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Comparison of Steel Manufacturing Off-Gas Utilization Methods via Life Cycle Analysis

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Abstract

This study utilizes life cycle analysis to compare three steel manufacturing off-gas utilization systems: a status quo system, which produces electricity via a low-pressure steam turbine; a combined cycle power plant (CCPP) system, which produces electricity using gas and steam turbines; and a methanol (MeOH) system, which converts coke oven gas (COG) and blast furnace gas (BFG) into MeOH (CBMeOH). This research seeks to compare the environmental impacts of each system based on equivalent raw material inputs. Since the systems have different products, system expansion is used to ensure that they have the same outputs and are therefore comparable. The system boundary consists of a combination of cradle-to-gate and gate-to-gate boundaries. The environmental effects of each system are compared at five locations—Ontario, the USA, Finland, Mexico, and China—using TRACI, CML-IA baseline, ReCiPe2016, and IMPACT2002+ in SimaPro v9. The results show that in Ontario, Finland, and China, CBMeOH systems had the lowest environmental impact, while the CCPP system had the lowest impact in the USA and Mexico. The status quo system had the greatest environmental impact for all of the studied locations, except for the USA. This environmental assessment, combined with previous economic analysis, demonstrates that the CBMeOH system is the optimal choice in Ontario, and China. In the USA, plants might be better off adopting CCPP systems when carbon taxes reach $50/tonne. For Mexico, the CCPP system is the most environmentally friendly choice, while the CBMeOH system is the most profitable. Finally, the results indicate that status quo systems are not recommended in Mexico or China in any foreseeable circumstance.

Keywords: coke oven gas, blast furnace gas, life cycle analysis, combined cycle power plant, methanol production.

1. Introduction

Steel manufacturing off-gas mainly consists of coke oven gas (COG), blast furnace gas (BFG), and basic oxygen furnace gas (BOFG). COG and BFG are continuously produced throughout the manufacturing process, while BOFG is only produced intermittently. COG has relatively greater higher heating value (HHV) compared to BFG and BOFG, while BFG is produced in the greatest quantities. In general, the life cycle of COG and BFG during the steelmaking process consists of four main stages [1]. First, they are used for constant consumption in various milling processes, such as sintering, coking, and blast furnace processing. Second, the surplus gas from these processes is then stored in gas holders for future use. Third, if the quantity of surplus gas is large enough, it will be used to produce electricity via a built-in power plant. Finally, any remaining gas is burned and emitted into the atmosphere, which is an undesirable outcome. The four stages of off-gas utilization methods might not be the best option, as they result in high CO_2 emissions and low energy recovery efficiency. Given this, considerable research on steel manufacturing off-gas valorization has been conducted to develop more effective methods of reducing CO_2 emissions and increasing energy recovery efficiencies. As noted by Deng and Adams, steel manufacturing off-gass is most commonly used to generate electricity via combined cycle power plants (CCPP) and for methanol (MeOH) synthesis [2] [3]. Deng and Adams analyzed the economic feasibility and CO_2 emissions of these two systems, and found that, due to a variety of factors, it was economically advantageous to build CCPP and MeOH plants in some countries, but not in others. This was demonstrated in a prior study by Deng et al.[3] wherein coke oven gas (COG) and blast furnace gas (BFG) were used to synthesize MeOH (called the CBMeOH process). As their results showed, lower MeOH market prices do not necessarily result in lower net present value (NPV) because NPV is impacted by lots of other factors, such as electricity price, carbon tax, electricity carbon intensity, power purchasing parity, and income tax. For example, although China has lower MeOH prices than the USA, retrofitting plants with CBMeOH systems will yield a much higher NPV within a Chinese setting. However, this study only consisted of a gate-to-gate analysis, which meant that it had some deficiencies. For example, it did not consider the related upstream carbon footprint. Additionally, since the products of each system were different, it was not possible to compare them directly. Finally, it did not consider other categories of environmental impact aside from greenhouse gas (GHG) emissions. Hence, it is desirable to do a thorough life cycle analysis (LCA).

The literature contains numerous LCAs of power co-production in steel plants and methanol production from COG. For example, Li et al. [1] conducted an LCA of a steel plant that had been outfitted with a combined cycle power plant. Specifically, they compared the results of a gate-to-gate LCA for this system to those of a coal-powered system that produces the same amount of electricity and steel off-gas, which is burned without energy recovery. The LCAs in this study were conducted using eBalance software, which is produced in China and uses data that is specific to a Chinese context. The results showed that, in producing the same amount of electricity, the steel plant with the combined cycle power plant used 54% less energy and emitted 29% less CO_2 than the other coal-powered system. Li's et al.'s LCA showed that building a CCPP plant in China would help to reduce CO_2 emissions. However, they did not factor in equivalent amounts of electricity from China's electricity grid. In addition, Li et al.'s LCA lacked data regarding other envrioenmental effect, such as acidification and eutrophication.

Several research groups have also conducted LCAs of methanol production from coal, COG, and NG [4-6]. Both Lee et al. [4] and Chen et al. [6] found that using COG to produce MeOH is cleaner than using coal, with NG being the cleanest option of the three. Similarly, Li et al. [5] performed LCAs for methanol production from coal gasification and coal-coking-produced COG, and found that the COG method was much cleaner than coal gasification. Other research groups, such as Ou et al. [7], have performed LCAs on the conversion of steel mill off-gas to ethanol via fermentation, and compared them to LCAs of traditional petroleum gasoline to ethanol conversion. As their results show, fermentation is capable of reducing GHG emmisions by approximately 50%, and requires significantly less fossil fuel consumption (0.51-0.74 MJ fossil fuel/MJ ethanol) than the conventional method (1.34 MJ fossil fuel/MJ ethanol). The above-mentioned COG-to-MeOH process [4-6] uses the traditional method, which acquires the additional CO_2 required for adjusting the H_2/CO mole ratio via coal gasification or CO_2 recycled from the MeOH synthesis process. However, in this work, BFG is used as an additional CO_2 source, which is a novel contribution. In addition, the proposed CBMeOH system's desulphurization process is much shorter than the traditional two-stage hydrodesulfurization process [3]. While prior studies have conducted LCAs of methanol production from COG [4-6], this is the first work to conduct an LCA of a CBMeOH plant.

Although the findings of the prior studies indicate that the production of electricity or methanol using off-gas from steel production is cleaner than traditional methods, it is unknown whether these processes are more environmental friendly given equivalent amounts of off-gas. To the best of our knowledge, no one has ever conducted LCA comparisons of the status quo, CCPP, and CBMeOH systems with equal levels of COG. Furthermore, the impact of factors such as the acquisition of raw materials, transportation distances, and traditional methanol production processes all vary based on the location of the plant. Thus, this research uses LCAs to understand the environmental impact of the status quo, CCPP, and CBMeOH systems in five locations: Ontario, the USA, Finland, Mexico, and China.

2. Systems Description and Methods

The status quo system used in this research is based on the off-gas utilization method used by ArcelorMittal Dofasco (AMD), located in Ontario, Canada. AMD's approach to off-gas utilization involves combusting the COG in order to boil low-pressure water into steam, which is then fed into the low-pressure steam turbine to generate electricity. Electricity is the only product of the status quo system.

The CCPP system uses the same amount of COG as the status quo system for electricity generation. However, instead of combusting the COG directly, the CCPP system uses MDEA desulphurization to remove bulk H_2S. In this process, the COG is compressed before being fed into the MDEA absorber to produce sweet COG, which leaves the stripper at about 16 bar, and with a sulfur content reduced to less than 1 ppmv. Next, the sweet COG is fed into a combustor to react with compressed air, creating combusted high-pressure exhaust gas which is passed through a gas turbine to generate electricity. After passing through the gas turbine, the exhaust gas still contains a high amount of thermal energy (temperature around 650 ℃), which is subsequently recovered using process water and low-, intermediate-, and high-pressure steam turbines. This process allows for a maximum amount of energy to be recovered. Optimizing the volume of process water is critical, as it enables the NPV of the CCPP system to be maximized. The results show that the CCPP system produces over twice as much overall electricity as the status quo system. As with the status quo system, electricity is the only product of the CCPP system.

The CBMeOH system uses the same amount of COG as the status quo and CCPP systems. However, unlike the status quo and CCPP systems, the CBMeOH system also uses BFG as raw material. Furthermore, the CBMeOH system also requires the COG to undergo fine desulphurization. Instead of the two-stage hydro desulphurization process used in the commercialized method, the CBMeOH system uses an energy-intensive CO_2 and steam reforming (CSR) process that not only cracks the methane in the COG into H_2 and CO, but that also breaks and converts the thiophene into H_2S. Following this CSR process, the converted H_2S is removed using a middle-temperature sulfur-removal process. The CO_2 recovered from the BFG via Rectisol is used as an additional carbon source, with the volume being adjusted to convert the methane in the COG, as well as to adjust the $(H_2\text{-}CO_2)/(CO+CO_2)$ molar ratio. Next, prepared syngas is supplied to a typical boiling water reactor for MeOH synthesis. Most of the unconverted syngas is recycled to the MeOH synthesis reactor, while the remainder is combusted and used in a gas turbine to produce electricity. The thermal energy created by the exhaust gas exiting the turbine is further used to preheat the water used in the boiling reactor for MeOH synthesis, and to control the reaction temperature. In this system, the remaining BFG (mainly CO, H_2, and N_2) contains a large amoung of energy, and is capable of providing the same amount of heat downstream as the status quo method. The major product of this system is MeOH, but it is also capable of recovering some heat. However, the CBMeOH system is reliant on electricity from the grid, as it only produces a small amount on its own.

The different products produced by the three systems poses a challenge, as a comparison of their relative environmental impacts requires the same outputs. This issue is addressed by using system expansion, which is detailed in Section 2.1. In addition, SimaPro V9 is used to conduct the life cycle analyses and comparisons of the environmental effects of the status-quo, CCPP, and CBMeOH systems. The LCA methods utilized in this work are in accordance with ISO 14040, which contains four main steps: goal and scope definition, inventory analysis, impact assessment, and interpretation.

2.1. Goal and Scope Definition

The goal of this study is to use LCA to compare the environmental effects of three different systems available to steel manufacturers. These results will expand upon the findings of previous economic analyses, and help steel plant operators select the most optimal off-gas utilization method. As such, this work's main target audience is steel manufacturers. The functional units used in all three systems are the combined co-products of 1 MWh of electricity and 1.37 MWh of heat.

The system boundary of this work is a combination of 'cradle-to-gate' and 'gate-to-gate' boundaries. Since the aim of this work is to analyze retrofitting options for AMD's off-gas utilization systems, the upstream production of raw material, COG, and BFG is irrelevant. Consequently, the mining and transportation of coal, the making of coke, the removal of tar, benzene, ammonia, and other compounds from COG, and the BFG produced by the steel plant will all be considered the same for all three scenarios. In this respect, a gate-to-gate boundary is sufficient. However, further traceback is required with respect to NG, electricity, oxygen, steel, solvent, and catalyst, as each of the three systems uses different amounts of these utilities and materials. Therefore, a cradle-to-gate boundary is also needed in order to consider these pathways.

Another issue that must be considered when drawing the system's boundary is where the system ends, and what falls inside or outside of the boundary. The status quo and CCPP system only use COG from steel manufacturing, while the CBMeOH system uses both COG and BFG. Additionally, the three systems have different products: the status-quo and CCPP systems produce electricity only, while the CBMeOH system produces MeOH and heat, but no electricity output. In order to conduct a fair comparison, it is critical to consider the same amounts of raw COG and BFG, and the same products for each system. In this study, both COG and BFG are taken into consideration, and the considered products are the amount of electricity and heat produced by the status quo system with an expansion. The detailed system boundaries are illustrated in Figures 1 to 3. The inputs for the status quo system (Figure 1) mainly consist of COG, water, and air, with BFG serving as the system expansion material, while the outputs include electricity, heat, and emissions into the atmosphere.

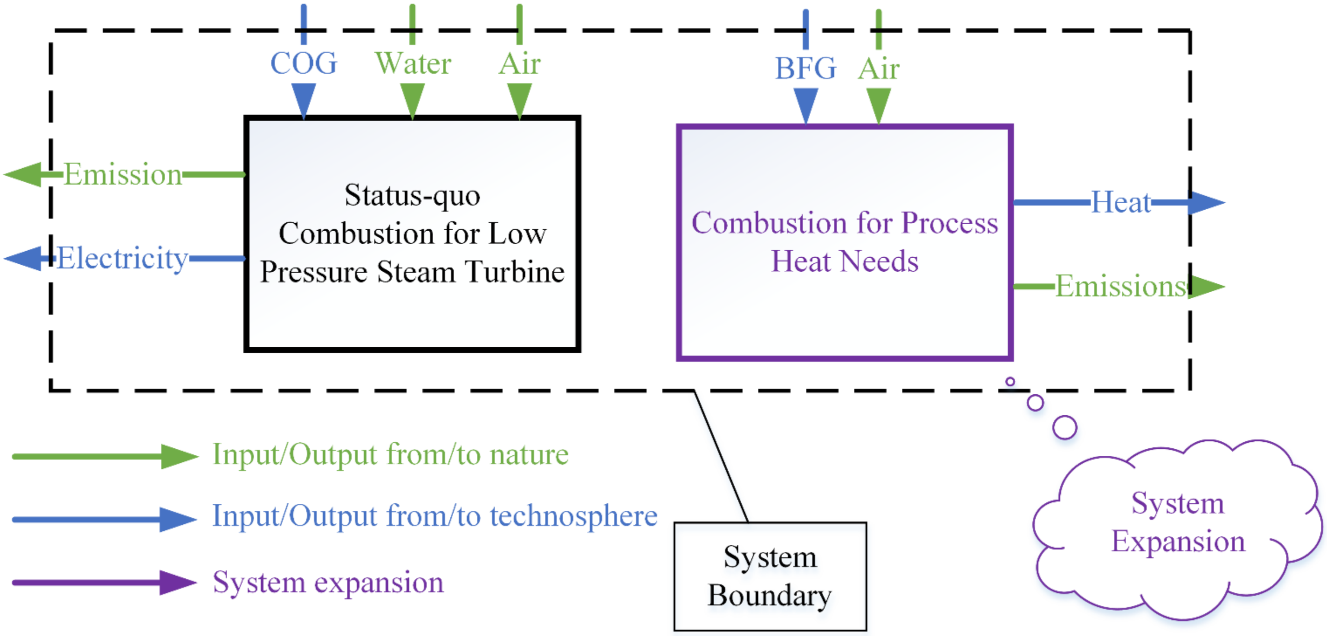

Figure 1. Status-quo COG utilization boundary

As shown in Figure 2, desulphurization is one of the major processes in a CCPP system. The major raw materials used in the CCPP system are COG and BFG, with NG serving as the heating utility for the desulphurization process. The cradle-to-gate environmental effects of NG and steel are represented by the dashed box. The Claus process is a waste treatment process. As can be seen in Figure 2, the upstream environmental effects of the oxygen supplied in this process are also included.

Compared to the COG flow rate, only a very small amount of MDEA is used as solvent in COG desulphurization (less than 1%). Thus, no further tracing back is considered. System expansion that combusts the same amount of BFG used as a carbon source in CBMeOH was also used. This system expansion is shown in purple in Figure 2. The major products of the CCPP system are electricity and heat.

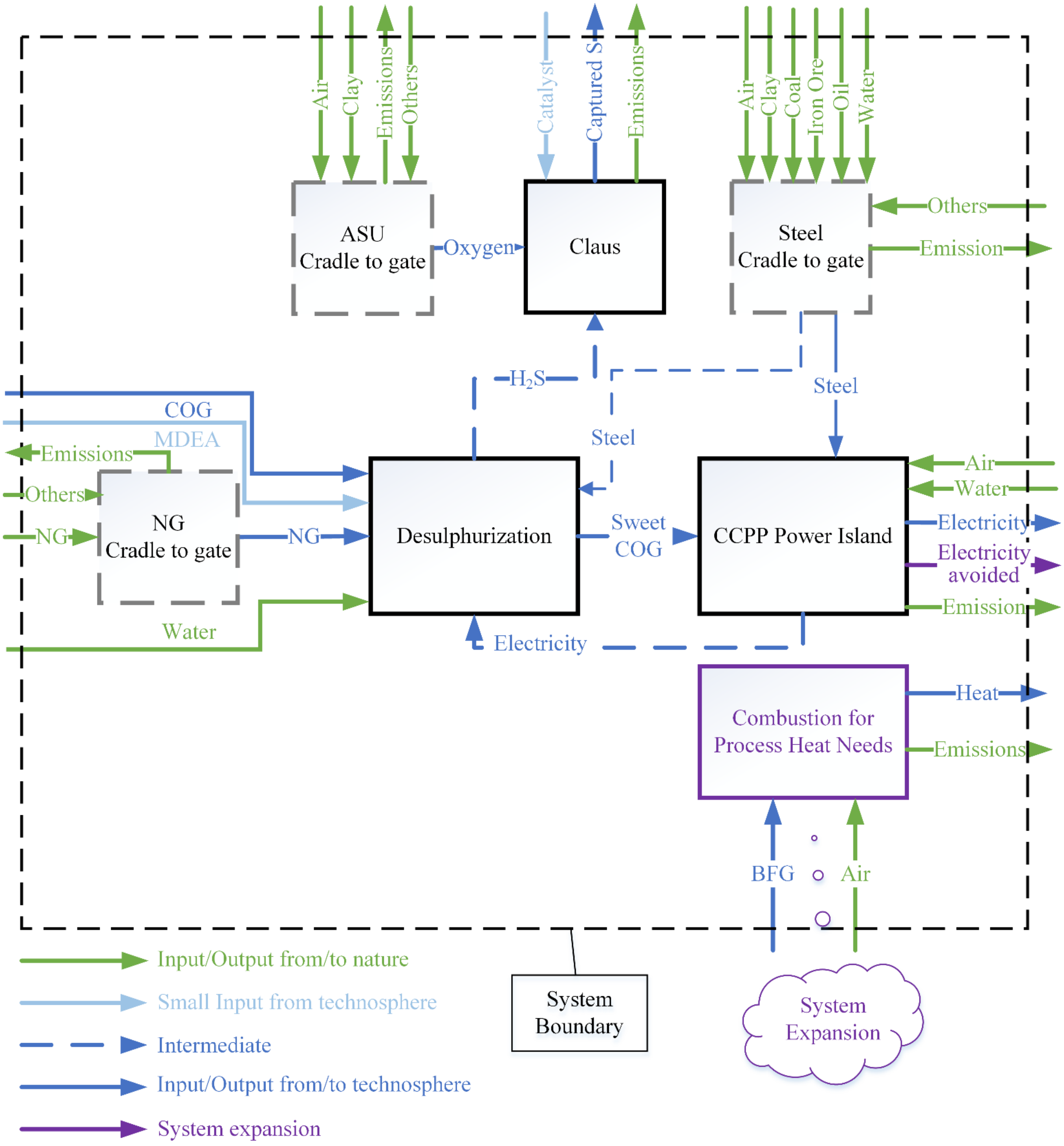

Figure 2. CCPP System boundary.

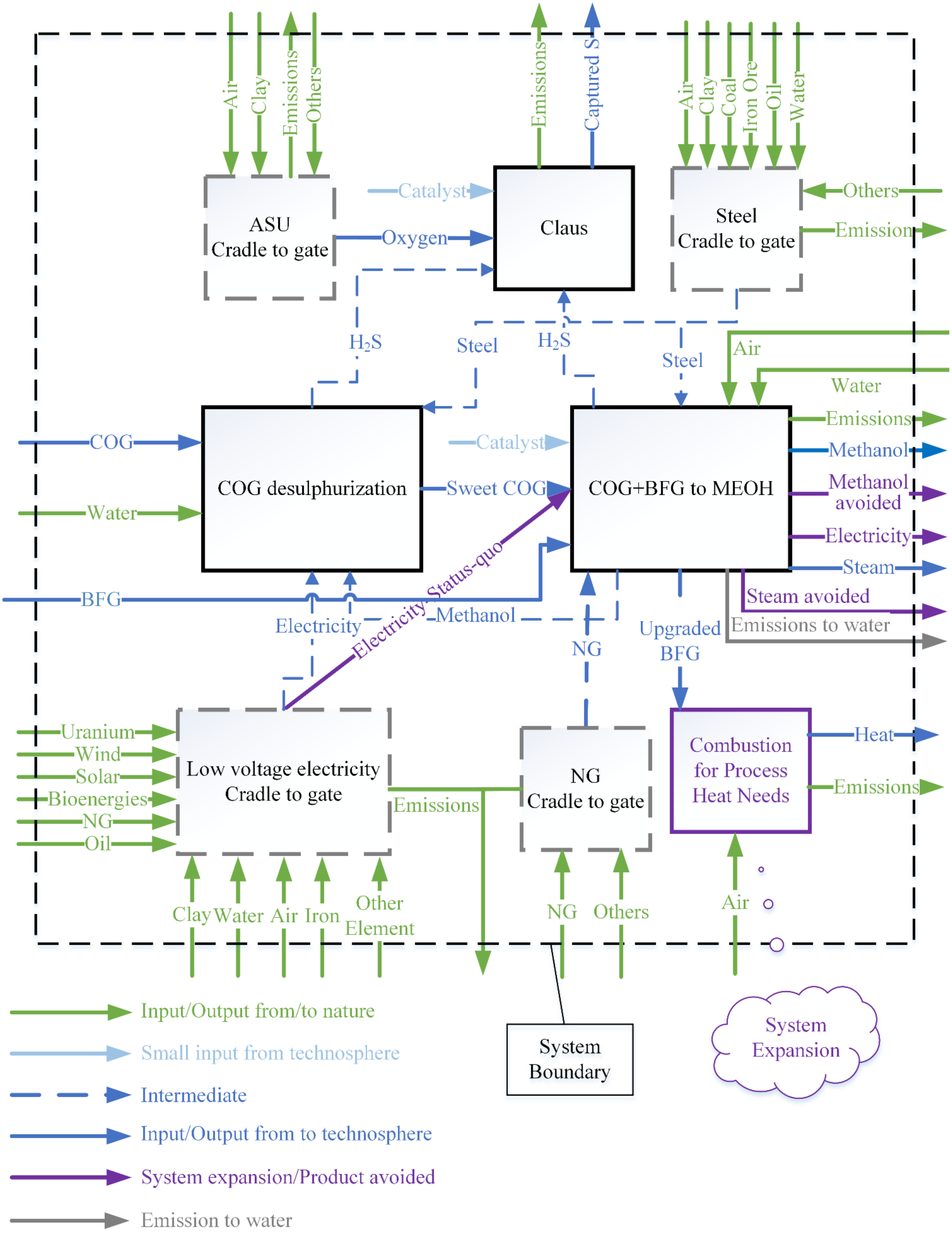

Figure 3. COG + BFG to MeOH system boundaries

The major inputs for the CBMeOH system are COG, BFG, air, water, NG, and electricity. The solvent used in the Rectisol process (methanol) is an intermediate of the system's products, while NG serves as the heating utility for the reboiler and process steam. The cradle-to-gate environmental impacts of steel, oxygen, NG, and electricity are also considered. As with the CCPP system, system expansion is used to enable an adequate comparison between the CBMeOH system and the status quo system. The same amount of electricity is consumed from what is assumed to be the local grid, and the same amount of methanol and steam is assumed to be produced as product avoided. Even though the CBMeOH system uses BFG as a carbon source, the heat rate of the remaining BFG remains the same as the original BFG, as up to 97.6 wt.% purity of CO_2 is removed from it. The other 2.4 wt.% mainly consists of H_2O in the removed CO_2 stream [3]. Hence, the upgraded BFG can still provide the same amount of heat when combusted in the downstream process. The major output of the CBMeOH system is electricity and heat.

The use of system expansion ensures that the three systems produce the same amount of COG and BFG from steel manufacturing, and the same products, namely, electricity and heat. Thus, the three systems are now comparable.

2.2. Life Cycle Inventory

The process data inputs and outputs for each system were consistent with those used in our prior work. Input and output data not included in the previous model, such as the cradle-to-gate impacts of NG, steel, electricity, and traditional MeOH, were obtained from the Ecoinvent v3.5 database in order to ensure the highest possible level of accuracy. We adhered to the ISO 14044 standard cutoff for material or energy flow comprising < 1% of the total input, which is not considered when evaluating the system, as the environmental impact of these streams is minimal [8]. In total, less than 5% of the input was unaccounted for.

In this work, the total catalyst used in the reactors for the CBMeOH process was less than half of the total fixed capital equipment [3], which in in turn is a trivially small percentage of the total mass consumed by the system over its lifetime (about 0.035%). As such, the effects of catalyst manufacturing are not accounted for in this analysis. The total amount of solvent required for the Rectisol process is also small, since it is continually regenerated, and the MeOH that is produced during the process can be used for the relatively small amount of makeup solvent required. Hence, the environmental impacts of the solvents in the Rectisol process are considered to be intermediate, and are calculated according to linear correlation to the process described by Sun et al. [9]

The difference between the three systems is largely related to the equipment used in each. For example, the status-quo system only requires a combustor, a pump, a heat exchanger, a steam turbine, and a condenser. In contrast, as described in a previous paper, the CCPP system requires six heat exchangers, three steam turbines, three pumps, one gas turbine, three compressors, two distillation columns, one reboiler, and two condensers. The CBMeOH process uses two distillation columns, one reboiler, two condensers, one CSR, one MeOH synthesis reactor, two flash drums, four compressors, one gas turbine, one stack, and eight heat exchangers. The environmental effects associated with the equipment used in these processes are modeled in a first-order model, which only considers the production and transportation of materials.

A Claus process is used in both the CCPP and CBMeOH processes for treating H_2S waste. The main inputs for the Claus process are oxygen, sour gas, and boiler feed water, while the products are solid sulfur, low-pressure steam, high-pressure steam, and tail gas. The materials and energy required for the furnace, reheating, and condenser utility were calculated using a linear correlation, which was detailed in a previous study by our group [10].

The wastewater from the CBMeOH plant contains trace amount of CO, CH_4, C_2H_2, H_2S, CH_4O, C_2H_4, SO_2, C_2H_6O, and $C_2H_4O_2$. Those organic and sulfide components‘ environmental impact are considered as emissions to water.

The electricity used in steel manufacturing is a mixture of medium-voltage and low-voltage electricity [11]. For simplification and conservation, this study assumes that all electricity used is low voltage. However, the emissions and losses associated with the conversion from medium- to low-voltage electric power are also considered.

Databases were carefully chosen in order to obtain the most representative information on heat avoided, NG, and methanol avoided for each location. With respect to heat avoided, due to lack of more representative data, the European database (RER) was selected for all locations except for China, as the global database offered the most representative data for this location. For NG and methanol avoided, the USLCI database was selected for Ontario, USA, and Mexico. For Finland, the RER database was used for NG avoided, while global market data was used for methanol avoided. For China, global market data was used for NG avoided, while methanol avoided data was obtained from the literature. In fact, IKE (Short name of Integrated Knowledge of our Environment) has developed life cycle analysis software, known as eBalance, which is based on Chinese data and normalization references. eBalance features a China-based life cycle database for methanol production [12] specifically. However, the data are not publically accessible. According to the literature, 58% of China's methanol supply is derived from coal-to-methanol (CTM), of which 17% comes from COG-to-methanol (COGTM), and 14% is produced via NG-to-methanol (NGTM). The remaining 11% is generated due to the coproduction of ammonia and methanol (CAM) [5], most of which is the result of coal conversion [13]. The rate of methanol to ammonia is adjustable and varies from plant to plant. For example, Li et al. [14] indicate that 4.5 million tonnes of methanol are produced for every 4.5 million tonnes of ammonia that are produced. Thus, according to Li et al., the methanol to ammonia ratio (MTA) is 1:1, though it can be as low as 0.201 [15]. In general, the environmental impact allocation in the CAM system is either based on mass or energy. As such, methanol produced via the CAM system will have a relatively lower environmental impact than methanol produced by the CTM method, as part of the burden is taken up by ammonia. There is no database regarding ammonia produced from coal, nor is there any literature regarding LCAs of the coproduction of ammonia and methanol from coal. This could be an interesting subject of study for future work. For now, however, we assume that the 11% of methanol produced via the CAM system has the same environmental impact as the methanol produced via the CTM system. Although Li et. al.'s [5] study on the cradle-to-gate life cycles of coal-to-methanol (CTM) and coke-oven-gas-to-methanol (COGTM) provides with detailed data on these methods, it does not provide data for the NG-to-methanol (NGTM) method. For this reason, Chen et al.'s [6] data was used for the NGTM method, as it was the most accurate data available.

Based on the above discussion, the following assumptions were made with respect to data utilization:

1. It is assumed that there are no upstream environmental effects associated with the raw material COG and BFG.
2. The Rectisol process for BFG washing mainly removes CO_2 and H_2S in the stream. Given that the change of energy in the upgraded BFG stream is negligible, we assume that the upgraded BFG in the CBMeOH system can produce the same amount of heat as the status quo and CCPP processes.
3. It is assumed that the retrofitted CCPP and CBMeOH plants are mainly constructed of steel. As such, the cement required for construction is not considered. Since the status quo system already exists in the plant, no construction is required. Hence, we assume that there is no construction footprint for the status quo system.
4. The weight of the construction materials used for the CCPP and CBMeOH plants is less than 0.03 wt.% and 0.07 wt.% of the total COG and BFG inputs over the process lifetime of 30 years. According to ISSO 1440, these materials can be

discounted, as they account for less than 1% of the total input. However, we consider the cradle-to-gate environmental impact of the required construction material, as it is one of the main areas of difference between the three studied systems.

5. The CBMeOH system requires the following amounts of catalyst each year: 73 tonnes for MeOH synthesis, 16.2 tonnes for the CSR unit, and 2867.7 tonnes for MTSR [3]. Assuming the catalyst is regenerable, the total weight required would be approximately 3 ktonnes over a plant lifetime of 30 years, or about 12.32 kg/h, which accounts for 0.7% of the CBMeOH system's total input. According to ISSO 1440, the cradle-to-gate environmental effects of the required catalyst can be neglected; however, we still account for their transportation footprint.
6. The makeup of the MDEA solvent is 7.03E-6 kg/kg COG. Thus, the effects related to the production and transportation of MEDA are neglected.
7. In order to compare the three systems, the extra electricity produced by the CCPP system is subtracted from electricity avoided from the grid, while the extra methanol produced by the CBMeOH system is subtracted from methanol avoided.
8. Although the COG and BFG are produced on site, the transportation of the process water that is required for the systems must be considered. However, as AMD is located on the shore of Lake Ontario, it can reasonably be assumed that the transportation impact for process water is zero. Given this, it is assumed that the steel plants in the other locations are located close to water resources as well.
9. The USLCI database is used for NG as utility and methanol avoided for the North American locations (Ontario, USA, and Mexico).
10. For Finland, the RER database is used for NG utility, while global data is used for methanol avoided.
11. For China, global data is used for NG as utility, while methanol avoided LCI data is obtained from two papers: CTM and COGTM from Changhang Li et al. [5], and NGTM from Chen et al. [6].
12. CAM in China comes from coal sources. The environmental impact of methanol in this process is assumed to be the same as in CTM.
13. Steel is assumed to be the main material required to construct the desulphurization, CCPP, COG desulphurization, and COG+BFG to MEOH plants. Thus, the cement required for the construction of these plants is not considered.
14. Combustion mainly provides heat for downstream processes, and it is assumed that the combustion chamber already exists in the steel plant. Hence the construction of the combustion chamber is not considered.

The detailed input and output data for each of the three systems are shown in Table 1. The input and output data listed in the table are directly related to the three systems (gate-to-gate), and do not consider any upstream factors. This means that the heat from NG, electricity, methanol avoided, and transportation are based on the cut-off data in the database. No details regarding the production of electricity are provided.

Table 1. Flow of elements into and out of the system boundaries based on functional units of 1MWh of electricity and 1.37 MWh of heat.

	Status quo	CCPP	CBMeOH	Unit
System Input				
COG	624	624	624	kg
BFG	0	0	2088	kg
Air	17791	17791	3413	kg
One-time process water for power generation (Recyclable)	1.67×10^{-5}	1.67×10^{-5}	0	m^3
Electricity from grid	0	0	1.34	MWh

Electricity from internal	0	0.13	0.86	MWh
Water for solvent	0	0.006	0	m^3
Heat from NG	0	23.5	40.7	MWh
MeOH from internal	0	0	0.42	kg
Refrigerant	0	0	0.062	MWh
Steel	0	0.35	0.79	kg
Steel transport, freight, Ontario	0	0.53	1.18	tkm
Catalyst transport, freight, Ontario	0	0	4.12×10^{-5}	tkm
Water for synthesis	0	0	0.4	m^3
Water for cooling	0		13.48	m^3
MDEA make up	0	0.004	0	kg
System Output				
Electricity product	**1**	**1**	0	MWh
Electricity to internal	0	0.133	0.86	MWh
MeOH	0	0	835	kg
System expansion				
Input				
BFG	2088	2088	0	kg
MeOH avoided	0	0	835	kg
Heat avoided from the process	0	0.37	2.31	MWh
Electricity avoided	0	1.04	0	MWh
Output				
Heat from BFG combustion	**1.37**	**1.37**	**1.37**	MWh
Electricity product, the same as status quo	0	0	**1**	MWh
Emissions to air				
Sulfur dioxide	13.69	0.71	3.50×10^{-6}	
CO_2 from process	995	995	402	kg
CO_2 from BFG as source	1368	1368	756	kg
Hydrogen	0	0	0.012	kg
Water	0	0	287	kg
Nitric oxide	0	0	4.22	kg
Nitrogen dioxide	0	0	0.14	kg
Emissions to water				
Methanol	0	0	0.001	kg
Ethanol	0	0	6.2×10^{-7}	kg
Methyl formate	0	0	4.0×10^{-9}	kg
Waste treatment: Clause process				
Acid input				
O_2 (99.44 wt.% purity)	0	3.4	3.7	kg
Boiling feed water	0	22.3	24.7	kg
H_2S content in acid gas	0	7	7.7	kg
CO_2 content in ACID gas	0	13	14.4	kg
N_2 content in ACID gas	0	3.2	3.5	kg

CH_4 content in ACID gas	0	3.1×10^{-6}	3.4×10^{-6}	kg
Total heat required (heater) (NG for temp. >200C)	0	2.6	2.9	kWh
Total heat required(utility) (NG)	0	0.17	0.2	kg
Total heat removed (utility) (steam 45 bar production)	0	22.3	24.7	kg
Total heat removed (condenser) （steam)	0	18.1	20	kWh
Output				
solid sulfur	0	6.4	7.13	kg
tail gas H_2S content	0	0.17	0.19	kg
Sour water total (H_2S content)	0	0.0002	0.0002	kg
Sour water total (NH_3 content)	0	0.0002	0.0002	kg
Sour water total (CO_2 content)	0	0.006	0.006	kg
Sour water total (SO_2 content)	0	5.7×10^{-14}	6.3×10^{-14}	kg
Sour water total (COS content)	0	1.2×10^{-7}	1.3×10^{-7}	kg
Sour water total (CH_4 content)	0	1.1×10^{-6}	1.2×10^{-6}	kg
Sour water electricity required	0	1.8×10^{-5}	2.0×10^{-5}	kWh

Table 1 shows the raw materials and elements from the environment and energy inputs from the technosphere required for each of the three systems. Each data column lists the gate-to-gate flows of the corresponding boxes in the system boundary figures. For example, the column, 'Status Quo,' represents the input/output of the 'Status-quo combustion' box in Figure 1; the column, 'CBMeOH,' represents the input/output of the boxes, 'COG desulphurization' and 'COG+BFG to MeOH,' in Figure 3; and the column, 'CCPP,' represent the boxes, 'Desulphurization' and 'CCPP,' in Figure 2. All five locations have the same data: for every 1 MWh of electricity produced, the system consumes about 624 kg of COG. For the CBMeOH process, 1.34 MWH of electricity and 2.2 kg of NG as heating utility are required. The fresh water requirements for the status quo and CCPP systems are very small, as the process water can be recycled. The other notable number relates to heat output. After applying the system expansion, the major output of the three systems are electricity and heat. The heat output here represents heat from BFG combustion, which is one of the products of system expansion. The emission from BFG combustion is CO_2; no other emissions are included. With respect to direct emissions into the atmosphere, the CBMeOH system produces almost no SO_2; however, it does emit some SO_2 into the waterways via wastewater from the MeOH purification process. The status quo and CCPP systems release approximately the same amount of CO_2 into the atmosphere because they combust the same amounts of COG and BFG within their system boundaries. The emission of ethyne, hydrogen sulfide, carbon disulfide, thiophene, methanol, ethene, ethane, ethanol, monoethanolamine, methyl formade, methane, and dimethyl ether to air and water as predicted by simulation were only trace amounts, which are not listed in the table. However, those computed values are still available in the source files uploaded to LAPSE: http://psecommunity.org/LAPSE:2020.0267.

2.3. Life Cycle Impact Assessment Method

This work utilizes two environmental assessment tools: TRACI 2.1 v1.05/US-Canadian 2008, and CML-IA EU25+3, 2000. TRACI includes categories such as ozone depletion, global warming, smog, acidification, eutrophication, carcinogenic, non-carcinogenic, respiratory effects, ecotoxicity, and fossil fuel depletion. CML's categories include abiotic depletion, abiotic depletion (fossil fuels), global warming, ozone layer depletion, human toxicity, freshwater aquatic ecotoxicity, marine aquatic ecotoxicity, terrestrial ecotoxicity, photochemical oxidation, acidification, and eutrophication. Although these tools have overlapping categories, there are variations between how they are measured. One example of this difference can be observed in how they respectively treat the global warming category. In TRACI, 1 kg of CH_4 is equivalent to 25 kg of CO_2, whereas the

CML tool considers 1 kg CH_4 as being equal to 28 kg of CO_2. These figures are current as of TRACI and CML's most recent updates, which occurred in March 2012 (IPCC report 2007) and September 2016 (IPCC report 2013), respectively. In addition, while CML considers more variables in relation to global warming, TRACI assesses more variables relating to ozone depletion. Thus, it is possible that the analysis results will be slightly different depending on the chosen method. Although TRACI's GHG data is outdated compared to CML's, it was selected because it is based on North American data. In contrast, the CML tool is based on European data. Since the four of the five locations in this study are located in either North America or Europe, TRACI and CML are appropriate tools for use in this study.

Though both TRACI and CML provide each system's midpoint emissions, the damage to the environment caused by those emissions is still unknown. Therefore, other methods that are capable of converting these emissions into damages are required. One selected endpoint method, ReCiPe2016, uses 17 categories to assess a system's midpoint impacts, which can then be converted into three damage categories at its endpoints [16]:

1. Human health: particulate matter, tropical Ozone formation, ionizing radiation, stratospheric Ozone depletion, human toxicity, human toxicity, global warming, water use.
2. Ecosystem: global warming, water use, freshwater ecotoxicity, freshwater eutrophication, tropical Ozone formation, terrestrial ecotoxicity, terrestrial acidification, land use/transformation, marine ecotoxicity, marine eutrophication.
3. Resources: mineral resources, fossil resources.

ReCiPe2016 allows users to choose from three time horizons: 20 years (I: individual), 100 years (H: hierarchies), and 100,000 years or infinite (E: Egalitarian) [16]. According to the ISO 14040 series, weighting is not allowed if the results will be used to compare (competing) products, and if they will be presented to the public. However, ReCiPe2016 allows for a triangle analysis between two products (or system in this work), which helps to eliminate the subjectivity that comes with weighting factors for each type of damage. While ReCiPe2016 uses IPCC report 5, which is the most recent, it should be noted that its midpoint-level characterization factor for the global warming effect is different from that used in CML. For instance, ReCiPe2016 classifies 1 kg of CH_4 as being equivalent to 34 kg CO_2 over a 100-year time horizon, which is much higher than CML's 28 kg CO_2 equivalent [16].

The other selected endpoint method, IMPACT 2002+, assigns 17 variables to one or more damage categories. IMPACT 2002+ is a combination of four methods: IMPACT 2002, Eco-indicator 99, CML and IPCC. The unit of all normalization is based on the number of equivalent persons affected during one year per unit of emission in Europe (persons × year/$\text{unit}_{\text{emission}}$). This method categorizes the impact into four damage groups [17]:

1. Human health: effects include human toxicity, respiratory effects, ionizing radiation, ozone layer depletion, photochemical oxidation, water turbined, water withdrawal, and water consumption.
2. Ecosystem quality: effects include ozone layer depletion, photochemical oxidation, aquatic ecotoxicity, terrestrial ecotoxicity, aquatic acidification, aquatic eutrophication, terrestrial acid, land occupation, water turbined, water withdrawal, and water consumption.
3. Climate change: global warming is the only effect considered in this category.
4. Resources: includes non-renewable energy and mineral extraction.

Normalization relates the magnitude of the calculated impact scores to a common reference, namely, the impact of society's production/consumption activities. As a result, LCA methods are able to provide a better understanding of how the product system under study impacts the reference system [18]. IMPACT 2002+ is a European method, while ReCiPe2016 is a global method. As such, both tools have their respective pros and cons. Thus, this work uses ReCiPe 2016, IMPACT 2002+, TRACI, and CML, as it was decided that this would provide the most robust analysis.

3. Results and Discussion

Since the CBMeOH system is the most complex of the three systems under review, it is worthwhile to examine which of its process stages has the greatest environmental impact. Figure 4 presents the emissions impact of the CBMeOH system producting the functional unit (1MWh of electricity and 1.37 MWh of heat) in stacked columns. In this figure, 'Desulphurization' represents the COG desulphurization process using Rectisol, and 'Electricity Product' refers to the output of the system expansion. Since the CBMeOH process does not produce electricity, the environmental impact from the electricity required from the grid is denoted as 'Electricity from Grid'. 'Steel' represents the environmental impact from the steel used to construct the CBMeOH synthesis system. This category does not account for the Rectisol washing process. 'Electricity for CBMeOH' denotes the total net electricity consumed throughout the CBMeOH process. 'NG for CSR' represents the heating utility effect of the CSR units used in the CBMeOH process. 'Heat for Reboiler' indicates the amount of heat required for the MeOH purification process via NG. 'Steel transport' and 'Catalyst transport' capture the environmental impact of transporting these materials from their production sites to the plant. For these categories, transportation is assumed to be within the country. 'Heat Avoided' denotes the amount of heat that is recovered during the CBMeOH process. This requires another system expansion stream in order to ensure that the product is the same as that of the status quo system. Similarly, 'Methanol Avoided' refers to the amount of methanol that is recovered during the CBMeOH process. Although methanol is the main product of the CBMeOH system, the status quo and CCPP systems do not produce any. Hence, the amount of MeOH produced is subtracted using product avoided. 'Claus process' denotes the waste treatment process. 'Heat from BFG' refers to another system expansion that mainly accounts for CO_2 emissions created by the combustion of upgraded BFG in order to provide heat. The red 'Sum' dot in each column represents the total process flow emissions.

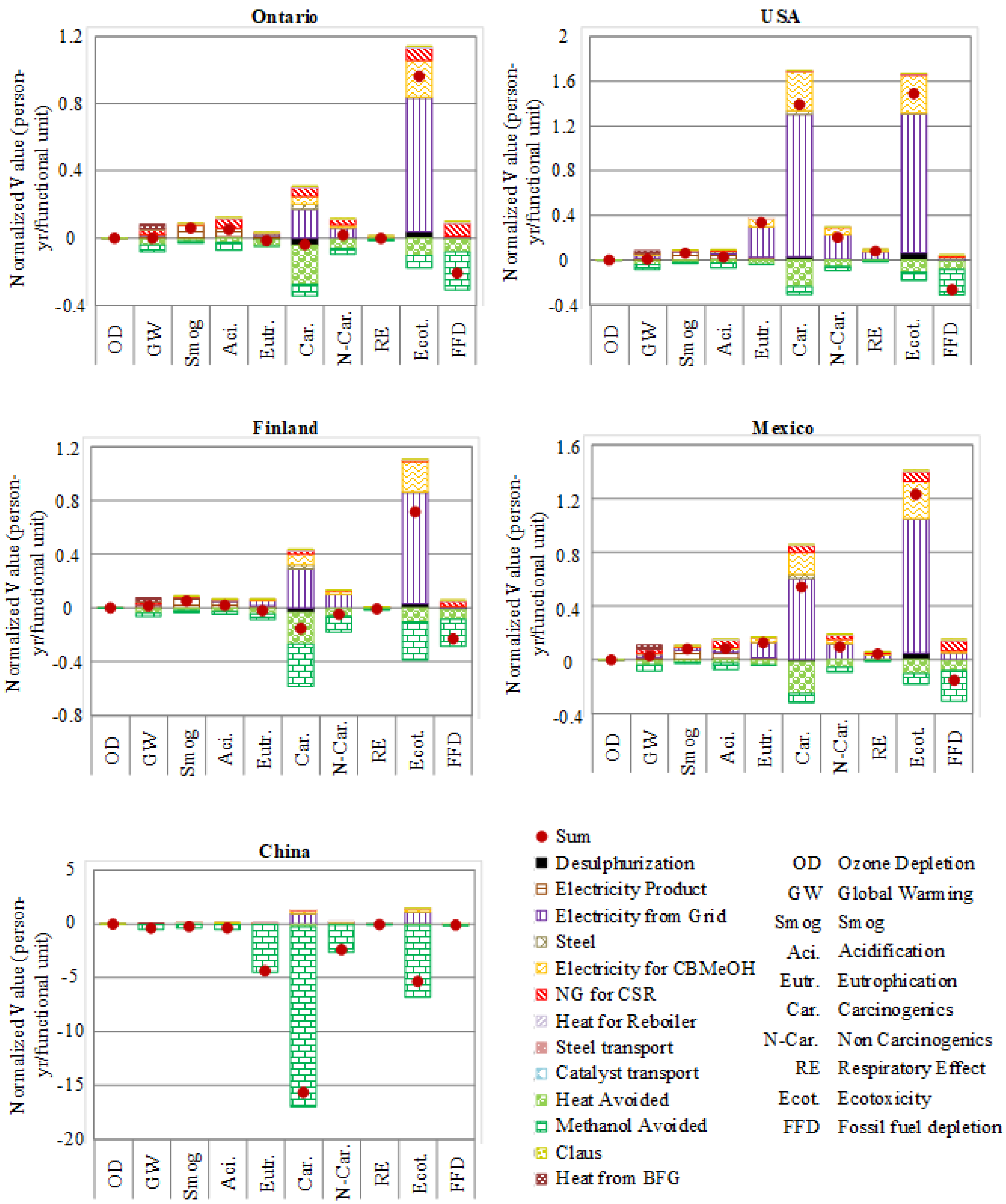

Figure 4. CBMeOH process emission contributions with NG as a heating utility: TRACI.

It is obvious from Figure 4 that, except for China, accounting for Heat Avoided and Methanol Avoided reduced major environmental impacts at all locations. One likely reason why similar effects were observed at these locations is that data for Heat Avoided was acquired from the RER database for each one. For Methanol Avoided, data for Ontario, the USA, and Mexico were obtained from the USLCI database, which is specific to an American context. In the USA, methanol is mainly produced via NG [19]; as such, USLCI uses NG for 100% of methanol production. In contrast, 69% of methanol in China is produced from coal, which is also the most environmentally damaging method [6]. Consequently, the environment impact of methanol production in China is significantly higher than in the USA. As illustrated in Figure 4, the negative effect of Methanol Avoided in China's case is obviously higher than in the North American countries. Methanol Avoided data for Finland was acquired using the global database; these results indicated that methanol production in the Finnish context produced a greater environmental impact than in North America, but less than in China.

Smog, Acidification, Global Warming, and Eutrophication are the main environmental effects produced when the CBMeOH system generates the same amount of electricity as the status quo system, which is the effect of Electricity Product. The other big effect produced by the CBMeOH system relates to the use of NG as a heating utility for the CSR unit. The utilization of Electricity from the Grid mainly impacts carcinogenics, respiratory effects, and ecotoxicity. The effects related to the fabrication and transportation of construction materials are trivial compared to the above categories.

The Desulphurization effect was more pronounced in Ontario and Finland than in the other three countries. Figure 4 also shows different impacts of NG utilization, Methanol Avoided, and Heat Avoided for all five locations. As discussed above, data for Ontario, the USA, and Mexico were obtained from the USLCI database, which indicated that NG, Methanol Avoided, and Heat Avoided all had similar trends across these three locations. The big difference affecting the stacked columns comes from electricity utilization. In the USA and Mexico, up to 65% and 79% of electricity is produced using fossil fuels [20], [21]; in contrast, only about 6.7% of Ontario's electricity is produced using fossil fuels, with the remainder being produced via nuclear energy (58.4%), hydro (23.9%), wind (8%), and solar PV (2.3%) [22]. Hence, the USA and Mexico's Electricity from Grid has a much higher impact on all categories than Ontario, especially regarding the effects on eutrophication, carcinogenics, non-carcinogenics, respiratory effects, ecotoxicity, and ozone depletion. In Finland, about 40% of Electricity from Grid is produced using fossil fuels [23]. Thus, the biggest impact of Electricity from Grid can be seen between Ontario and the USA/Mexico. Although up to 70% of of China's electricity is produced from fossil fuels [24], the effects related to Methanol Avoided are much higher than those related to electricity consumption or production. Hence, Electricity from Grid has a relatively lower environmental impact for China.

3.1. System Comparison

The system comparisons from the TRACI analysis are shown in Figure 5. As can be seen, with the exception of ozone depletion, the CBMeOH process had a negative effect on all categories for the Chinese case, making it the most environmentally friendly process for this context. The ozone depletion effect was almost invisible for all three systems at all five locations. The status quo system had the highest global warming effect of the three systems, while the CBMeOH system generally had the lowest. With the exception of China, the CBMeOH system produced more smog effects than the status quo and CCPP systems at all locations. The status quo system had the largest acidification effects, while the CCPP had the lowest. Again, this held for all locations with the exception of China. The CCPP system had a negative eutrophication effect for all five locations; the CBMeOH system's eutrophication effect was unneglectable in the USA and Mexico. The CBMeOH and CCPP systems both had large carcinogenic effects. The CBMeOH system had a positive impact on carcinogenic effects for the locations in Mexico and the USA, but a negative impact for all of the other locations. In contrast, the CCPP system had a negative impact on carcinogenic effects for all locations. A similar trend was observed for non-carcinogenic effects. The impacts on respiratory effects were minimal for all five locations. Additionally, the CBMeOH process had a very large positive impact on eco-toxicity for all locations (except for China), while the CCPP process had significant negative effect. Moreover, the CBMeOH system was the most effective at reducing fossil fuel depletion.

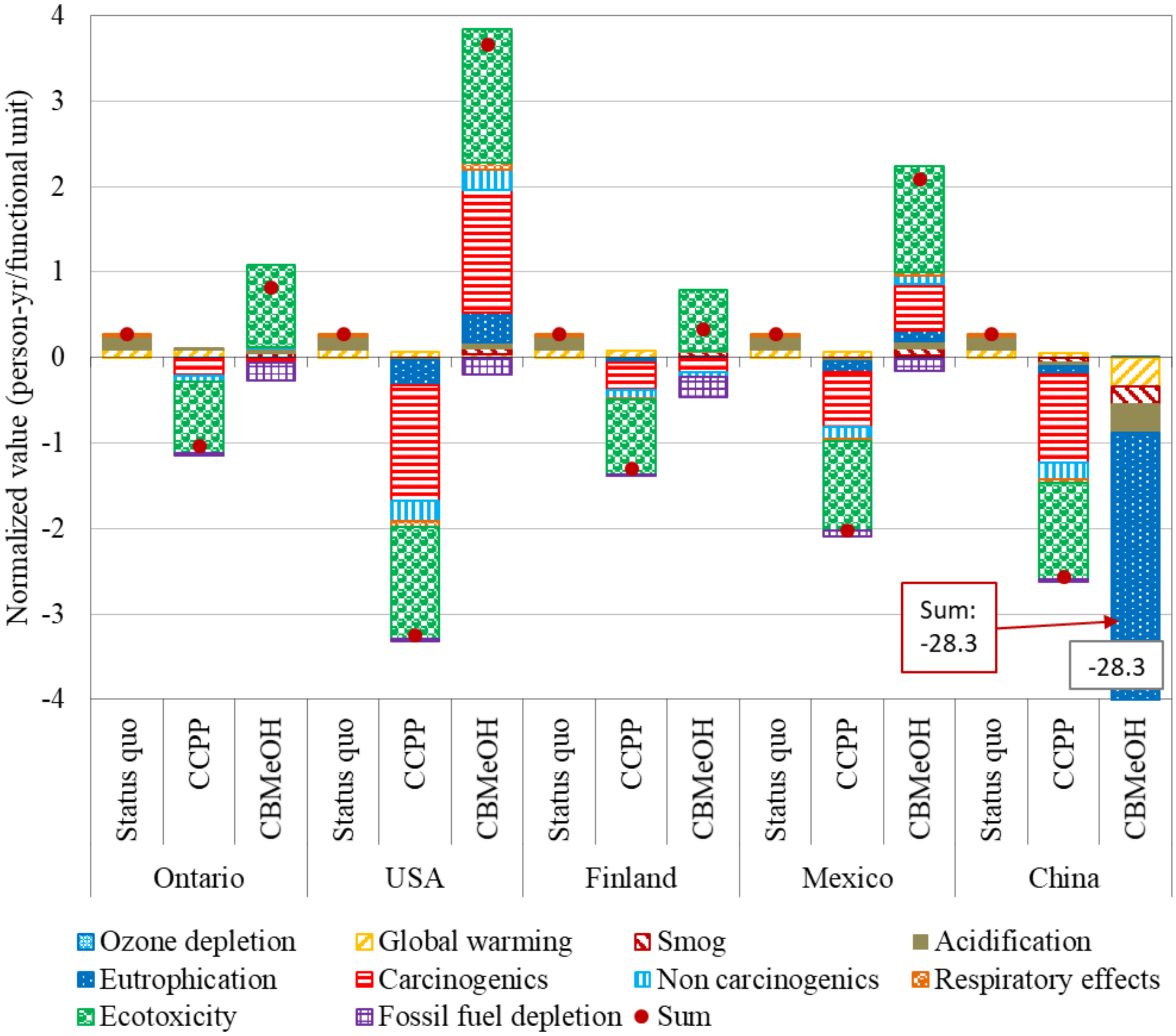

Figure 5. LCA of status quo, CCPP, and CBMeOH systems in five locations using the TRACI tool with normalization. The normalized value is equal to the number of equivalent persons affected during one year in the US-Canada region [25].

The sum data points in Figure 5 indicate that, with the exception of China, the CCPP system yielded the lowest equivalent person affected per year for all studied locations. Conversely, the CBMeOH system produced relatively higher effects for Ontario, the USA, Finland, and Mexico, but the lowest for China.

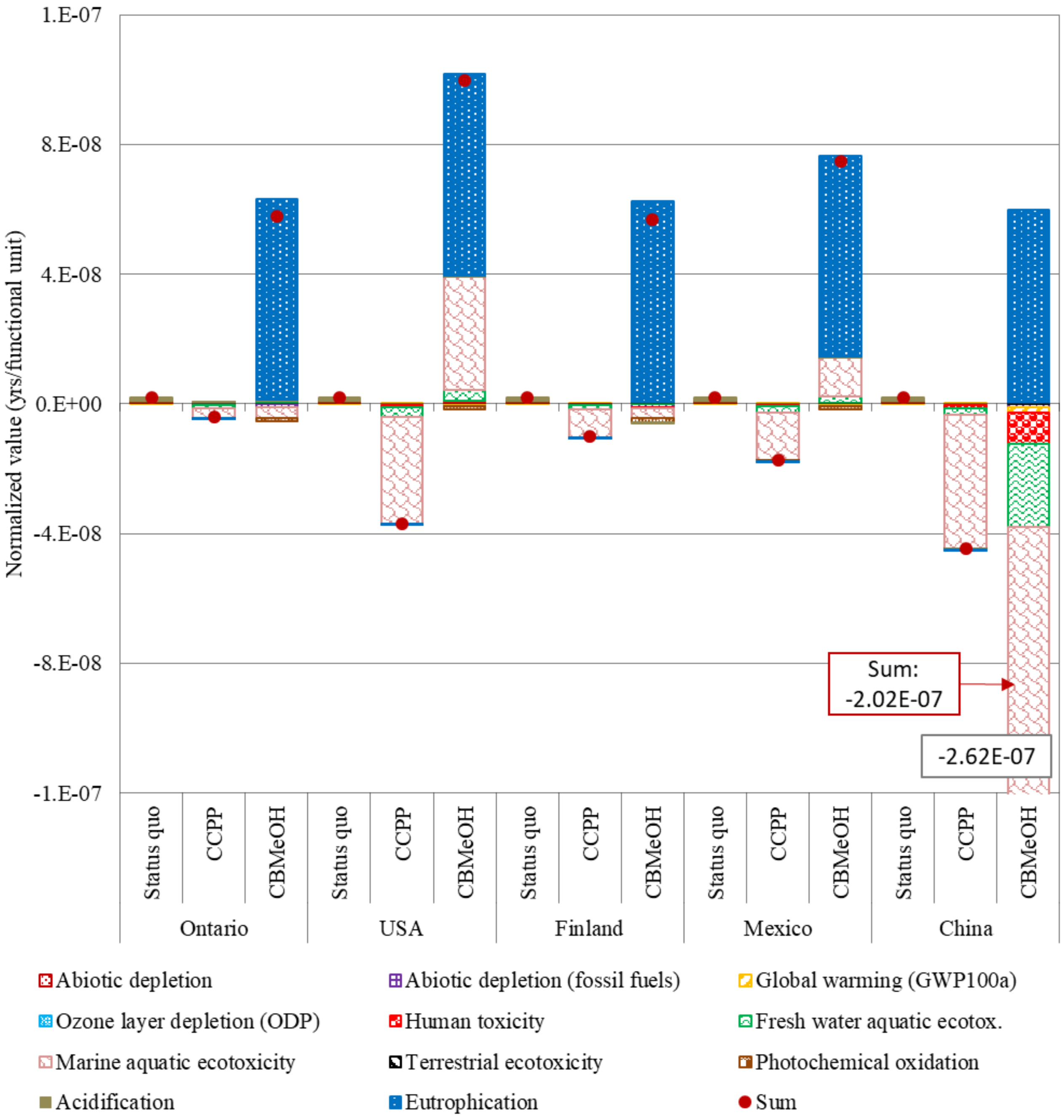

Figure 6. LCA of the status quo, CCPP, and CBMeOH systems in five locations using the CML tool with normalization. The normalized value is equivalent amount of emissions produced in the Europe in the span of one year [25].

The value of each category is seven or eight orders of magnitude smaller for CML than in TRACI (Figure 6). This is difference is due to the fact that CML uses the total amount of emissions in Europe in one year as its normalization reference, while TRACI uses the total emissions in the US-Canada area in one year per person [Roland Hischier, 2010]. The CBMeOH system had a very large positive effect on eutrophication, while the CCPP system had almost none. Amonia is an important factor to account for with regards to eutrophication. Amonia's effect in the CML analysis was more than three times greater than its effect in TRACI. In addition, the eutrophication impact related to Methanol Avoided was very large due to the amount of electricity required in the methanol production process. As discussed earlier, cut-off methanol production data from the USLCI database was used for the Ontario, USA, and Mexico locations. Consequently, these locations all had very high eutrophication effects.

In the USA and Mexico, the CBMeOH system yielded increased marine aquatic ecotoxicity effects. In contrast, the use of this sytem in China resulted in significant negative effects on marine aquatic ecotoxicity. The status quo system had the highest impact on acidification across all five locations, while the CBMeOH system was most effective at reducing fossil fuel depletion. These two results are consistent those obtained using the TRACI tool. The sum of each system's normalized value with the CML method indicates that the CCPP system produced the lowest emissions in Ontario, the USA, Finland, and Mexico, while the CBMeOH system produced the lowest emissions in China.

Although the normalized values obtained using TRACI and CML are able to indicate each category's relative emissions, these tools are unable to capture each category's ability to cause damage and their total damage to human health, ecosystems, and resources. Hence, it is necessary to convert these emission categories into damage categories. For this reason, ReCiPe2016 and IMPACT2002+ are used.

In ReCiPe2016, all midpoint emissions are converted to three damage categories, which were discribed Section 2.3. However, the conversion equations and methods are outside the scope of this work. In SimaPro, the conversion equations are embeded, and the endpoint method can be used to obtain a triangle for each location, thus enabling the comparison of two systems at a time. For such analyses, the system with the lower impact will show on the figure, while the system with higher impact will not. The results indicated that the staus quo system was the most environmental unfriendly system for all five locations. Thus, the area representing the status quo system will never show up in the triangle. As shown in *Figure 7*, the sum of the weighting factors (i.e., human health, ecosystems, and resource damages) will be 100% at any point of the triangle, with each weighting factor varing from 0% to 100%. For Ontario, Finland, and China, the CBMeOH system had a clear environmental advantage over the status quo and CCPP systems. In contrast, the CCPP system provided greater environmental benefits than the status quo and CBMeOH systems for the locations in the USA and Mexico. Hence from an environmental perspective, it is recommended that Ontario, Finland, and China utilize CBMeOH systems, and that the USA and Mexico pursue the use of CCPP systems.

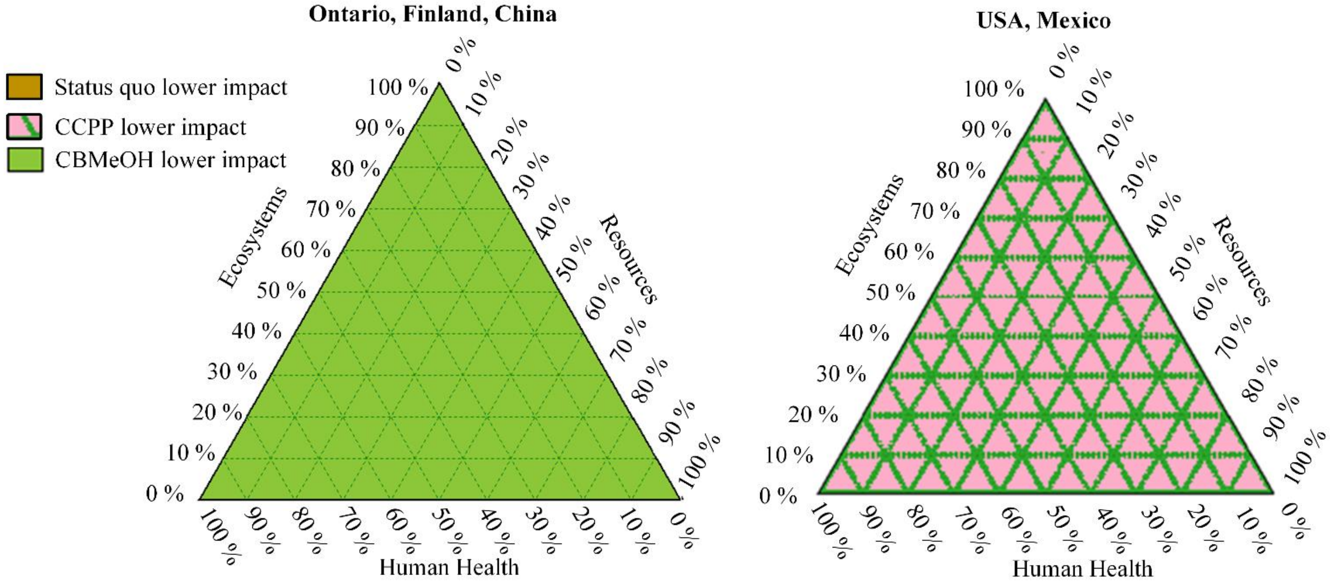

Figure 7. System comparison among five locations using ReCiPe2016.

IMPACT2002+ offers another useful tool for converting emissions categories into damage groups, as it summarizes all 17 impact categories into four damage categories: human health, ecosystem quality, climate change, and resources. Each category is assigned a weighting factor of 1 and is then summarized into a total number. As shown in Figure 8, the analysis using IMPACT2002+ returned similar results to those obtained using ReCiPe2016. That is, the CBMeOH system was the most environmentally friendly for the locations in Ontario, Finland, and China, while the CCPP system was most environmentally friendly for the locations in the USA and Mexico. Figure 8 also shows that the CBMeOH system produced the most environmental damage for the US location, which means that, from an environmental perspective, under no circumstances should steel plants in the USA use CBMeOH systems. Furthermore, the status quo had the highest impact for the other four locations, and still far worse than the CCPP system in the US location. Thus, from an environmental perspective, the status quo system is not recommended.

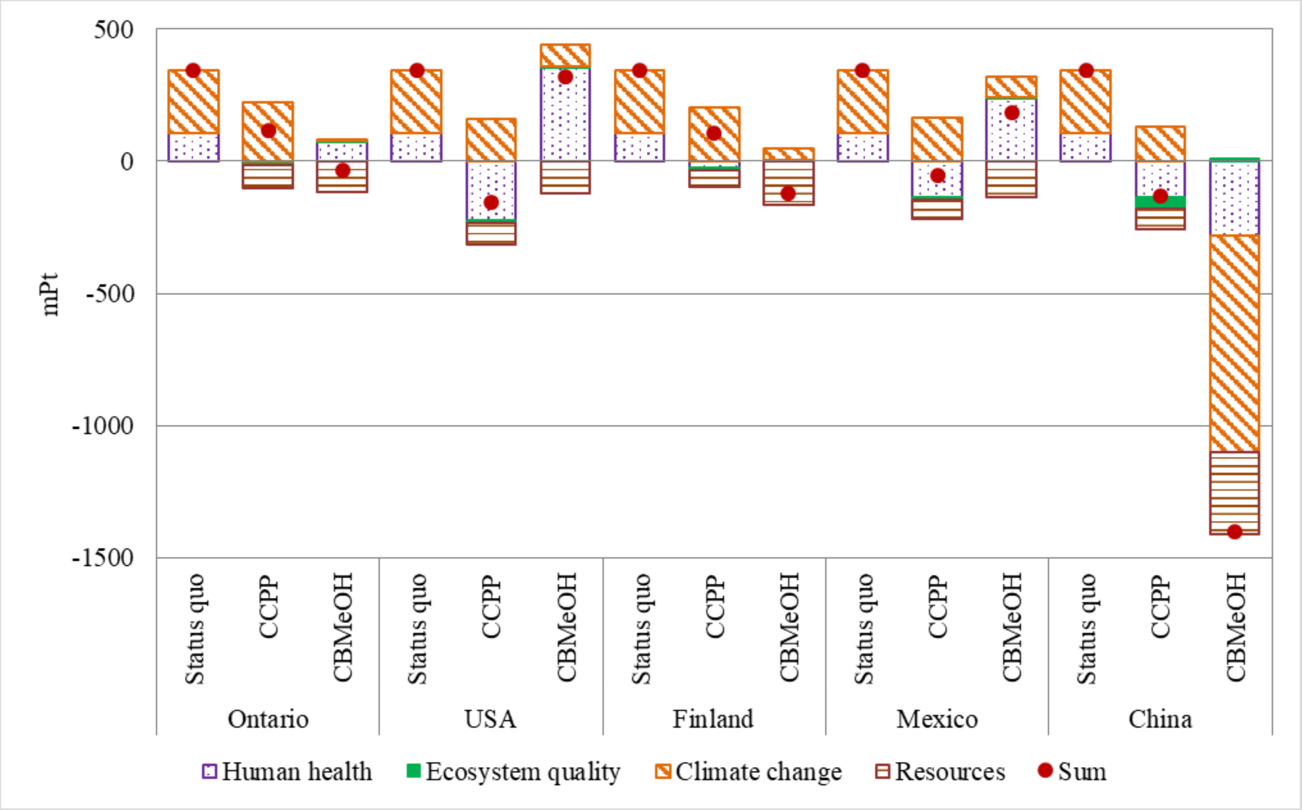

Figure 8. System comparison at five locations with IMPACT 2002+. The weighting factor for each damage category is 1.

Taken in conjunction with our earlier economic analysis [3], these results indicate that it would be profitable to build CBMeOH plants at the Ontario, USA, Mexico, and China locations. While the construction of a CCPP plant in the USA would result in a negative NPV with no carbon tax, it would produce a positive NPV if the carbon tax was increased to \$50/tonne when accounting for the benefit of avoided CO_2 taxes from the status quo [3]. In Finland, CCPP is expected to have a positive NPV in just 6 years over past 13 years studied. For China and Mexico, both CCPP and CBMeOH plants can produce NPVs of more than \$190 million. However, it would be even more profitable to build CBMeOH palnts in Mexico and China. Hence, CBMeOH plants offer more overal environmental and economic benefits for locations such as Ontario, and China, while locations in the USA would see the biggest benefits form building CCPP plants once the carbon tax is increased to \$50/tonne. For Mexico, CCPP plants are the best option in terms of environmental impact, but CBMeOH plants are the best choice in terms of economics. Overall, the results show that it is not recommended that more status quo systems are built in Mexico or China in any circumstance.

4. Improvement and Limitations

The biggest limitation of this work is region-specific data availability and accuracy. The same products are likely to have significantly different environmental impacts at each of the locations due to a variety of factors, such as how electricity is produced in that country. However, data on NG and MeOH production is not yet available for all of the locations examined in this study. Future work on this subject may have the benefit of more complete databases, or it could focus on developing our own database in order to obtain results that are more representative. In addition, it is always very difficult to estimate transportation distances, especially when considering systems as a concept rather than a specific case study. However this variable has a relatively insignificant impact on the overall system.

Another limitation to this work is that each method used different impact factors. For example, most of the chemical compounds considered in the environmental categories had different factors, and some of the tools took more components into consideration than others. Furthermore, most of the analytical tools were developed for European and North America contexts, which means they are not very representative when applied to Asian countries, especially considering huge differences in the normalization reference among locations. The development of a tool that is more specific to an Asian context would be immensely helpful in producing more representative LCA results.

5. Conclusions

In conclusion, from both economic and environmental analysis, the overall results could be represented in the following table.

Table 2. Conclusion from both environmental and economic aspect

	Ontario	USA	Finland	Mexico	China
Environmentally	CBMeOH	CCPP	CBMeOH	CCPP	CBMeOH
Economically (In recent 13 years)	CBMeOH	CBMeOH	CCPP	CBMeOH	CBMeOH

Under no circumstances was the status quo system the best option in terms of environmental impact. When considered in terms of both economic benefit and environmental effects, it is clear that the CBMeOH plant is the best option for Ontario, and China, while the CCPP plant is the best option for the USA provided the carbon tax is increased to 50$/tonne. Mexico could realize big economic gains from building either CCPP or CBMeOH plant. On the one hand, a CBMeOH plant would result in higher NPV, but on the other hand it would have a more negative environmental impact than a CCPP plant. Thus, the system that is ultimately chosen will depend on the shareholders' preferences.

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