Life cycle assessment of emerging chemical technology systems: challenges and future needs

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Chapter 4: Ex-ante Life Cycle Assessment of polyols using carbon captured from industrial process gas

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Abstract

The steel industry needs to significantly reduce greenhouse gas (GHG) emissions as it is considered as one of the major industrial contributors to global GHG emissions. Since CO and CO_2 occur in high concentrations in steel mill gases, one of possible options to do this is utilizing CO and CO_2 for the production of value added chemicals. Following this goal, a Carbon Capture and Utilization (CCU) technology was developed transforming CO and CO_2 from the blast furnace gas (BFG) of a steel mill to building blocks for polyols. These polyols were then used to produce polyurethane (PUR) for the manufacturing of coatings and rigid foam for insulation boards. For assessing and comparing the life cycle environmental impacts of this novel CCU system to the incumbent steel and polyols system, ex-ante Life Cycle Assessment (LCA) was carried out. Three possible scenarios of the CCU system were compared to the incumbent steel and polyols systems, assessed by performing LCAs and identifying hotspots. All three scenarios of the CCU technology showed improved environmental performance compared to the incumbent technology although limited to a maximum of about 10% reduction in carbon footprint. Energy and chemicals used to produce CCU polyols were identified as the main hotspots to the life cycle impacts of all three scenarios.

4.1 Introduction

Global warming caused by greenhouse gas (GHG) emissions has been recognized as a severe problem on a global scale that needs to be tackled. The European Union (EU) set up an objective to reduce GHG emissions of 80%-95% till 2050 compared to 1990 (European Commission, 2011). The steel industry is one of the largest industrial emitters of CO_2, being responsible for 7%-9% of direct CO_2 emissions from the global use of fossil fuel (World Steel Association, 2021). Carbon Capture Utilization (CCU) using CO_2 for chemical synthesis is currently seen as one of the possibly promising approaches to mitigate carbon emissions (Ariyama et al., 2019). CCU allows to transform carbon emissions CO/CO_2, e.g., from steel mills, into value-added chemical products.

The Carbon4PUR project, funded by the European Union's Horizon 2020 research and innovation program, aimed at transforming carbon emissions from the blast furnace gas (BFG) of a steel mill to valuable intermediates (chemical building blocks) for the production of polyols in the polyurethane industry (Carbon4PUR, n.d.). Polyurethanes (PUR) are a large group of polymers that covers a broad range of various applications. It can be used for the manufacture of coatings, adhesives, sealants, rigid foam for thermal and sound insulators, flexible foam for furniture, elastomers, etc. (Akindoyo et al., 2016). The Carbon4PUR project developed polyols for PUR that can be used in the production of coatings and rigid foam for insulation boards. In this study, the technology developed within the Carbon4PUR project is from here on referred to as "CCU technology".

Life Cycle Assessment (LCA) is a method to assess the environmental impacts related to products and services. It is, along with other assessment methods such as e.g., techno-economic assessment, often used to support the development of new technologies. Generally, LCA is used to assess existing technologies operating at the industrial scale, for which data at the industrial scale is available. The application of LCA to the CCU technology is more challenging as it has so far only been developed at the laboratory and the pilot scales. Consequently, this technology is lacking industrial scale data which is essential for regular LCA studies.

Ex-ante LCA can be defined as LCA studies those that a) scale-up an emerging technology using likely scenarios of future performance at full operational scale, b) compare the emerged technology at scale with the evolved incumbent technology (Cucurachi et al., 2018), or as "performing an environmental life cycle assessment of a new technology before it is commercially implemented in order to guide R&D decisions to make this new technology environmentally competitive as compared to the incumbent technology mix." (van der Giesen et al., 2020). Some LCA practitioners use the term "prospective LCA" rather than "ex-ante LCA" for this type of assessment (Arvidsson et al., 2018). In this work, we will refer to LCA of emerging technology as "ex-ante LCA".

Several LCA studies have been published on CCU technologies used for the production of chemicals (Artz et al., 2018; Thonemann, 2020), most of which were focusing on the production of polyols from CO_2 (Carvalho et al., 2021; Fernández-Dacosta et al., 2018; Meys et al., 2019; Von Der Assen and Bardow, 2014). However, to the best of our knowledge, there have been no LCA studies carried out for the joint production of both CO-based polyols and CO_2-based polyols from the CO and CO_2 fractions of BFG.

In this study, we perform an ex-ante LCA of a CCU technology that converts CO and CO_2 gases from BFG to valuable intermediates for the production of polyether-ester polyol (CO-based polyol) and polyether-carbonate polyol (CO_2-based polyol). The environmental performance of three scenarios of the CCU technology were compared to the existing commercial technology (baseline system), and the main contributors (hotspots) to the impacts were identified.

4.2 Methodology

4.2.1 Goal definition

The CCU technology assessed in this LCA study converts carbon emissions from steel production to intermediates to produce polyols. These polyols then are used to produce polyurethane for the manufacturing of coatings and rigid foam for insulation boards. The purpose of the LCA study was to assess life cycle impacts of the CCU technology (using a part of the BFG for the production of polyols), to compare the CCU technology to the baseline system (incumbent way of using the BFG by the steel industry itself and of producing

polyols). The details of our approach are provided in section 4.2.2. The approach we developed aimed at determining whether the integrated new symbiotic system of the CCU technology performed environmentally better than the two independent incumbent systems using BFG for the production of energy for the steel production and the production of polyols from fossil fuels.

Three research questions were formulated:

1. What is the overall environmental performance of the CCU technology system compared to the baseline system as described above?
2. How can differences in environmental performances be explained in terms of main contributors (hotspots) and components differing between the CCU technology and the baseline system?
3. Do the identified hotspots in the CCU technology system offer options for further improvement?

4.2.2 Scope definition

The geographical coverage for this LCA study was Europe. A cradle-to-gate approach was applied meaning that the LCA included the processes starting from the raw material extraction and ending with the production of polyols. The background processes were modelled using the ecoinvent v3.4 (cut-off version) database (Wernet et al., 2016). The foreground processes were based on data provided by project partners. LCA followed ISO 14044 framework (ISO International Standard 14044, 2006). The AB (Activity Browser) (B. Steubing et al., 2021; Steubing et al., 2020) and the CMLCA software (version 6.1) (R. Heijungs, 2018) were used for the LCA calculations, and calculation results were mutually validated between these two software programs.

For the comparison of the baseline system to the CCU technology system, we excluded those parts of the steel production that were qualitatively and quantitatively the same for both systems (Figure 4.1). The use of a portion of the BFG produced from the pig iron production was the only part of the steel production that was different between the baseline and the CCU technology systems. In the baseline system, BFG, produced from the pig iron production process, was incinerated to produce heat (5%) and electricity (75%) to be recycled back for use by the steel production processes, and a part was flared as waste (20%) (Collis et al., 2021). In the CCU technology system, a part of

BFG produced from the pig iron production was used to produce polyols. As a result, this part of the BFG could not be used to produce heat and electricity, and thus, less heat and electricity was recycled back to the steel production processes. Therefore, the amount of heat and electricity that could be produced from BFG needed to be substituted in the steel production processes by heat from an industrial boiler and electricity from the grid.
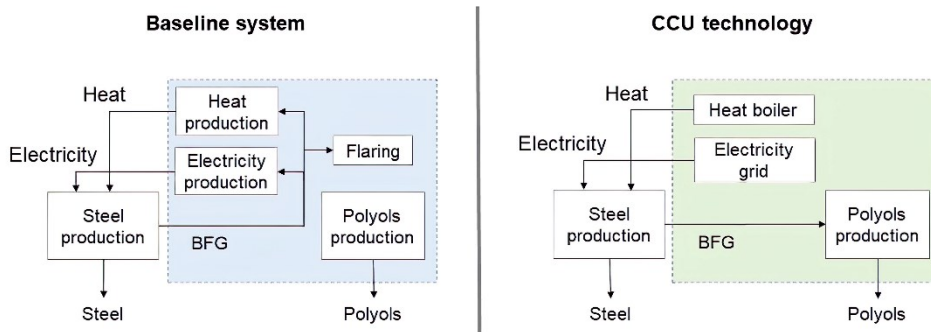

Figure 4.1 *The comparison adopted in this study. The CCU polyols production is an aggregate representation of several processes.*

In the CCU technology system, not all BFG components were used in the polyols production process. During this process, a waste BFG gas was produced that was returned to the steel mill. This waste BFG had a different chemical composition compared to the BFG gas generated from the pig iron production process. The BFG waste was composed of unreacted vapor components: CO, CO_2, N_2, H_2, THF, ethanal, acrylic acid, dioxan, etc. The waste BFG had lower carbon content and calorific value than the BFG gas. However, the quantity of the waste BFG gas was so small compared to the total BFG flow that we assumed that it could be mixed with the BFG at the steel mill, so that the carbon and calorific content of the total BFG flow would not be affected. Thus, the assumption was made that the waste BFG returned to the steel mill had the same carbon content and calorific value as the BFG produced from the pig iron production and was used at the steel mill in the same way for production of electricity (75%), heat (5%), and flared (20%). By doing this, we could calculate an amount of the BFG used for polyols production by subtracting returned waste BFG to the steel mill from the BFG delivered by the steel mill.

The CCU technology reflects a technology readiness level (TRL) between TRL 2 and TRL 6 (different parts of the CCU technology including gas

conditioning and production of polyols are at different TRL levels from TRL 2 to TRL 6). The data derived from these laboratory scale and pilot scale implementations cannot be applied in the environmental assessment of a future technology operated at full scale since these data are far from the industrial scale data (TRL 9). Thus, the laboratory scale and the pilot scale data were upscaled to the projected industrial scale following the upscaling framework presented by Tsoy et al. (2020) to get an estimate of its potential full-fledged future performance. According to this framework, the upscaling of an emerging technology in ex-ante LCA is composed of three steps: 1) Projected technology scenario definition, 2) Preparation of a projected LCA flowchart, and 3) Projected data estimation.

It should be noted that different kinds of expertise are required to upscale a new technology in ex-ante LCA, and thus it is recommended that the experts from different fields are involved in the upscaling, e.g., technology developers, engineers, and LCA practitioners (Tsoy et al., 2020). In the case of the upscaling of the CCU technology in this study, steps 1 to 3 of the upscaling were performed by the technology developers of the CCU technology with support from the LCA experts in steps 2 and 3. Next, LCA calculations were performed using the results of the upscaling steps as input.

The next sections of this paper (Sections 4.2.2.1-4.2.3.2) provide a more detailed description of the three upscaling steps performed: 1) Projected technology scenario definition, 2) Preparation of a projected LCA flowchart, and 3) Projected data estimation.

4.2.2.1 Projected technology scenario definition

Several laboratory scale and pilot scale implementations of the CCU technology were developed (Aly et al., 2022; Flores-Granobles and Saeys, 2022; Machat et al., 2022) according to three scenarios. Aspen Plus process flow sheets were developed by technology developers deciding on installations and process operating conditions and showing the equipment of the three upscaled CCU technology scenarios. The general overview of these three scenarios is shown in Figure 4.2. All three scenarios were composed of two main processes: conditioning of the BFG gas and production of polyol.
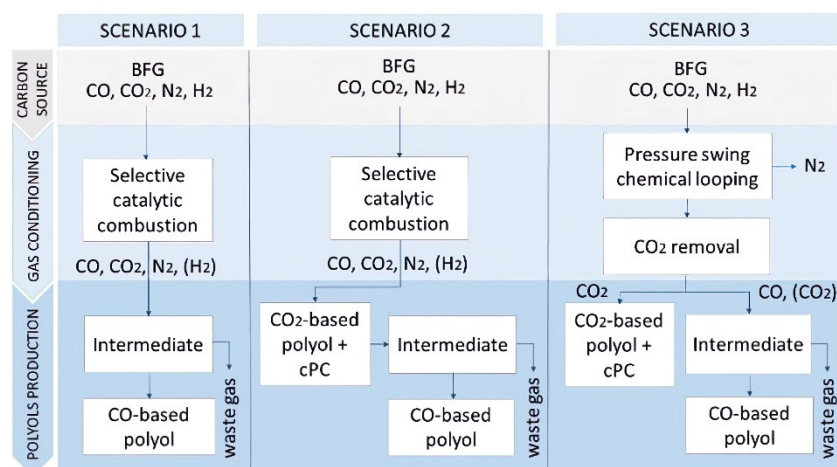
Figure 4.2 *Overview of scenarios of the CCU technology.*

4.2.2.1.1 Scenario 1: BFG to CO-based polyol

Selective catalytic combustion was analysed as a gas conditioning method in scenario 1. Selective catalytic combustion is a process where pure O_2 is used to decrease the amount of H_2 in the BFG via selective oxidation reaction (Aly et al., 2022). With regards to the polyols production, CO-based polyol was assessed, while CO_2-based polyol was not considered. Scenario 1 avoids the dependency between two products observed in scenarios 2 and 3.

4.2.2.1.2 Scenario 2: Sequential process – BFG to CO_2-based polyol and CO-based polyol

Scenario 2 represents the sequential production of CO_2-based polyol and CO-based polyol. Similar to Scenario 1, selective catalytic combustion was used to condition BFG. Conditioned BFG containing CO/CO_2 and inert N_2 is used to produce CO_2-based polyol. Next, the CO_2 depleted stream is used in the production of succinic anhydride which is an intermediate to produce CO-based polyol. After the CO-based polyol is produced, the used gas stream is disposed as waste.

4.2.2.1.3 Scenario 3: Parallel process – BFG to CO_2-based polyol and CO-based polyol

Pressure swing chemical looping (Flores-Granobles and Saeys, 2022) and a CO_2 removal process (the DMX[TM] process) (Aleixo et al., 2011; Dreillard et

al., 2017) were used as a gas conditioning method in Scenario 3. Pressure swing chemical looping produces a CO/CO_2 stream almost free of H_2 and inert gas N_2. After that a CO_2 removal process is used to remove most of CO_2 from this CO/CO_2 stream. As a result, two gas streams are produced: a CO-rich stream and a pure CO_2 gas stream that can be used in the production of CO-based polyols and CO_2-based polyols separately in a parallel process. Since the gas conditioning method in this scenario produces more pure gas streams for the polyols production, the overall polyol production processes are more efficient: less gas volume is needed, thus the reactors are much smaller, and less compression is required. In this study, Scenario 3 was only investigated as a holistic scenario (scenario, where both CO-based polyol and CO_2-based polyol are produced) to compare to Scenario 2.

Function, functional unit, and reference flows were defined for each scenario. As explained before, the function of the compared systems was defined as *the production of polyols and the provision/compensation of heat and electricity for steel production*. The functional unit was different for each scenario as the quantity of the BFG used for the polyol production in each scenario was different, affecting the amount of heat and electricity to be delivered to the steel production. Table 1.1 shows function, functional unit, and reference flows for each scenario.

4.2.3 Inventory analysis

4.2.3.1 Preparation of a projected LCA flowchart

Figure 4.3 shows the LCA flowcharts for the three scenarios. In this paper, each of three scenarios was divided into three main processes: supply of the BFG, gas conditioning, and polyols production. A description of these processes is provided below.

4.2.3.1.1 Supply of the BFG

The ecoinvent v3.4 database (Wernet et al., 2016) was used to model the production of steel including processes such as coke production, pig iron production, steel production and steel rolling. The alternative use of a portion of the BFG from the pig iron production process was modelled partly as a source of heat and electricity and partly flared in the baseline system or as a

carbon source for the polyols production in the CCU technology system. All other parts of the steel mill model were excluded in LCA, as those parts were qualitatively and quantitatively the same in both the baseline and the CCU technology systems. The data for the energy production and consumption

Table 1.1 *Function, functional unit, and reference flows for three scenarios.*

Function	Scenario	Functional unit	Reference flows	
			Baseline system	*CCU technology*
Production of polyols and the provision/ compensation of heat and electricity for steel production	Scenario 1: BFG to CO-based polyol	*Polyols production:* 1 kg CO-based polyol *Energy for steel production:* 0.035 megajoules (MJ) of heat and 0.223 MJ of electricity	1 kg of phthalic acid polyester polyol 0.035 MJ of heat and 0.223 MJ of electricity from BFG	1 kg of CO-based polyol 0.035 MJ of heat by an industrial boiler and 0.223 MJ of electricity by the average European grid
	Scenario 2: Sequential process – BFG to CO_2-based polyol and CO-based polyol	*Polyols production:* 1 kg of CO-based polyol and 1.99 kg of CO_2-based polyol *Energy for steel production:* 0.083 MJ of heat and 0.526 MJ of electricity	1 kg of phthalic acid polyester polyol and 1.99 kg of a polyether polyol 0.083 MJ of heat and 0.526 MJ of electricity from BFG	1 kg of CO-based polyol and 1.99 kg of CO_2-based polyol 0.083 MJ of heat by an industrial boiler and 0.526 MJ of electricity by the average European grid

	Scenario 3: Parallel process – BFG to CO_2-based polyol and CO-based polyol	*Polyols production:* 1 kg of CO-based polyol and 2.23 kg of CO_2-based polyol *Energy for steel production:* 0.227 MJ of heat and 1.444 MJ of electricity	1 kg of phthalic acid polyester polyol and 2.23 kg of a polyether polyol 0.227 MJ of heat and 1.444 MJ of electricity from BFG	1 kg of CO-based polyol and 2.23 kg of CO_2-based polyol 0.227 MJ of heat by an industrial boiler and 1.444 MJ of electricity by the average European grid

in the steel mill, thermal and electrical efficiencies for the production of heat and electricity from the BFG were provided by a steel producer.

4.2.3.1.2 Gas conditioning

BFG consists of 49% N_2, 22% CO_2, 22% CO, 3.6% H_2, 3.2% H_2O and further impurities (Machat et al., 2022). The H_2 gas in BFG can interfere with the reaction of the polyols production (Aly et al., 2022; Machat et al., 2022). Thus, BFG should be conditioned prior to the production of polyols to decrease the H_2 content in BFG. For this, a **selective catalytic combustion** method for conditioning BFG was developed (Aly et al., 2022). In this method, the H_2 content is decreased in BFG via selective oxidation of H_2 over a Ni-based catalyst. Currently, selective catalytic combustion reflects a TRL 5.

Pressure swing chemical looping is another method developed to condition BFG (Flores-Granobles and Saeys, 2022). This method uses solid chemical intermediates (CO_2 sorbent and oxygen storage material) in reaction-regeneration cycles and produces CO/CO_2 stream almost free of H_2 and N_2. In addition, a **CO_2 removal step** is used to remove CO_2 from produced CO/CO_2 stream using DMX^{TM} (Demixing solvent) process (Aleixo et al., 2011; Dreillard et al., 2017). In the CO_2 removal step, about 90% of CO_2 content is removed. In the current CCU technology system, the pressure swing chemical

looping reflects TRL 2. Selective catalytic combustion was modelled as a gas conditioning method in scenarios 1 and 2, while pressure swing chemical looping and CO_2 removal were assessed in Scenario 3 (Figure 4.3).

4.2.3.1.3 Polyol production

4.2.3.1.3.1 Production of CO-based polyol

The developed production process of the intermediate and CO-based polyol (Machat et al., 2022) was assessed in all three scenarios (Figure 4.3). In this process, CO from the BFG is used in a double carbonylation reaction with ethylene oxide (EO) to produce succinic anhydride (an intermediate). This reaction is carried out using a catalyst in tetrahydrofuran (THF). In the first carbonylation step, CO reacts with EO to produce β-propiolactone, and in the second carbonylation step, CO reacts with the produced β-propiolactone to form succinic anhydride. Then the co-polymerisation of the formed succinic anhydride and EO in the presence of the catalyst results in the formation of polyether-ester polyol (CO-based polyol). In the current CCU technology system, the intermediate production was developed up to TRL 5 and the CO-based polyol production to TRL 6.

4.2.3.1.3.2 Production of CO2-based polyol

Production of CO_2-based polyol was analysed in scenarios 2 and 3 (Figure 4.3). For the development of the CO_2-based polyol production process, a slightly adopted version of the existing CO_2-based polyol production technology (Langanke et al., 2014) was taken. The production of CO_2-based polyol in the CCU technology assessed in this LCA study is similar to that in the existing CO_2-based polyol production technology: CO_2 and propylene oxide (PO) are converted to polyether-carbonate polyol (CO_2-based polyol) in the presence of a starter and a double metal cyanide (DMC) catalyst (Machat et al., 2022). However, in the case of the CCU technology assessed in this study, mixed CO/CO_2-containing BFG gas stream is used in the polyol production, while in the existing CO_2-based polyol production technology, pure CO_2 is used.

4.2.3.2 Projected data estimation

When the LCA flowcharts (Figure 4.3) for the three scenarios were prepared, data was estimated for each unit process of these flowcharts. The technology experts and the LCA experts estimated missing data using the data estimation methods reviewed by Tsoy et al. (2020) and Parvatker and Eckelman (2019). For the three scenarios presented here, data estimation was mainly done using *process simulation*: first, technology experts calculated the mass and energy data for the novel gas conditioning and the polyols production technologies using Aspen Plus (Aspentech, n.d.). Next, the LCA experts used other data estimation methods to approximate missing data. For instance, *manual calculations* (stoichiometric calculations) were performed to estimate emissions for the thermal oxidation processes. Finally, the upscaled data of the CCU technology scenarios were used in the LCA calculations.

4.2.3.3 Data collection for the baseline system

The data for the baseline polyols phthalic acid polyester polyols and polyether polyols (comparable to the novel CO-based polyols and the CO_2-based polyols, respectively) were provided by a chemical company. These data are confidential and therefore, cannot be shared in this paper.

4.2.3.4 Multifunctionality and allocation

Since the BFG is a useful co-product of the multifunctional pig iron production process, a part of the environmental burdens of the steel process needed to be allocated to this BFG. However, the amount of burden allocated to the BFG in the baseline system exactly matches the amount of burden allocated to the BFG in the CCU technology system. Since the allocated burdens to the BFG are equal for the baseline system and the CCU technology system, the method of allocation does not matter. In this study, we applied mass allocation as basis for the results.

In scenarios 2 and 3, two types of polyols are co-produced: CO_2-based polyol and CO-based polyol. Mass allocation was applied to allocate environmental burdens between these polyols.

4.2.4 Impact assessment – characterization

The potential impact of the three scenarios were assessed applying following the characterization methods recommended by the International Reference

Life Cycle Data System (ILCD) 2.0 2018 (Institute for Environment and Sustainability, 2012). Thirteen impact categories were included: 1) Climate change (CC), 2) Ecosystem quality, freshwater and terrestrial acidification (FTA), 3) Ecosystem quality, freshwater ecotoxicity (FEC), 4) Ecosystem quality, freshwater eutrophication (FEU), 5) Ecosystem quality, marine eutrophication (MEU), 6) Ecosystem quality, terrestrial eutrophication (TEU), 7) Human health, carcinogenic effects (HHC), 8) Human health, ionizing radiation (HIR), 9) Human health, non-carcinogenic effects (HHNC), 10) Human health, ozone layer depletion (OLD), 11) Human health, photochemical ozone creation (POC), 12) Resources, fossil resources (FR), 13) Resources, minerals and metals (MM).
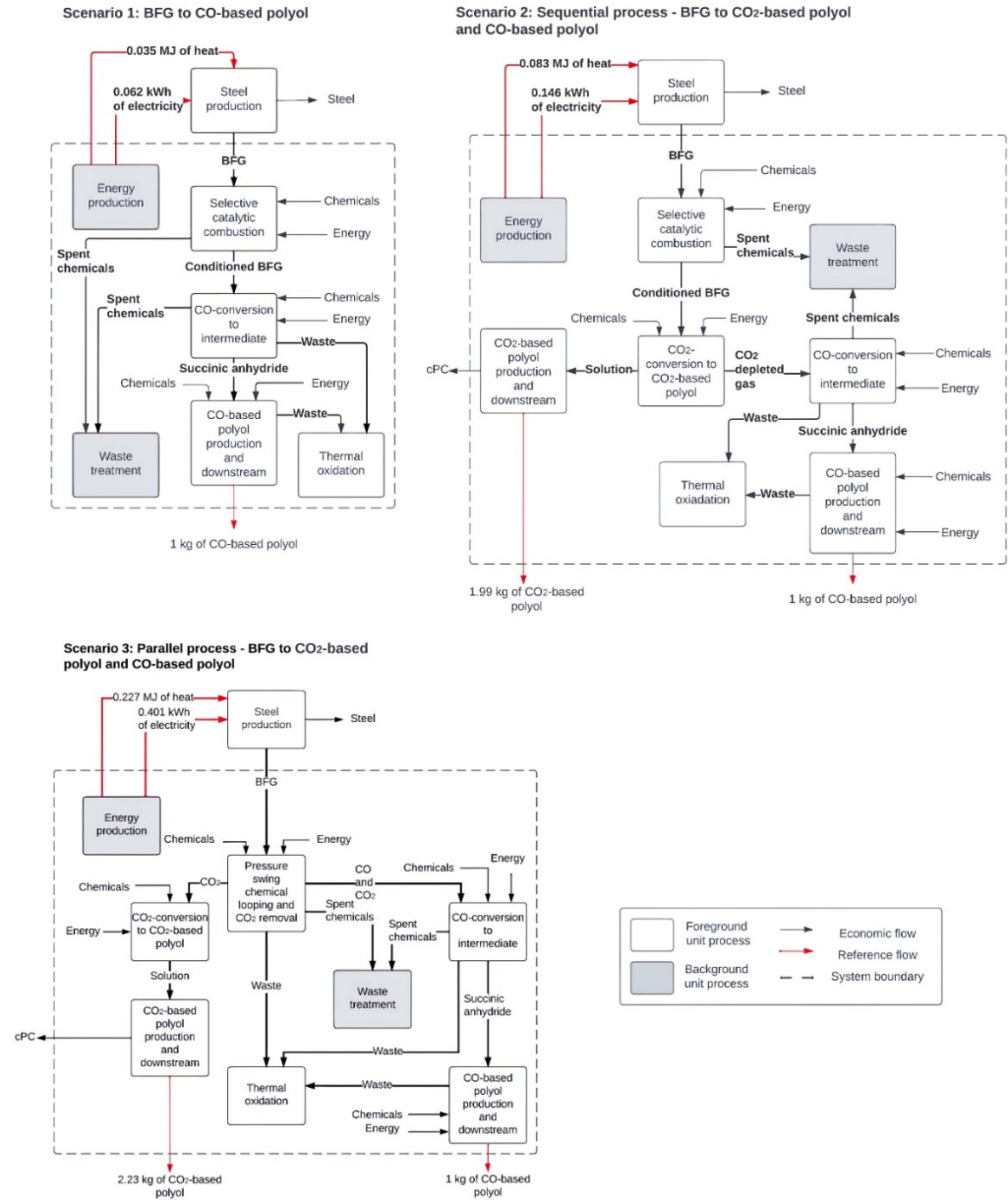
Figure 4.3 *LCA flowcharts for three scenarios of the CCU technology.*

4.3 Results

4.3.1 Characterization results

4.3.1.1 Scenario 1: BFG to CO-based polyol

The results show that the carbon footprint of the CCU technology system is better than the footprint of the baseline system by 8%. Both the baseline and the CCU technology systems show the same (mass-) allocated footprint to the BFG 0.34 kg CO_2-equivalents. The footprint results of heat from an industrial boiler, electricity from the grid and the CO-based polyol in the CCU technology system are slightly better than the ones for heat and electricity produced from the BFG, and phthalic acid polyester polyol in the baseline system, respectively. The impact results for other impact categories show a diverse pattern (Figure 4.4). The CCU technology system shows slightly lower impact results for human health (non-carcinogenic and carcinogenic effects), fossil resources, climate change, ozone layer depletion and freshwater ecotoxicity (1-25%), while the baseline system shows slightly better results for all other impact categories.
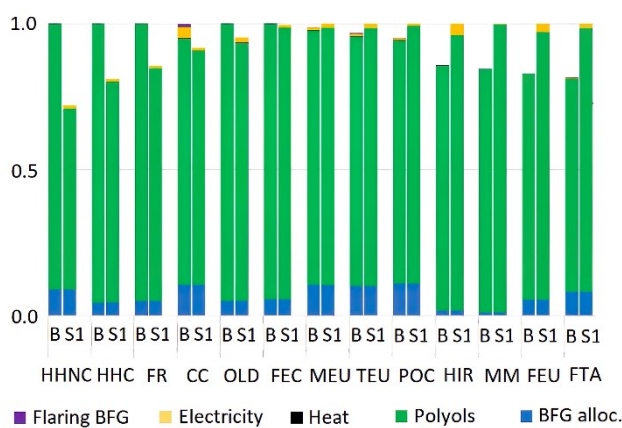

Figure 4.4 ILCD 2.0 (2018) characterisation results for the baseline system (B) compared to the CCU technology system for Scenario 1 (S1), scaled to the alternative showing the highest results for a given impact category.

4.3.1.2 Scenario 2: Sequential process – BFG to CO2-based polyol and CO-based polyol

The results show that the carbon footprint of the CCU technology system is better than the footprint of the baseline system by 9%. Both the baseline and the CCU technology systems show the same (mass-) allocated footprint to BFG 0.71 kg CO_2-equivalents. The footprint results of the CCU polyols are again slightly better than those of the baseline polyols. Furthermore, the footprints for heat from an industrial boiler and electricity from the grid are slightly better than the ones for heat and electricity produced from the BFG. The CCU technology system shows a better performance with regards to other impact categories compared to the baseline system by 0.5-12.5% (Figure 4.5). Ionizing radiation is the only impact category on which the baseline system performs slightly better (by 4%) than the CCU technology system.
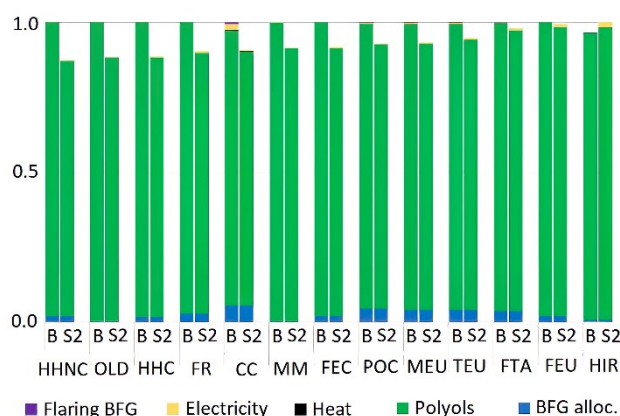

Figure 4.5 *ILCD 2.0 (2018) characterisation results for the baseline system (B) compared to the CCU technology system for Scenario 2 (S2), scaled to the alternative showing the highest results for a given impact category.*

4.3.1.3 Scenario 3: Parallel process – BFG to CO2-based polyol and CO-based polyol

The results show that the carbon footprint of the CCU technology system is better than the footprint of the baseline system by 11%. Both the baseline and the CCU technology systems show the same (mass-) allocated footprint to the

BFG 2.18 kg CO_2-equivalents. The footprint results of the CCU polyols are again slightly better than those of the baseline polyols. Furthermore, the footprints for heat from an industrial boiler and electricity from the grid are better than the ones for heat and electricity produced from the BFG. The CCU technology system shows a better performance with regards to all impact categories compared to the baseline system by 4-15% (Figure 4.6).
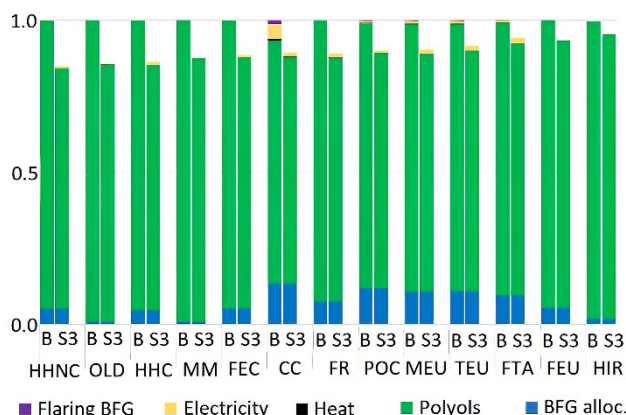

Figure 4.6 *ILCD 2.0 (2018) characterisation results for the baseline system (B) compared to the CCU technology system for Scenario 3 (S3), scaled to the alternative showing the highest results for a given impact category.*

4.3.2 Interpretation

This section presents the contribution analysis results for three CCU technology scenarios, focusing on the main contributors to the total impacts of the CCU technology. Firstly, for each scenario an analysis of the contributions of the individual processing steps of the CCU technology to the total environmental impacts was conducted, i.e. at the aggregation level that corresponds to the LCA flowcharts in Figure 4.3: BFG energy substitution, gas conditioning, CO-conversion to intermediate, CO-polyol production and downstream, CO_2-conversion to CO_2 polyol (in scenarios 2 and 3), and CO_2-polyol production and downstream (in scenarios 2 and 3).

Secondly, an analysis of sectors (by means of grouping processes within the same sector) to the total environmental impacts over the life cycle of producing the polyols was performed. Six sectors were defined: fossil energy

carrier supply, energy generation, waste treatment, chemicals production, metals production, other. The sectors "fossil energy carrier supply" and "energy generation" in Figure 4.7 (b, d, f) relate to energy. It should be noted that the results for sectors refer to not only the CCU technology, but to the entire product system, thus including supply chains as modelled in the ecoinvent database. The sectors aggregate one or several processes. For example, the sector "energy generation" sums up the impact across the life cycle of the polyols production related to the production of electricity and heat. A cut-off value of 5% was used at the product level. This means that if a product related to a process contributes by more than 5%, this process is associated with one of the sectors (or "other" if no sector fits). If the product contribution is less than 5%, the process related to this product is accounted in the category "other".

4.3.2.1 Contribution analysis results

4.3.2.1.1 Scenario 1: BFG to CO-based polyol

Figure 4.7 (a) shows the results of the contribution analysis for the production of CO-based polyol in Scenario 1 by processing steps. CO-conversion to intermediates and polyol production have the highest impact on almost all impact categories. BFG energy substitution and gas conditioning account for a smaller share of impacts.

Figure 4.7 (b) presents the results of the contribution analysis for the CO-based polyol production in Scenario 1 by sectors. Energy (that includes "fossil energy carrier supply" and "energy generation") has the highest contribution to most impact categories. Also, chemicals are responsible for a large part for the production of polyols. To be specific, EO and the precursor ethylene used in the production of chemicals for the polyol production have high contributions to the impact categories as climate change, acidification, eutrophication (marine and terrestrial), ozone creation and resource depletion. The production of metals is the largest contributing factor to the impact category resources, minerals and metals and plays only subordinate role in acidification, ecotoxicity, and human health effects (carcinogenic and non-carcinogenic).

4.3.2.1.2 Scenario 2: Sequential process – BFG to CO2-based polyol and CO-based polyol

CO_2-conversion to CO_2-based polyol has the highest contribution to all impact categories in Scenario 2 (Figure 4.7 (c)). The other processes play only a minor role.

In Scenario 2, CO_2-conversion to CO_2-polyol is a multifunctional process, and the impacts of this process are allocated over the production of CO_2-based polyol and the production of CO-based polyol.
Thus, the production of CO-based polyol has a share of the impacts of the process CO_2-conversion to CO_2-polyol, although the production of CO-based polyol does not include the CO_2-conversion step (Figure D1 (a) in Appendix D). The process CO_2-based polyol downstream does not contain any direct emissions or environmentally relevant inputs, and thus, does not have any contribution to impact categories (Figure D1 (b) in Appendix D).
The results for contribution analysis for Scenario 2 by sectors (Figure 4.7 (d), Figure D3 (a, b) in Appendix D) are similar to the results in Scenario 1. The environmental impacts across almost all impact categories are driven by energy (that includes "fossil energy carrier supply" and "energy generation") and the production of chemicals. The sector "Chemicals production" is mostly dominated by precursors ethylene and propylene, contributing 8% and 18% to the climate change, respectively. Sodium hydroxide and gaseous chlorine which are the precursors for PO have the highest contribution to non-carcinogenic effects and ozone layer depletion. The production of metals has the highest impact on resources, minerals and metals and a small contribution to ecotoxicity, and human health effects (carcinogenic and non-carcinogenic).

4.3.2.1.3 Scenario 3: Parallel process – BFG to CO2-based polyol and CO-based polyol

The results in Scenario 3 (Figure 4.7 (e)) show the same pattern as in Scenario 2: all impact categories are dominated by the process CO_2-conversion to CO_2-based polyol. However, unlike in Scenario 2, gas
conditioning separates conditioned CO_2 and CO rich streams before the step CO_2-conversion to CO_2-based polyol, and the production of CO-based polyol is not linked to the step CO_2-conversion to CO_2-based polyol. Thus, in the production of CO-based polyol in Scenario 3 (Figure D2 (a) in Appendix D),

the contribution analysis results show the same pattern as in Scenario 1: the main contributors to all impact categories are CO-conversion to intermediate and the production of CO-based polyol and downstream. Similar to Scenario 2, production of CO_2-based polyol and downstream do not show up in the results for the preparation of CO_2-based polyol (Figure D2 (b) in Appendix D).

The contribution analysis results for Scenario 3 by sectors (Figure 4.7 (f), Figure D4 (a, b) in Appendix D) show similar results to those in Scenario 1 and Scenario 2. Overall, the main contributors to almost all impact categories are energy (that includes "fossil energy carrier supply" and "energy generation") and chemicals. However, one difference to Scenario 2 is that the process of the production of CO-based polyol is not linked to the process CO_2-conversion to CO_2-based polyol (using PO). Thus, in the production of CO-based polyol in Scenario 3, the sector "Chemicals production" is dominated by ethylene (contributing approximately one third of the impacts for climate change, acidification, eutrophication (marine and terrestrial), 46% for ozone creation and 62% for fossil resources) (Figure D4 (a) in Appendix D). Also, Scenario 3 differs from scenarios 1 and 2 by the fact that the unconverted BFG is not delivered back to the steel mill and is incinerated onsite by thermal oxidation (without the energy recovery), contributing approximately 15% of the impacts for climate change in the production of CO-based polyol.
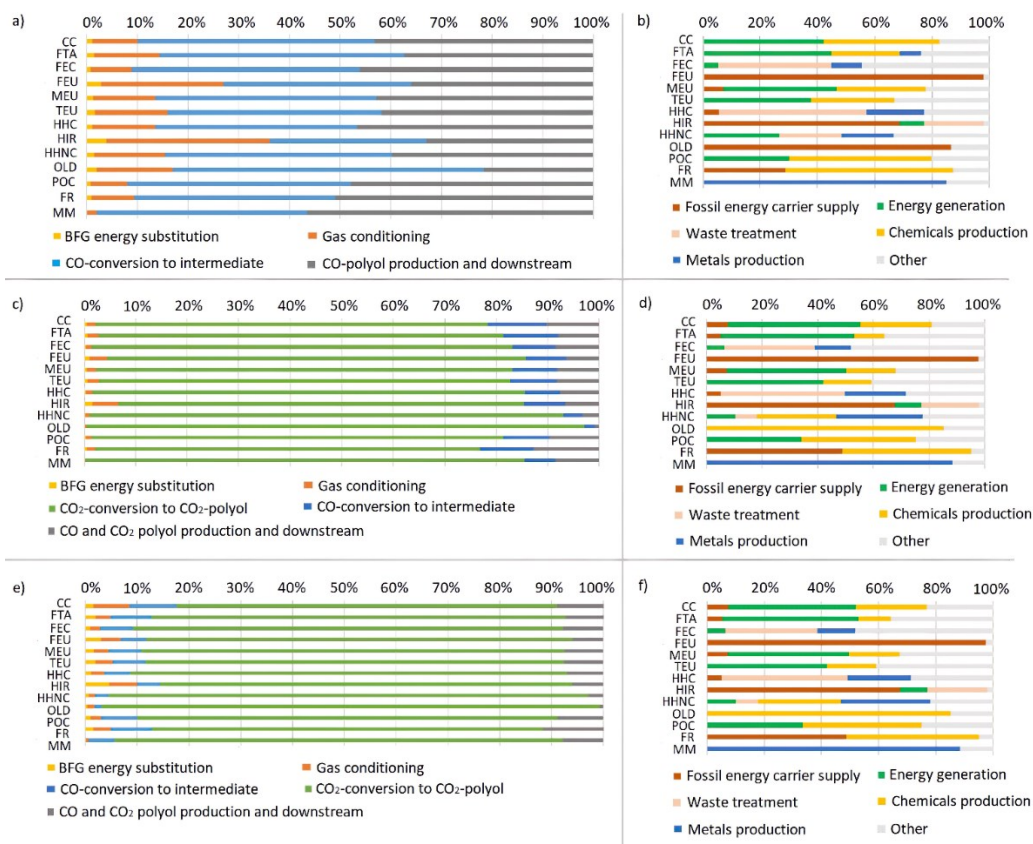
Figure 4.7 *Contribution analysis results by processing steps for a) CO-based polyol for scenario 1, c) for both polyols, CO-based polyol and CO2-based polyol, for scenario 2 and e) for both polyols, CO-based polyol and CO2-based polyol, for scenario 3; Contribution analysis results by sectors for b) CO-based polyol for scenario 1, d) for both polyols, CO-based polyol and CO2-based polyol, for scenario 2 and f) for both polyols, CO-based polyol and CO2-based polyol, for scenario 3.*

4.3.2.2 Scenario comparison

The results of three scenarios cannot be compared directly as the functional units adopted in those scenarios were different. A functional unit for each scenario was formulated as the production of a certain quantity of polyols, a certain quantity of heat and a certain quantity of electricity. However, the quantities of polyols, heat and electricity were different, and thus, resulting in different functional units for scenarios. If the quantity of polyols produced in each scenario were the same and scaled linearly with the quantities of heat and

electricity, three scenarios could be compared directly, however, that is not the case. Instead, we can scale three scenarios to an annual production scale of the CO-based polyol of 50 kt/a, and after that compare their environmental potencies. Specifically, we scaled the differences in the carbon footprint between the baseline system and the CCU technology systems to a production scale of 50 kt/a of the CO-based polyol. It should be noted, that in scenarios 2 and 3, CO_2-based polyol is produced together with the CO-based polyol, and the total quantity of polyols in these two scenarios are much higher than in Scenario 1. Figure 4.8 shows the results of this comparison.

The results show that the environmental potency of Scenario 3 is the most promising among all three scenarios. In Scenario 3, the largest quantity of polyols is produced, and the highest GHG saving is attained of about 90 kt CO_2-eq. per year.

All three CCU technology scenarios 1, 2 and 3 have lower carbon footprint compared to the baseline system. In Scenario 1, the main reasons for having lower footprint are changing the production of heat and electricity from the BFG at the steel mill in the baseline scenario to the production of cleaner heat from an industrial boiler and electricity from the average European grid in the CCU technology scenario, and the reduction of the GHG emissions associated with polyols production. In scenarios 2 and 3, the GHG savings in the production of polyols are dominated by the substitution of PO by CO_2 in the CO_2-based polyol production process. However, in Scenario 3 (unlike in scenarios 1 and 2), the unconverted BFG is not delivered back to the steel mill but is incinerated onsite by thermal oxidation without energy recovery. As a result, the environmental impact caused by the emissions from thermal oxidation decrease partly the substitution effects mentioned above. Possibly, in a future technology implementation, it would be better to recover energy from the unconverted BFG instead of incinerating it.
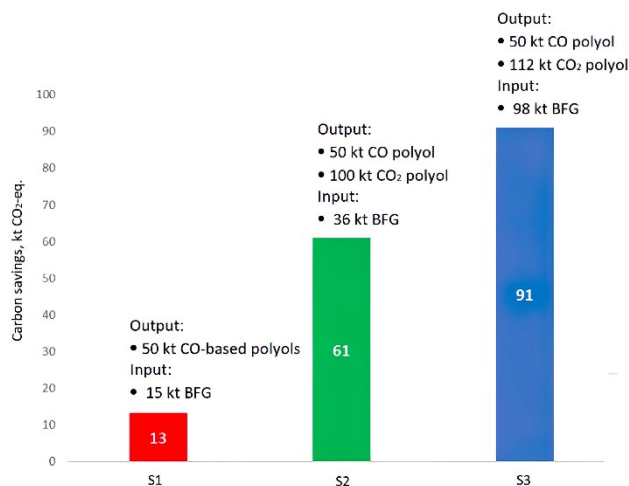
Figure 4.8 *Indication of yearly carbon savings (in kt CO2-eq.) for a 50 kt/a plant CO-based polyol for each scenario; S1 – scenario 1, S2 - scenario 2, S3 – scenario 3.*

4.4 Discussion

Three scenarios of the polyols production from the BFG from the steel production (the CCU technology system) were compared to a baseline system, in which the BFG was partly used to cover the steel mill's heat and electricity needs and partly flared. The comparison excluded those parts of the steel production system that were qualitatively and quantitatively the same in both systems. This approach was adopted as we aimed to determine whether the integrated CCU technology system performs environmentally better than the incumbent system, not focusing on how benefits may be divided between different products. Production of polyols, heat and electricity were all included in the functional units of the systems.

Scenario 3 showed the most promising results. In comparison to the baseline system, this scenario is expected to have 4-15 % lower impacts in most of the impact categories. The context of these results should be interpreted carefully, however. The CCU technology reflects TRL from TRL 2 to TRL 6 (TRL 2 for pressure swing chemical looping, TRL 5 for selective catalytic combustion, the CO-based intermediates production is at TRL 5, and the CO-polyol production and downstream processes are at TRL 6). Ex-ante LCA was carried out for the CCU technology that was upscaled using mainly process simulation

to TRL 9. Since ex-ante LCA of the CCU technology was done at an early phase of development (TRL 2 to TRL 6), there is a possibility for the technology developers to implement improvements to future implementations of the CCU technology to further decrease its environmental impacts. One of the possibilities for improvement determined by this study for the foreground processes of the CCU technology is the use of energy in all three scenarios. Another improvement option could include the use of particularly EO for the production of CO-based polyol in all three scenarios and the use of PO for the production of CO_2-based polyol in scenarios 2 and 3. Most impacts come from the background processes that the technology developers could not affect directly, for example, production of precursors EO and PO. However, a possibility could be to use precursors based on alternative, non-fossil feedstocks, e.g., chemicals from biobased materials or for which higher shares of renewables are applied in their manufacturing process. Furthermore, in the future, other options could be possibly explored to lower the amount of these precursors used in the polyols production by using larger amount of CO/CO_2 from the BFG in polyols and related products. Based on current knowledge and data, Scenario 3 shows ~ 10% reduction in climate change. However, this footprint result is reached by using only up to ~20% CO/CO_2 in the polyols production. This implies that a high improvement potential exists for the current CCU technology scenarios by applying larger amount of CO/CO_2 in the production of polyols by further optimizing technology and addressing new application areas.

Another limitation of our study and of ex-ante LCAs, in general, is that our current (lower TRL) knowledge of the process data may only be a snapshot of what we may know in the end. For example, we currently have no knowledge and were not able to estimate possible emissions related to the novel foreground processes and thus assumed them to be negligible for the time being. Adding improvements related to energy and chemical usage (see above) may result in even better environmental performance of this system, however, filling emissions data gaps may decrease the performance. Thermal oxidation was the only foreground process in the CCU technology system for which the emissions were estimated applying stoichiometric calculations. To be more specific, these calculations allowed to estimate carbon related emissions from incineration of the waste gas containing organic compounds. However, these

emissions may be only a part of the thermal oxidation emissions as other kinds of emissions may also occur depending on the quality of incineration.

Another limitation of this study is that the baseline polyols (phthalic acid polyester polyol and polyether polyol for the novel CO-based polyol and CO_2-based polyol, respectively) were not included at the same level of detail as for the CCU polyols. This is due to confidentiality issues related to the datasets of these baseline polyols. Thus, there is a possibility that the results could as yet change with better data. Also, cyclic propylene carbonate (cPC), that is co-produced with CO_2-based polyol, was excluded from the comparison. This was due to the absence of a baseline chemical for cPC available in the market. Thus, cPC was allocated away on a mass basis, however, this should not significantly affect the comparative results reported in this study since the quantity of co-produced cPC is very small.

Also, we assumed that the waste BFG from the CCU polyol production returned to the steel mill had the same calorific value as the BFG generated from the pig iron production process (see section 4.2.2). In practice, this waste BFG may have 30%-50% less energy, and therefore, may not generate the same quantity of heat and electricity as the BFG produced from pig iron production. However, the results in section 4.3.1 showed that the contribution of producing heat and electricity from the BFG and flaring BFG was very small. Based on these results, it is expected that this assumption would have a negligible effect on the results.

Also, datasets from the ecoinvent v3.4 database (cut-off version) were applied for modelling background processes in the CCU technology system. Better datasets may become available or new assumptions should be made in the future when the CCU technology develops further. Thus, the current results are only valid for the current system, datasets, knowledge, and assumptions applied in this study.

Lastly, it was assumed that the end-of-life of the PUR products using the CCU technology polyols would remain the same as using the baseline polyols, which would imply incineration with associated emissions of CO_2. A possible solution might be to use Carbon Capture and Storage of the CO_2 emitted due to incineration of used PUR products or to adopt a more circular system of reusing the products.

4.5 Conclusion

Ex-ante LCA was carried out to assess the environmental performance of three scenarios of the production of polyols from the BFG from the production of steel (CCU technology system). These scenarios were compared to the baseline system, in which the same amount of the BFG was utilized to produce heat and electricity for the use in the steel mill and flared. The comparison excluded those parts of the steel production system that were qualitatively and quantitatively the same in the CCU technology and the baseline systems. Three research questions were formulated at the beginning of the ex-ante LCA study. These research questions are answered below.

1) What is the overall (integrated system) environmental performance of the CCU technology system compared to the baseline (incumbent) system?

Overall, three scenarios of the CCU technology showed better environmental performance than that of the baseline system, ranging from approximately -20% to +25% for Scenario 1, from 0.5% to 12.5% for most impact categories for Scenario 2 except for ionizing radiation (-4%), and from 4% to 15% for all impact categories for Scenario 3. The scenario comparison showed that Scenario 3 is the most promising among all three scenarios. In this scenario, the GHG saving of about 90 kt CO_2-eq. per year may be achieved assuming yearly levels production of 50 kt/a of CO-based polyol and ~110 kt/a of CO_2-based polyol.

The current results of Scenario 3 showed ~10% reduction in carbon footprint. However, taking into consideration the low-medium TRL level of the CCU technology processes and the possibility of using more CO/CO_2 in polyols in the future, it can be concluded that the current CCU technology scenarios have a considerable potential for further improvement.

2) How can differences in environmental performances be explained in terms of main contributors (hotspots) and components differing between the CCU technology and the baseline system?

In the CCU technology system, thermal oxidation is the only foreground process that was determined as a direct contributor to the carbon footprint (e.g., up to approximately 15% for CO-based polyol in Scenario 3). This is due to thermal oxidation currently being the only foreground process for which it was possible to estimate emissions.

Mostly, environmental impacts are due to chemicals and energy that were used to produce polyols in the CCU technology system.

The carbon footprints of the three scenarios were all identified to be lower than that of the baseline system. This is mainly due to substitution of the production of heat and electricity from the BFG in the steel mill in the baseline system by cleaner heat from industrial boiler and electricity from the average European grid in the CCU technology system, and the reduction of the GHG emissions associated with the use of chemicals utilized in the production of polyols.

3) Do the identified hotspots in the CCU technology system offer options for further improvement?

Contribution analysis showed that possibilities for improvement of the CCU technology scenarios were mostly related to the production of energy and chemicals used to produce the CCU polyols. Using more renewable energy in the CCU technology processes may seem to be an obvious option, but this may help all systems equally not only the CCU technology scenarios but also baseline system. However, using less energy in the CCU technology even after transition to renewable based energy would help to decrease impacts compared to the baseline system. With regards to the improvement possibility for chemicals - EO (all scenarios) and PO (scenarios 2 and 3) used for the CO-based polyols and CO_2-based polyols production, respectively - precursors could be used based on alternative, non-fossil feedstocks, e.g., chemicals from biobased materials or for which higher shares of renewables are applied in their production process. Also, in the future, other ways may be explored to reduce the amount of these chemicals used in the polyols production by using more CO/CO_2 from the BFG in polyols and related products by optimizing the recipes of the polyol production and addressing new application areas.

The conclusions are only valid for the current scenarios developed by the technology developers. The scenarios may show better environmental performance at higher TRLs, however, filling data gaps or including changes in the current LCA assumptions may decrease the performance. It should be noted that the conclusions above are "if …then …" conclusions. *If* the scenarios developed are implemented in practice according to their specifications, *then* the above conclusions can be drawn.

Finally, the purpose of ex-ante LCAs performed for technologies at lower TRLs is to determine possibilities for the environmental improvement and communicate them to the developers of those technologies rather than to estimate their exact environmental impact. This is also true for the CCU technology processes that reflect a TRL between TRL 2 and TRL 6. Therefore, the numerical results presented in this study should not be used in the comparative assertion or benchmarking exercise of product alternatives since the novel technologies assessed might yet change significantly at higher TRLs (so that in practice they may be different from the upscaled technologies using process simulation).

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