

Figure 1. Flow diagram of the materials inputs for the production of 1,000 kg HDPE (calculated based on US LCI database (2016) as cited in Franklin Associates (2011))

(Abbreviations used: NG: Natural gas; RFO: residual fuel oil; LPG: liquefied petroleum gas; PP: petroleum products; L: liter; kwh: kilowatt hours; kg: kilogram)

Table 1 shows the unit processes included in the HDPE production with all inputs and outputs. All inputs and outputs to or from ecosphere and technosphere were organized in a spreadsheet for each stage of the production processes of HDPE.

Table 1. Unit processes of HDPE production with all inputs and outputs

Unit processes	Inputs	Outputs
Natural gas extraction	• Energy • Raw materials	• GHG emissions • Raw natural gas
Natural gas processing	• Raw natural gas • Energy	• GHG emissions • Processed natural gas
Crude oil production	• Energy • Raw materials	• GHG emissions • Crude oil
Refining petroleum products	• Crude oil • Energy	• GHG emissions • Refined petroleum products
Transportation	• Processed natural gas	• GHG emissions

	• Refined petroleum products • Energy	• Refined petroleum products • Processed natural gas
Ethylene production	• Processed natural gas • Refined petroleum products • Energy • Water	• GHG emissions • Ethylene
HDPE manufacture	• Ethylene • Energy • Water	• GHG emissions • HDPE

Transportation distances calculations

Regarding the transportation of processed natural gas from the natural gas plant to the petrochemical company, we conducted some search to determine the specific case for Dow Chemical Canada. We found that Dow Chemical Canada has a long term contract with Keyera (specifically Rimbey gas plant) to supply ethane (processed natural gas) [2]. Some search has been done to determine the transportation system and distance to supply ethane to Dow Chemical Canada. According to Keyera website, a 32 km pipeline was built to transport ethane from Rimbey gas plant to an ethane transportation pipeline system running through Alberta [2]. Then, the transportation distance is estimated from the ethane transportation pipeline system to Dow Chemical Canada facility in Fort Saskatchewan using google maps (144 km).

This was not possible for refined petroleum products, therefore, we assumed a potential supplier and estimated the transportation distance using google maps. Specifically, we are assuming that Repsol oil and gas, Alberta, Canada is the supplier of refined petroleum products and the transportation distance is estimated using google maps from Repsol oil and gas to Dow Chemical Canada facility in Fort Saskatchewan (131.5 km).

These pipelines distances are used to calculate the amounts of GHG emissions associated with transportation of processed natural gas and refined petroleum products. Transportation emissions data is collected from the US LCI database for Canada and US (for natural gas) and from the ecoinvent unit processes database (for petroleum products) after calculation of tonne-kilometers [3].

Calculation of tonne-Kilometers (tkm):

tkm = (Material Weight kg / 1000)*Distance Travelled km

e.g. Natural gas weight = 940 kg

Distance travelled = 176 km

tkm = (940/1000)*176 = 165.44 tkm

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SUPPLEMENTARY MATERIAL 3: LCC inventory analysis

This section presents more detailed calculations and information on the LCC inventory data.

For all processes included in the flow diagram of the HDPE production, the costs of the inputs are calculated according to the functional unit of this study which is "1,000 kg HDPE". The amounts of inputs for each process have been already identified for LCA. These amounts are used to calculate the costs. The selling prices of materials and energy are obtained from online sources (such as Natural Resources Canada; Natural Gas Exchange INC; Direct Energy Regulated Services) [1-3].

Table 1 presents the detailed life cycle inventory (LCI) of energy and raw materials costs along the HDPE production per functional unit (FU).

Table 1. LCI energy and raw materials costs for HDPE

(Note: all costs for raw materials and energy are calculated using the average of 2007-2016 prices whenever data is available. In other case, the costs were calculated using the average of prices of all available previous years)

(Abbreviations used: m³: cubic meters; kwh: kilowatt hours; kg: kilogram)

HDPE processes	Types of inputs	Amounts of inputs per FU	Costs per FU	Source
Natural gas extraction	Raw materials (Natural gas)	980 kg	$146.3	Natural Gas Exchange INC [1]
	Electricity at grid	36.8 kwh	$2.9	Direct Energy Regulated Services [2]
	Natural gas (fuel)	23 kg	$3.43	Natural Gas Exchange INC [1]
	Diesel	1.2 liter	$0.9	Natural Resources Canada [3]
	Residual fuel oil	0.75 liter	$0.35	US Energy Information Administration [4]
	Gasoline	0.75 liter	$0.5	Natural Resources Canada [5]
Natural gas processing	Electricity at grid	20.04 kwh	$1.6	Direct Energy Regulated Services [2]
	Natural gas (fuel)	24 kg	$3.6	Natural Gas Exchange INC [1]
	Diesel	0.05 liter	$0.04	Natural Resources Canada [3]

	Residual fuel oil	0.05 liter	$0.023	US Energy Information Administration [4]
	Gasoline	0.04 liter	$0.028	Natural Resources Canada [5]
Crude oil production	Raw materials (petroleum)	222 kg	$124	Alberta Energy [6]
	Electricity at grid	8.3 kwh	$ 0.66	Direct Energy Regulated Services [2]
	Natural gas (fuel)	5.2 kg	$ 0.78	Natural Gas Exchange INC [1]
	Diesel	0.28 liter	$ 0.21	Natural Resources Canada ([3]
	Residual oil	0.17 liter	$ 0.080	US Energy Information Administration [4]
	Gasoline	0.14 liter	$ 0.01	Natural Resources Canada [5]
Refining of petroleum products	Electricity at grid	30.03 kwh	$ 2.4	Direct Energy Regulated Services [2]
	LPG	0.24 liter	$ 0.18	Natural Resources Canada [3]
	Natural gas (fuel)	1.7 kg	$ 0.25	Natural Gas Exchange INC [1]
	Residual fuel oil	5.7 liter	$ 2.7	US Energy Information Administration [4]
Transportation processed natural gas	Fuel (natural gas)	1.48 kg NG	$0.22	Natural Gas Exchange INC [3]
Transportation refined petroleum products	Fuel (electricity)	0.41 kwh	$0.03	Natural Gas Exchange INC [3]
Ethylene production	Electricity at grid	78 kwh	$6.2	Direct Energy Regulated Services [2]

	Electricity at cogeneration[1]	67.2 kwh	$5.3	Direct Energy Regulated Services [2]
	Natural gas (fuel)	105.4 kg	$15.74	Natural Gas Exchange INC [3]
	Diesel	0.083 liter	$0.062	Natural Resources Canada [3]
	Gasoline	0.091 liter	$0.063	Natural Resources Canada [5]
	Water	1,611 liter	$2.54	Alberta Utilities Commission, Corix Utilities Inc. [7]
	Processed natural gas[2]	940 kg	$230	Alberta Energy [8]
	Refined petroleum products[3]	210 kg	$117.6	Alberta Energy [8]
HDPE manufacture	Electricity at grid	178 kwh	$14.2	Direct Energy Regulated Services [2]
	Electricity at cogeneration	221 kwh	$18	Direct Energy Regulated Services [2]
	Natural gas (fuel)	26.15 kg	$3.9	Natural Gas Exchange INC [3]
	Residual fuel oil	6.01 liter	$2.82	US Energy Information Administration [4]
	LPG	0.038 liter	$0.0285	Natural Resources Canada [9]

[1] Assumed to be electricity at grid rate due to data availability issues
[2] Assumed ethane price
[3] Assumed naphtha price

	Water	1,494 liter	$2.36	Corix Utilities Inc, Alberta Utilities Commission [7]

Labor costs are also calculated for every process and presented in Table 2.

Table 2. Labor costs for all processes of HDPE production per functional unit

HDPE processes	Labor cost per hour (Alberta government [10])	Labor costs per FU
Natural gas extraction	$40.81	$0.07
Natural gas processing	$40.81	$0.48
Crude oil production	$40.81	$0.002
Petroleum products processing	$40.81	$0.006
Transportation (processed NG)	$29.31	$0.45
Transportation (refined petroleum products)	$29.31	$0.001
Ethylene production	$29.38	$0.107
Polyethylene manufacture	$29.38	$0.166

Labor costs are calculated using the production capacity per year from potential assumed companies across the life cycle and labor cost per hour from Alberta Government [10]. Table 3 is an example of the labor cost calculations for ethylene production process:

Table 3. Labor cost calculation for ethylene production process
(Abbreviations used: kt: kilotonnes; kg: kilogram; $: dollars)

Ethylene production	**Value**	**Unit**	**Source**
Production capacity per year for Dow Chemical Canada facility at Fort Saskatchewan	1,304	Kt	Dow Chemical Canada
Production capacity in kg per year	1,304,000,000	kg	
Assuming:			
300 days of work per year			
4800 hours of work per year with two shifts of workers for 8 hours per shift			
Number of hours needed to produce 990 kg of ethylene	0.003644172	hours	

Labor cost per hour for manufacturing sector	29.38	$/hour	Alberta Government [10]
Labor cost per FU	0.107	$	

Total costs for each process are presented in Table 4. An aggregation of the costs from the different perspectives along the cradle-to-gate life cycle of HDPE is calculated.

Table 4. Total costs for all HDPE processes

HDPE processes	Total costs
Natural gas extraction	$153.55
Natural gas processing	$6
Crude oil extraction	$126
Refining petroleum products	$5.53
Transportation	$0.7
Ethylene production	$378
Polyethylene production	$42
Total costs	$712

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