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"Carbon4PUR - Turning industrial waste gases (mixed CO/CO_2 streams) into intermediates for polyurethane plastics for rigid foams/building insulation and coatings"

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Deliverable *6.2*: *Baseline LCA on conventionally produced polyol/PUR and steel mill gas treatment*

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Except for ecoinvent v3.4 data, all other data were provided by partners from the Carbon4PUR consortium.

The Carbon4PUR Consortium

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5.	Universiteit Leiden	UL	Netherlands
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7.	Technische Universität Berlin	TUB	Germany
8.	Commissariat à l'énergie atomique et aux énergies alternatives	CEA	France
9.	Arcelormittal Maizières Research SA	AMMR	France
10.	South Pole Carbon Asset Management Ltd.	SPG	Switzerland
11.	Grand Port Maritime de Marseille	MFPA	France
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13.	PNO Consultants BV	PNO	Netherlands
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* At the RWTH two departments are involved: RWTH-AVT (Aachener Verfahrentechnik) and RWTH-CAT (Catalytic Center)

Acronyms and Definitions

Acronym	Defined as
BF	Blast furnace
BFG	Blast furnace gas
BOF	Basic oxygen furnace
BOFG	Basic oxygen furnace gas
CCU	Carbon capture and utilization
CML	Institute of Environmental Sciences – Leiden University
CMLCA	LCA software used at CML
COG	Coke oven gas
EAF	Electric arc furnace
Steel mill gases	COG, BFG, and BOFG
GHG	Greenhouse gas
IPCC	Intergovernmental Panel on Climate Change
IPDI	Isophorone diisocyanate
ISO	The International Organization for Standardization
LCI	Life Cycle Inventory
LCT	Life Cycle Thinking
LCA	Life Cycle Assessment
MDI	Methylene diphenyl diisocyanate
PUR	Polyurethane
R&D	Research and Development
TDI	Toluene diisocyanate

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1. The Carbon4PUR project

Carbon4PUR aims at **turning steel mill gases** (COG, BFG, and BOFG, i.e. mixed CO/CO_2 streams) **into intermediates for polyurethane plastics for rigid foams/building insulation and coatings.**

The industrially driven, multidisciplinary consortium will develop and demonstrate a novel process based on direct chemical steel mill gas mixture conversion, **avoiding expensive physical separation**, thus substantially **reducing the carbon footprint**, and also **contributing to high monetary savings**. The interdisciplinary consortium consists of 14 partners from 7 European countries and across sectors: 4 industries (COV, Recticel, Megara, AMMR), 5 universities (UGent, UL, TUB, RWTH, ICL), 1 association (Dechema), 1 research organization (CEA), 2 service providers (PNO, SPG) and the Grand Port Maritime de Marseille-Fos.

Both the consortium and the work are **organized along the full value chain** starting with the provision and conditioning of industrial emissions **from a steel** (AMMR, UGent) **to a chemical company** (COV) in line with the **concept of industrial symbiosis** exemplarily at *Marseile Fos*, going through the transformation into **chemical building blocks** (CEA, RWTH and COV), which both will be further transformed **into polymer intermediates** (RWTH, COV) and flow into desired sustainable **polyurethane applications of rigid foams and coatings** (Recticel, Megara). **LCA and technology evaluation** will be done (UL, RWTH, TUB, SPG) and **replication strategies** to transfer the technology to other applications will be elaborated (Dechema, PNO, ICL).

The distinctive feature of the developed process is avoiding resource-intense separation of the gas components before the synthesis, and developing a chemo-catalytic process to deal directly with the gas mixture instead. The challenge and innovation is coming up with an adjustable process in terms of on-purpose and demand tailor-made production of required products, taking into account all variables at the same time: the available steel mill gases characteristic from the steel plant, material and process parameters, and the market requirements for the end product, thus flexibly involving the whole value chain with best results and possibly lower the prices.

2. Objectives and Overview

Climate change due to greenhouse gas (GHG) emissions and oil depletion are global challenges, which need to be addressed. The European Union set up a goal of the reduction of the GHG emissions by 40% by 2030 (from 1990 levels) (European Commission, 2014). In order to reach this target, a substantial decrease in carbon emissions in the industrial sector should be made. The iron and steel industry is one of the main industrial CO_2 emitters, producing 4-7% of global emissions (Arens, 2010). The Carbon4PUR project aims at decreasing GHG emissions and dependency on oil by converting steel mill gas CO/CO_2 emissions from steel industry to polyols for polyurethane (PUR) production.

Alternative, renewable feedstocks for the synthesis of PUR building blocks have been investigated. Examples include the production of polyols from vegetable oils (Zlatanić et al., 2002) and from oleochemicals (Heidbreder et al., 1999). More recently, the usage of carbon dioxide for the production of polyols at industrial scale has become an emerging field of carbon capture and utilization research (CCU) (von der Assen and Bardow, 2014). Likewise, the project Carbon4PUR addresses CCU. As a novelty the Carbon4PUR technology shall use gas mixtures and thus omit the energy intensive step of CO/CO_2 separation and purification from steel mill gases (COG, BFG, and BOFG).

Typically, Life Cycle Assessment (LCA) is carried out for mature and implemented technology systems. However, awareness of the need of applying LCA and Life Cycle Thinking (LCT) for emerging technology systems at an early stage of their development has been raised over the past few years. Identification of possible environmental impacts at an early stage of Research and Development (R&D) allows redirecting technology development towards improved environmental performance levels with relatively low costs and high impact, whereas design changes are more difficult to realize during later stages when a technology is close to market implementation.

This is the first LCA report within the Carbon4PUR project and presents the results of the LCA of the conventional fossil-based polyols/PUR production system and current use of the steel mill gas from the steel production system, referred to as the *baseline system*. These results will serve as a reference for evaluating the environmental performance of the novel Carbon4PUR technology (to be published at a later stage of the project).

3. Introduction to Life Cycle Assessment

Life cycle assessment (LCA) has been widely used as a method for the environmental assessment of a product or service. It quantifies environmental impacts of the product system taking into consideration all processes related to the product’s life-cycle and all relevant environmental impacts (Guinée et al., 2002). The life-cycle and multi-impact approach are essential features of LCA as they enable identification of environmental burden shifting to other phases of the life cycle or to other impact categories.

The LCA framework is composed of four phases: Goal and scope definition, Inventory Analysis, Impact Assessment, and Interpretation (ISO 14040 International Standard, 2006). LCA is a highly iterative method. Iteration may be required at any point of an LCA study, which is reflected by the arrows in Figure 1.

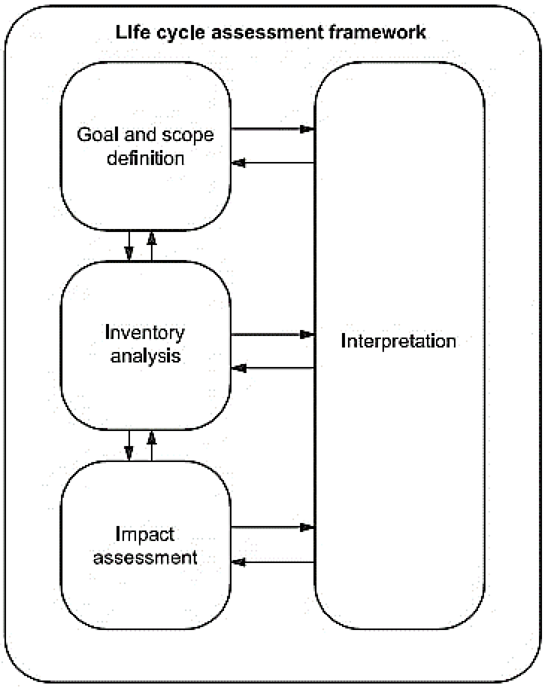

Figure 1: The phases of an LCA (ISO 14040 International Standard, 2006)

The description of each of the LCA phases are as follows (ISO 14040 International Standard, 2006):

1. Goal and scope definition

The goal definition includes the formulation of the aim of the study and the research questions, gives the reasons for performing the research, discusses the possible application(s) of the study and determines the target audience. As part of the scope definition, the system boundaries are defined, the data requirements for the LCA study are defined, and the limitations of the study are discussed.

2. Inventory Analysis

The Inventory Analysis phase includes data collection and calculation of the Life Cycle Inventory (LCI) results. A unit process is the “smallest element considered in the life cycle inventory analysis for which input and output data are quantified” (ISO 14040 International Standard, 2006). Examples of unit processes are coal mining, steel production, refining of oil, production of polyurethane, use of a insulation panel, recycling of waste, and transport by lorry. Each process converts inputs into outputs. Inputs may include products (including components, materials, and services), waste for treatment, and natural resources (including fossils, ores, biotic resources, and land). Outputs may include products, waste for treatment, and residuals to the environment (including pollutants to air, water, and soil). In LCA inputs from the environment and outputs to the environment are referred to as ‘elementary flows’ or ‘environmental interventions’. Eventually, an inventory table is calculated showing all environmental interventions associated with the product system.

3. Impact Assessment

The Impact Assessment phase of life cycle assessment aims at understanding and evaluating the magnitude and significance of the potential environmental impacts for a product system throughout the life cycle of the product” (ISO 14040 International Standard, 2006). Amongst others, this phase includes the classification and characterisation steps. In the classification step, the inventory results are assigned to predefined impact categories on a purely qualitative basis. In the characterisation step the contributions of the classified inventory results to a particular impact category are quantified, using so-called characterization factors, in terms of a common unit for that category, allowing aggregation into a single score: the indicator result. The IPCC Global Warming Potentials provide one example of a set of characterization factors for greenhouse emissions such as CO_2, CH_4, N_2O, etc.

4. Interpretation

Interpretation is the "phase of life cycle assessment in which the findings of either the inventory analysis or the impact assessment, or both, are evaluated in relation to the defined goal and scope in order to reach conclusions and recommendations" (ISO 14040 International Standard, 2006). Several elements are mentioned by ISO (Guinée et al. 2002):

- identification of significant issues;
- an evaluation that considers completeness, sensitivity and consistency checks;
- conclusions and recommendations;
- appropriateness of the definitions of the system functions, the functional unit and system boundary;
- limitations identified by the data quality assessment and the sensitivity analysis.

Additional analyses can be performed as part of the interpretation phase including contribution analysis, sensitivity analysis, perturbation analysis, and uncertainty analysis. The LCA framework reflects an iterative process. Therefore, this LCA study was revised whenever uncertainties appeared to be too high or sensitivity analysis showed that some decisions are crucial. Eventually, conclusions and recommendations are drawn as part of this phase.

4. Outline of the deliverable

The Carbon4PUR project is developing a novel technology that will convert CO/CO_2 gases emitted from steel mill to polyols. A concept of industrial symbiosis will be exemplarily investigated at Marseille Fos, where AcelorMittal has a steel mill and Covestro a PUR production side. PUR produced from novel polyols will be tested by Recticel and Megara for use in rigid foam production for insulation panels and wood coatings. Figure 2 summarizes the concept of the novel Carbon4PUR technology.

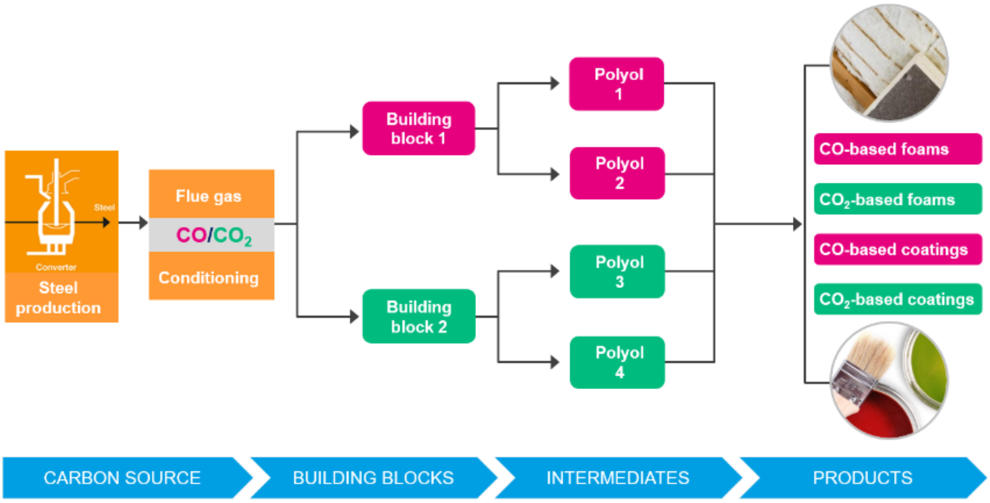

Figure 2: Overview of the novel Carbon4PUR technology

This deliverable reports on the LCA of the baseline system. The baseline system reflects the current steel and fossil-based PUR production systems as they exist before introducing the novel Carbon4PUR technology. The PUR production system can be further divided into two parts: the use of PUR in the manufacture of rigid foam for insulation panels and wood coatings. This deliverable will report on these two parts in two separate chapters:

1. Steel production and current use of steel mill gas in the ArcelorMittal steel mill
2. Conventional way of PUR production

Each of the chapters includes an introduction, method, and results part. The introduction provides a general overview of the baseline system. The method part describes how the different LCA phases are implemented for the analysed production system, and the results section presents and discusses the environmental impact results for different impact categories (results of the impact assessment phase), the results of hot-spot analysis named as *contribution analysis*, and sensitivity analysis results (results of the interpretation phase). Discussion and conclusions are provided at the end of the report.

5. Steel production and current use of steel mill gas in the ArcelorMittal steel mill

5.1 Introduction

The European Union (EU) as a whole is the second largest steel manufacturer in the world. Its production amounts over 177 million tons annually, which is 11% of global production **(**European Commission, n.d.). Two main routes in steel production are generally distinguished: Blast Furnace (BF)/Basic Oxygen Furnace (BOF) route and Electric arc furnace (EAF). The LCA reported in this deliverable concerns a steel production system using the BF-BOF route as it is expected that the BF-BOF route will continue to be the major technology in the steelmaking industry (OECD, 2015).

The BF-BOF route is a complex process, but in general, four main processes can be distinguished: coke production, pig iron production, steel production, and steel rolling. In the coke production, hard coal is converted to coke via destructive distillation in the coke oven at temperatures from 900ºC to 1100ºC for 15 to 30 hours (Michael and Gallaher Brooks, 2002). Next, coke together with iron ore burden is fed to the blast furnace (BF) to produce pig iron. In BF, CO gas released from the coke combustion reduces iron oxides in the iron ore to metallic iron (Geerdes et al., 2015). The steel manufacturing process is carried out in a basic oxygen furnace (BOF). In this process, pig iron and scrap are loaded to the BOF, and oxygen is injected to react with the metal. In BOF, carbon content of pig iron is reduced from approximately 4% to less than 0.1% to produce steel (Barker et al., 1998). In the final stage of the steelmaking process, steel is hot rolled for its final application as plate, sheet, or coil.

The gases released during the steelmaking processes - coke oven gas (COG), blast furnace gas (BFG), and basic oxygen furnace gas (BOFG) - are currently used as energy sources. Energy is recovered from COG, BFG, and BOFG in the power plants of ArcelorMittal to produce heat and electricity. A small part of the steel mill gas is flared.

5.2 Method

Below we describe how the case study on the Goal definition, Scope definition, Inventory Analysis, Impact Assessment, and Interpretation was implemented for the LCA on the steel production and current use of steel mill gas in the ArcelorMittal steel mill.

5.2.1 Goal definition

The aim of this study was to assess the environmental impacts for steel production and the current use of steel mill gas by ArcelorMittal steel mill in Fos-sur-Mer. The research questions were formulated as follows:

1. *What are the environmental impacts of the production of steel?*
2. *Which of ArcelorMittal's processes contribute the most to the impact categories?*

5.2.2 Scope definition

The geographical boundary for this LCA study is France, since the Carbon4PUR industrial symbiosis will be investigated between ArcelorMittal steel mill and Covestro chemical plant in the Port Maritime de Fos-sur-Mer in France.

A cradle-to-gate approach was adopted meaning that assessment of the baseline system was performed starting from the extraction of raw materials and ending with the production of rolled steel.

The energy production and consumption of the steel mill were modelled based on data provided by ArcelorMittal. This data is based on the years of 2014-2015 and is representative for the current state of ArcelorMittal's technology. The ecoinvent version 3.4 (ecoinvent v3.4) database (Wernet et al., 2016) was used for the construction of foreground and background processes. CMLCA software (version 6.0), developed by the Institute of Environmental Sciences (CML) at Leiden University, was used for the LCA calculations.

The function of the steel mill was to produce steel, and the functional unit was defined as the production of 1 kg of hot rolled steel. Likewise, the reference flow was the production of 1 kg of hot rolled steel.

5.3 Inventory Analysis

5.3.1 Flowchart

Figure 3 depicts a simplified version of the flowchart for the baseline system of steel production and the current use of ArcelorMittal steel mill gas.

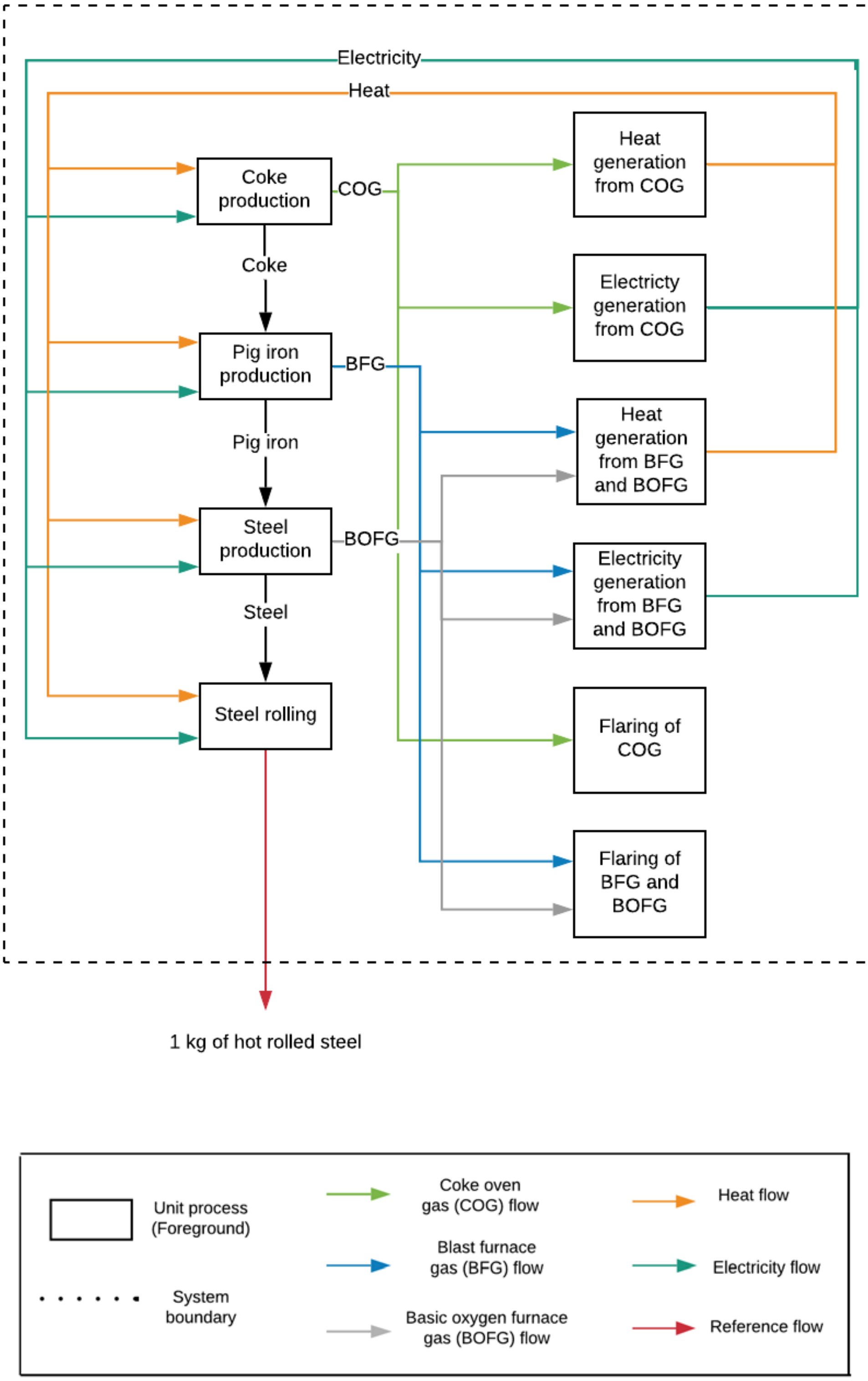

Figure 3: Flowchart for the baseline system of steel production and current use of ArcelorMittal steel mill gas

Note: In this flowchart, heat generation, electricity generation, and flaring are combined for BFG and BOFG as the technosphere flows (except of inputs of BFG and BOFG) and elementary flows associated with the BFG and BOFG heat and electricity generation processes were assumed to be the same.

5.3.2 Data collection

In the LCA of the baseline system for the steel production and current use of ArcelorMittal steel mill gas, coke production, pig iron production, steel production, and steel rolling were modelled using ecoinvent v3.4 processes. The data on the production and consumption of electricity and heat produced from steel mill gas and the data for natural gas and electricity bought from the market were provided by ArcelorMittal. The datasets represent the years 2014-2015, and the average of those years was used for the modelling. According to ArcelorMittal, the thermal and electrical efficiencies for heat and electricity generation from steel mill gas are 0.85 and 0.36, respectively. These efficiency values were used in the construction of the gas treatment processes in the LCA model. Appendix A provides the assumptions and data used for the LCA model of the baseline steel production system.

5.3.3 Multi-functionality and allocation

Coke production, pig iron production, and steel production are multifunctional processes meaning that they represent a unit processes yielding more than one functional flow. In this case all three multifunctional processes are an example of a co-production process, i.e. a process producing more than one valuable product as output. The functional flow of a process is a flow that constitutes the goal of the process, in other words, the product outflows of a production process (Guinée et al. 2002). In the processes mentioned above, coke and COG, pig iron and BFG, steel and BOFG are co-produced, respectively. The non-functional flows of a multifunctional process, i.e. product inflows, waste outflows and emissions, should be allocated to each of the products of these co-production processes. Economic allocation was used for this. Tables 2-4 in Appendix A show the allocation factors.

5.4 Impact Assessment and Interpretation

The ILCD 1.0.8 2016 recommendations for the best available methods were adopted for the characterisation of the inventory results (European Commission JRC-IES, 2012). Nine impact categories were selected:

1. Climate Change
2. Ecosystem quality, freshwater and terrestrial acidification
3. Ecosystem quality, freshwater ecotoxicity
4. Ecosystem quality, freshwater eutrophication

5. Ecosystem quality, terrestrial eutrophication
6. Human health, ozone layer depletion
7. Human health, photochemical ozone creation
8. Human health, respiratory effects, inorganics
9. Resources, mineral, fossils and renewables

5.4.1 Characterisation results

Table 1 shows the characterisation results for 1 kg of hot rolled steel.

Table 1: Characterisation results for 1 kg of hot rolled steel

Impact category	Impact	Unit[1]
Climate change	3.26E+00	kg CO_2 eq.
Acidification	9.21E-03	Mole of H+ eq.
Freshwater ecotoxicity	1.36E+01	CTUe
Freshwater eutrophication	7.70E-04	kg P eq.
Terrestrial eutrophication	1.98E-02	Mole of N eq.
Ozone layer depletion	6.69E-08	kg CFC-11 eq.
Photochemical ozone creation	5.96E-03	kg NMVOC eq.
Human health-respiratory effects, inorganics	1.22E-03	kg PM2.5 eq.
Resource depletion-mineral, fossils and renewables	2.91E-05	kg Sb eq.

5.4.2 Contribution analysis results

The contribution of processes responsible for these characterisation results was analysed and the results are shown in Figure 4. The impacts displayed in Figure 4 for coke production, pig iron production, steel production, and steel rolling represent the aggregated impacts associated with these processes, with the operations of the BF and BOF heat and electricity generation and the steel mill gas flaring processes, and with the supplying or management processes of the production of raw materials, energy, and waste treatment required for these processes.

[1] A comprehensive overview of the ILCD impact assessment methods including units and abbreviations readers are invited to refer to page 3, table 1 of http://eplca.jrc.ec.europa.eu/uploads/LCIA-characterization-factors-of-the-ILCD.pdf

The results of the contribution analyses show that most of the impact categories are dominated by the impacts related to pig iron production. A similar result was obtained by Hu et al. (2014).

Steel production has the highest contribution to resource depletion, constituting about 63% of the total impact of steel. Steel rolling related impacts contribute 10%-25% to all impact categories. Coke production has the lowest impact results among other processes.

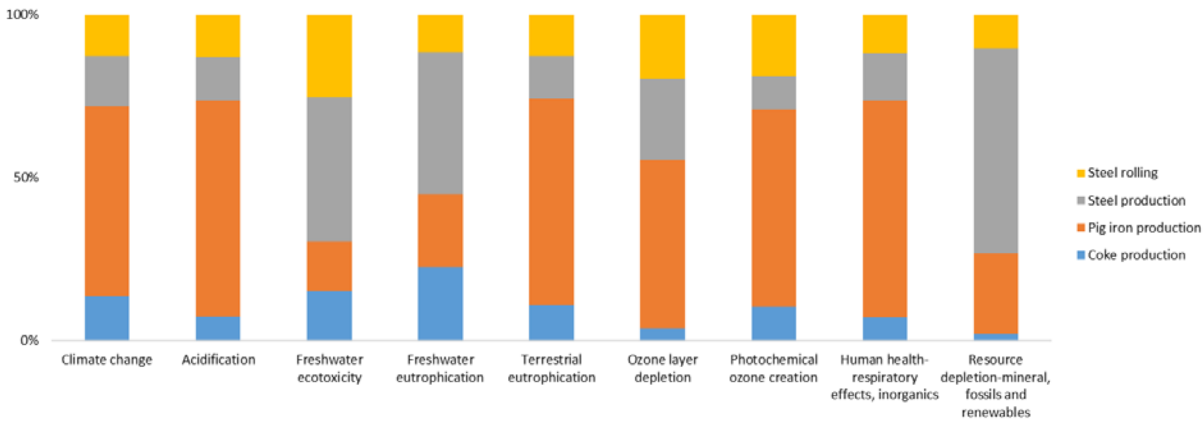

Figure 4: Process contributions for hot rolled steel

Figures A1-A10 in Appendix A show the results from more detailed contribution analyses. Contribution analyses were performed at the level of processes and elementary flows in order to determine, which of the supply-chain processes and emissions are responsible for which impacts. The results showed that the climate change results were mainly caused by carbon dioxide emissions to air from pig iron production, heat production from BFG, and electricity production from BOG (Figure A.2). The acidification results appeared to be mainly caused by the release of sulphur dioxide to air from sinter production and from transport by transoceanic ship (Figure A.3). Freshwater ecotoxicity is caused by the release of chromium ions to ground water from the treatment of BOF waste in a landfill, and by zinc ions released to ground water from the treatment of spoil from hard coal mining in a landfill (Figure A.4). Freshwater eutrophication is mainly dominated by the release of phosphates to ground water from the treatment of spoil coming from hard coal mining in a landfill, and from the treatment of BOF waste in a landfill (Figure A.5). Nitrogen oxides released to air from transport by transoceanic ship and sinter production are the main contributors to terrestrial eutrophication (Figure A.6). Bromotrifluoromethane (Halon 1301) emitted to air from petroleum and gas production is the main contributor to ozone layer depletion (Figure A.7). Photochemical ozone creation is mainly caused by the emission of nitrogen oxides to air from transport of goods by transoceanic ship (Figure A.8). According to Figure A.9, respiratory health effects are mainly originating from particulates emissions to air from the sinter production and the iron mine operation. Resource depletion is mainly dominated by the use of nickel silicates and nickel ore in Ferronickel production and by mining of indium sulphide, lead, zinc, silver, and cadmium.

5.4.3 Sensitivity analysis results

The impact results of the baseline system were compared to the impacts of the production of rolled steel as modelled in the ecoinvent database version 3.4. The steel mill model developed in this analysis will be referred to as the *ArcelorMittal model*, and the steel mill model as present in the ecoinvent database will be called *ecoinvent model*. As shown in Figure 5, the characterisation results for the *ecoinvent model* differ from those for the *ArcelorMittal model* (biggest difference is observed in the category “climate change”).

The most important difference between the two models is the underlying energy model for the production of process heat and electricity for steel production. While the *ArcelorMittal model* assumes that process heat and electricity are mostly internally produced from the steel mill gases, the *ecoinvent model* assumes that heat and electricity are supplied by regional consumption mixes (meaning that heat and electricity are supplied by a mix of technologies, e.g. natural gas, nuclear, and renewables). Different impact assessment results should be expected due to the different energy carriers and technologies involved in the heat and electricity production, i.e. from steel mill gases that stem from hard coal combustion in the *ArcelorMittal model* versus regional consumption mixes for heat and electricity from Germany, Europe, and Global markets in the *ecoinvent model*.

In order to assess the influence of the different energy supply models, Figure 5 presents a sensitivity analysis for the case that the *ArcelorMittal model* would use *electricity from the market* instead of producing it from steel mill gases and for the case that the *ArcelorMittal model* would use *heat and electricity from the market* instead of producing these from steel mill gases.

While this sensitivity analysis is not capable of explaining the observed differences between the two models for all impact categories, it shows that the impact on climate change is highly sensitive to the energy sources used in the steel mill. It further indicates that ecoinvent may be underestimating the climate change impact of steel production as it does not include the production of heat and electricity from steel mill gases in the steel production, but instead builds upon the assumption that (cleaner) heat and electricity can be obtained from the market. Therefore, our model is likely to be a more realistic representation of steel production as it includes the internal use of steel mill gases for heat and electricity based upon site-specific data.

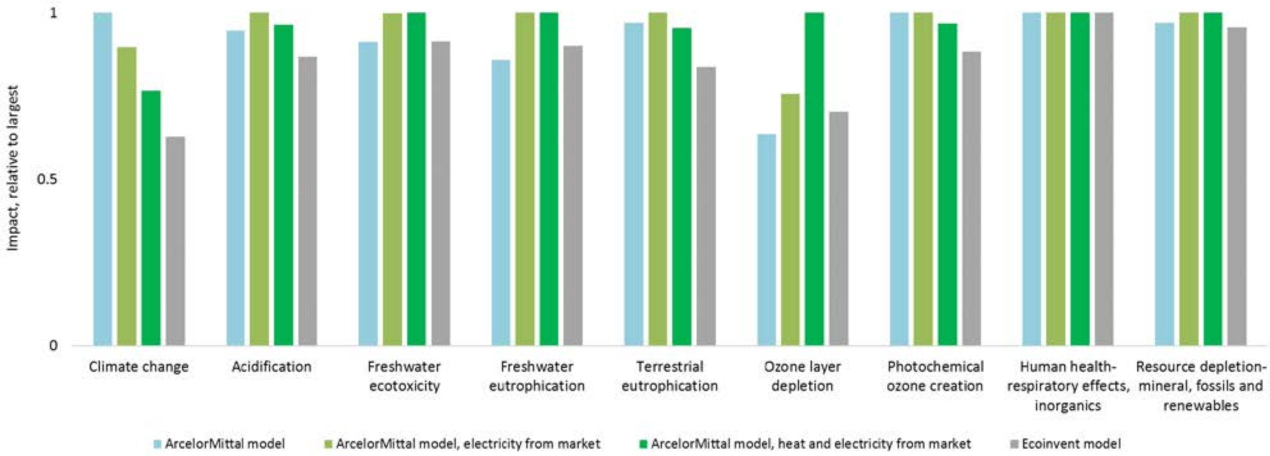

Figure 5: Sensitivity analyses for different assumptions on electricity and heat sources for the steel mill process and comparison with steel from the ecoinvent v3.4 database

6. Conventional way of PUR production and its applications

6.1 Introduction

Polyurethane (PUR) is one of the most widely used polymers worldwide. It covers a broad range of different applications. It can be used for the manufacture of flexible foam for furniture, rigid foam for roofs and insulation walls, for the production of paints, adhesives, sealants, elastomers for automotive interiors and floors, and as thermoplastic for footwear and medical devices such as biofilms and catheters (Melo and Cavaco, 2012). PUR is characterised by urethane groups (-$NHCO_2$) in its backbone chain, and is traditionally produced from alcohols (mainly polyols) and isocyanates (Ionescu, 2005):

$$\underbrace{R{-}N{=}C{=}O}_{\text{isocyanate}} + \underbrace{HO{-}R'}_{\text{alcohol}} \longrightarrow \underbrace{R{-}NHCOO{-}R'}_{\text{urethane}}$$

Equation 1: ***PUR synthesis from alcohol and isocyanate (Ionescu, 2005)***

The structure of PUR is comprised of soft segments and hard segments formed from polyols and isocyanates, respectively (Bajsic et al., 1996). Factors such as volume fractions and chemical composition of soft and hard segments, their distribution, and the degree of cross-linking all affect chemical, physical, and thermal properties of PUR (Kong and Narine, 2007). These factors could be controlled by varying the stoichiometric ratio between polyols and isocyanates. Different types of polyols are used in the production of PUR, and the most common are polyester polyols and polyether polyols. The most well-known isocyanates that are used for PUR production are aromatic diisocyanates such as toluene diisocyanate (TDI) and methylene diphenyl diisocyanate (MDI) and aliphatic diisocyanates, e.g. hexamethylene diisocyanate (HDI) and isophorone diisocyanate (IPDI).

In the LCA of the baseline system, polyester polyols were considered for the conventional PUR production processes as the structure of this type of polyols might be comparable to the structure of the novel polyols produced from CO/CO_2 steel mill gas. In general, polyester polyols are synthesised from polyhydric alcohol with polycarboxylic acid, its derivative or a polycarboxylic anhydride (Singh, 1997). In this LCA, it was assumed that MDI was used for the production of PUR for rigid foam and aliphatic diisocyanate was used for the production of PUR for coatings based on data provided by Recticel and Megara.

Preparation of rigid foam for insulation panels is carried out in one step by mixing polyols (polyester or polyether polyols), diisocyanates, and additives such as fire retardants, surfactants, catalysts, water, and blowing agents (Roth, 2003). The insulation panel is produced from rigid foam and the multi-layer facing made of aluminium foil. The multi-layer facing is used as a protective layer in the insulation panel (Hansbro et al., 2013).

In the production of wood coating, a PUR dispersion is prepared, and then blended with an aqueous paste of water and adjuvants in the mixing apparatus (Jahns et al., 2017). The PUR dispersion is achieved by the reaction of polyols, e.g. polyester, polyether, or polycarbonate polyols and aliphatic diisocyanates, and then dispersed into the mixture of water/neutralizing agent at a temperature between 20-100ºC (Zander et al., 2003). Different kinds of additives can be used such as catalysts, thickeners, defoamers, dispersing assistants, emulsifiers, and matting agents depending on the exact application (Munzmay et al., 2004).

6.2 Method

6.2.1 Goal definition

The goal of this LCA was to evaluate the environmental performance of the conventional way of PUR production and its applications.

The research questions were defined as follows:

1. *What are the environmental impacts of the production of an insulation panel?*
2. *Which processes in the insulation panel production system contribute the most to the impact categories selected?*
3. *What are the environmental impacts of wood coating?*
4. *Which processes in the wood coating production system contribute the most to the impact categories selected?*

6.2.2 Scope definition

The geographical boundary was defined to be Europe. A cradle-to-gate approach was adopted again for the LCA performed. Recticel and Megara provided data for the manufacturing processes of the insulation panel and wood coating. This data covers the present state of production technology for the manufacture of insulation panels and wood coatings. Ecoinvent v3.4 was used for the construction of the background processes for insulation panels and wood coatings. CMLCA software (version 6.0) was used for LCA calculations.

The function of the insulation panel is to provide thermal insulation properties to a building wall. The lifetime of the insulation panel was assumed to be approximately 60 years. The functional unit was defined as the coverage of 1 m² of a building wall with a U-value maximum of 0.24 W/m²K for 60 years. The reference flow was defined as the use of 2.85 kg of PUR to produce the insulation panel with a U-value maximum of 0.24 W/m²K for the coverage of 1m² of a building wall for 60 years.

The function of the coating (applied as a paint) produced from PUR is to protect a wooden panel against rotting. The lifetime of the coating was assumed to be approximately 10 years. The functional unit was defined as the coverage of 1m² of a wooden panel by an exterior coating for 10 years. 0.1 litre or 0.125 kg of coating is needed to paint 1m² of wooden panel. The reference flow was defined as the use of 0.125 kg of PUR-coating to paint 1m² of a wooden panel for 10 years.

6.3 Inventory Analysis

6.3.1 Flowcharts

Figures 6 and 7 show the flowcharts for the baseline systems of the insulation panel and wood coating, respectively.

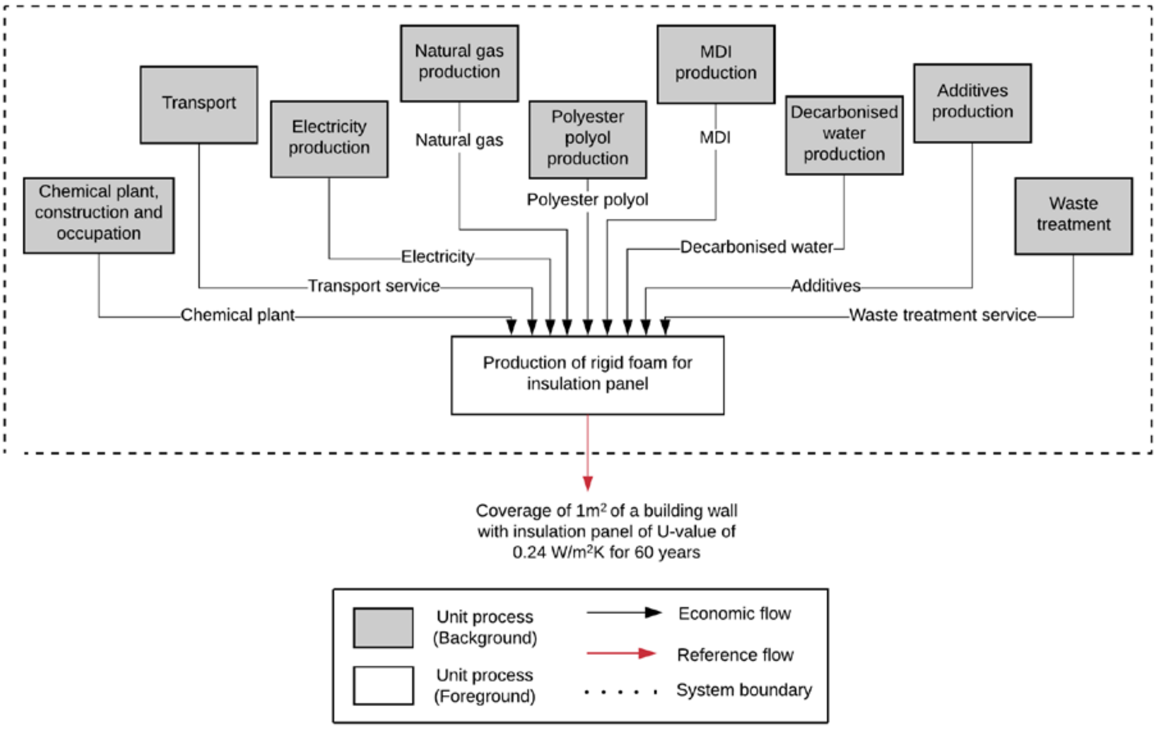

Figure 6: Flowchart for the baseline system of the conventional way of PUR production and PUR use in the insulation panel manufacture

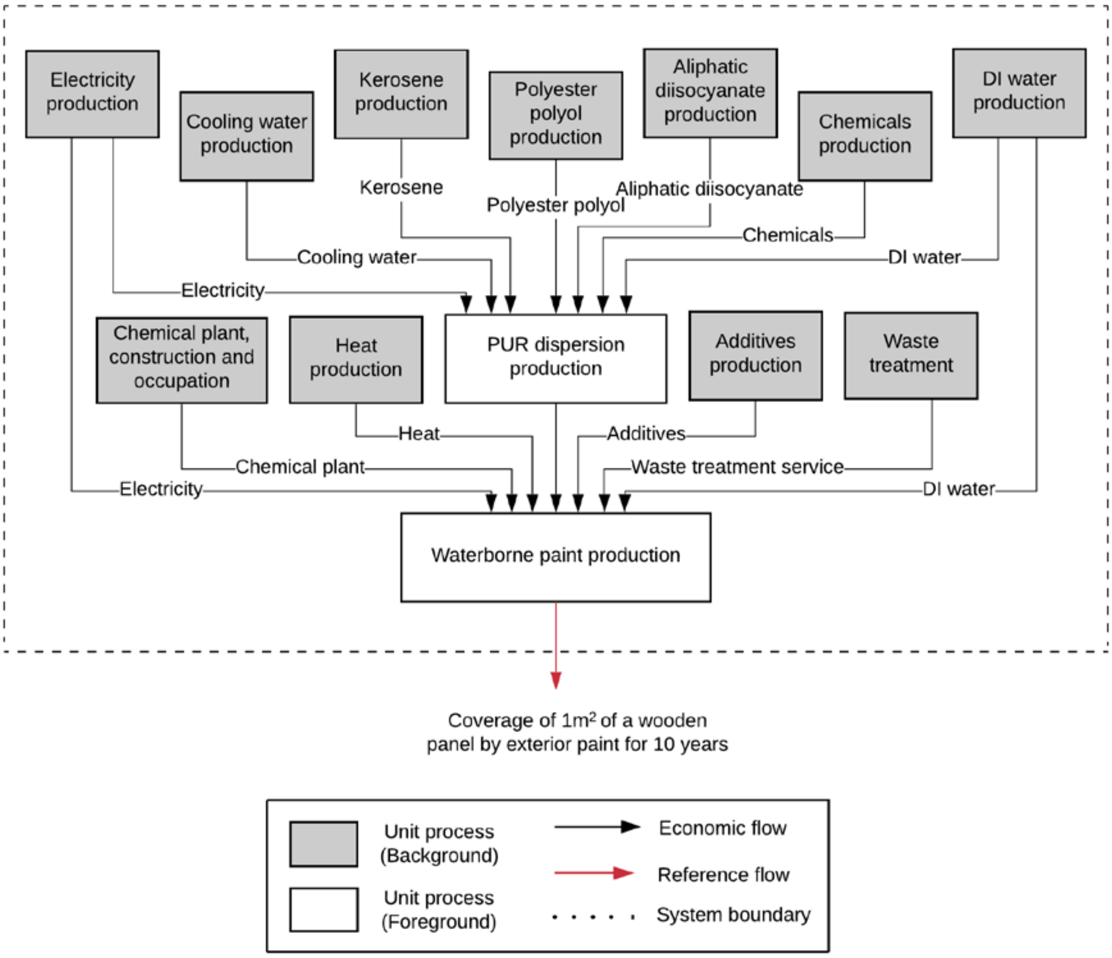

Figure 7: Flowchart for the baseline system of the conventional way of PUR production and PUR use in the wood coating manufacture

6.3.2 Data collection

Ecoinvent v3.4 was used for modelling background processes for the insulation panel and the wood coating (paint) production. The inputs and outputs for the insulation panel and wood coating production systems were modelled based on confidential data provided by Recticel and Megara, respectively. The amount of energy used in the PUR dispersion production for wood coating had to be estimated. The amounts of heating oil and cooling water, the energy for heating and cooling the reaction were calculated by TUB based on data provided by Megara. Production of kerosene was modelled in LCA as the heating oil. The energy required for stirring the PUR dispersion was not included in the LCA model. The amount of energy used for the production of the coating was adapted from the ecoinvent process of paint production. The value for the chemical plant construction was obtained from the ecoinvent process.

Data for adipic acid polyester polyols, phthalic anhydride polyester polyols, and aliphatic diisocyanate were kindly provided by Covestro. This data was due to incompatibility of software tools, not available as unit process data, but instead had to be combined with our process models at the level of impact assessment results using a separate spreadsheet.[2] For this reason, detailed process and elementary flow contributions could not be calculated for these three products. While this represents the most practical approach to include these products within our model, it may have introduced some inconsistencies, e.g. in terms of the underlying impact assessment models (cf Herrmann and Moltesen, 2015; Speck et al., 2015).

Due to these difficulties, the LCA data for wood coating and insulation panels should be considered as rather uncertain. While it was not possible to obtain better data within the deadline for this deliverable, further data collection is ongoing in order to ensure fair baseline scenarios for the comparison with the technologies developed in the Carbon4PUR project (future deliverables). Due to the uncertainty of the data we refrain from showing the impact assessment results.

6.4 Impacts Assessment and Interpretation

The ILCD 1.0.8 2016 recommended midpoint methods (European Commission JRC-IES, 2012) were used for the LCAs of the insulation panel and wood coating. The same impact categories were selected as for LCA on the steel production and steel mill gas treatment system.

6.4.1 Characterisation results

As discussed in 6.3.2, midpoint indicator characterisation results were calculated, but are not reported here in order to prevent a literal citation of the numbers given the likelihood of high uncertainties. Instead process contribution analyses are provided in the following.

[2] Data from Covestro was calculated in the GaBi (version 8.5) software using the ILCD 1.0.8 2016 impact assessment method. It was also available as elementary flows (aggregated inventory). However, due to different naming conventions in GaBi and the ecoinvent database, attempts to import this data into the CMLCA software used by Leiden University were not successful.

6.4.2 Contribution analysis results for the insulation panel production system

Figure 8 represents the results of the contribution analysis (interpretation) for insulation panel production. The results show that most of the impact categories are dominated by the impacts related to the use of MDI for PUR production and the use of aluminium for the manufacture of the multi-layer facing. The production of phthalic anhydride polyester polyol does not show a high contribution to any of the characterisation results (0-9% depending on the impact category).

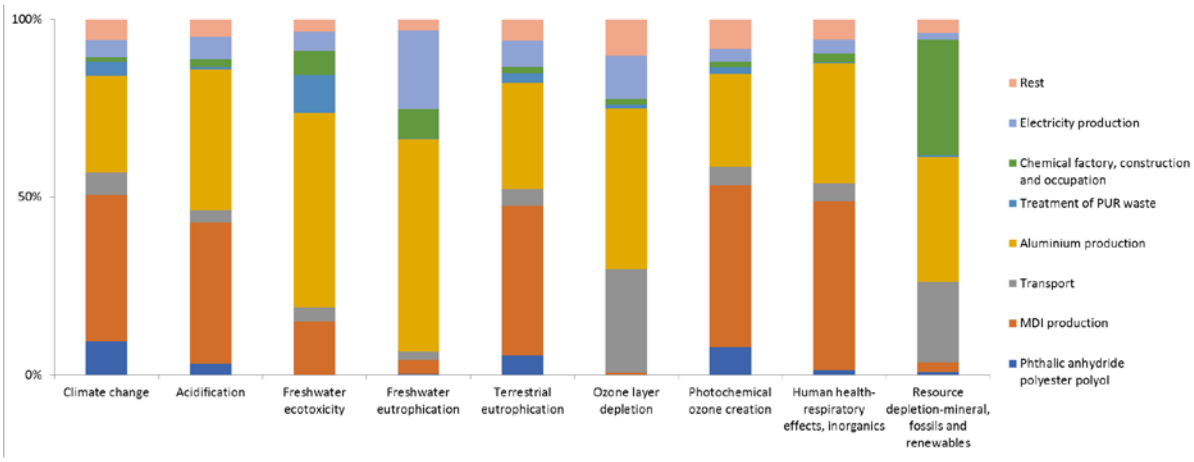

Figure 8: Process contributions for insulation panel production

6.4.3 Contribution analysis results for wood coating production system

Figure 9 shows the process contributions for the coating production. The results show that most of the impact categories are dominated by the production of PUR dispersion (21-74%). The second largest driver for impacts is process energy demand (heat and electricity). For the impact categories freshwater ecotoxicity, freshwater eutrophication and resource depletion the construction and use of the chemical factory additionally is of some importance, however, mainly driven by the absence of other relevant impact sources in these categories.

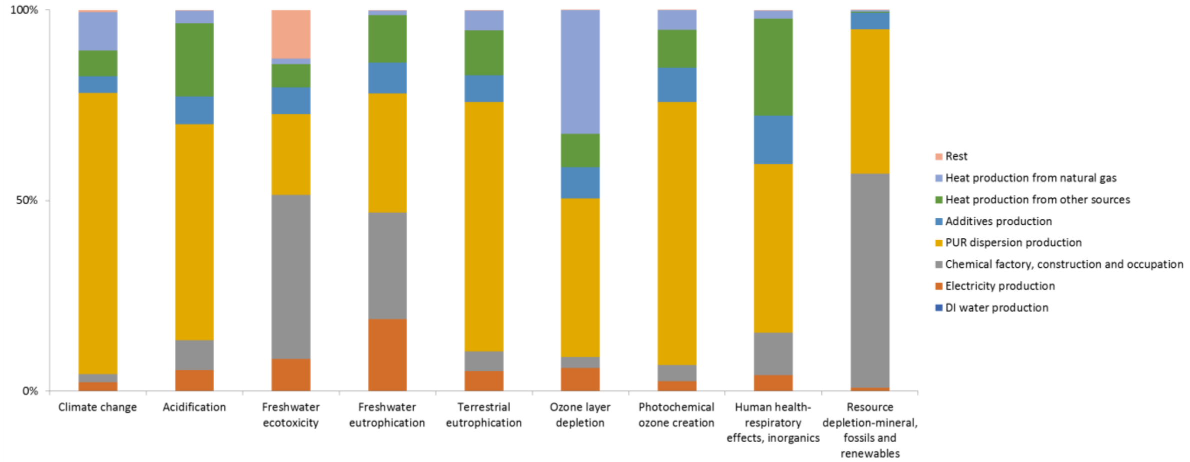

Figure 9: Contribution analysis results for wood coating

6.4.4 Contribution analysis results for the PUR dispersion production process of the wood coating system

Production of the PUR dispersion is the main cause of the environmental impacts in the coating production system for most of the impact categories. Therefore, an additional contribution analysis of PUR dispersion was performed in order to determine the sources of high impacts of this specific process. Figure 10 shows the process contributions of PUR dispersion. The results show that the production of adipic acid polyester polyol has high contributions to climate change, acidification, terrestrial eutrophication, and photochemical ozone creation. Aliphatic diisocyanate production contributes the most to resource depletion accounting for 70% of impacts. The production of kerosene, which is used for heating the reaction, has high contributions to ozone layer depletion (46%). The production of other chemicals contributes between 8% - 60% depending on the impact category considered. A further disaggregation of these chemicals was not possible due to the confidentiality of the data.

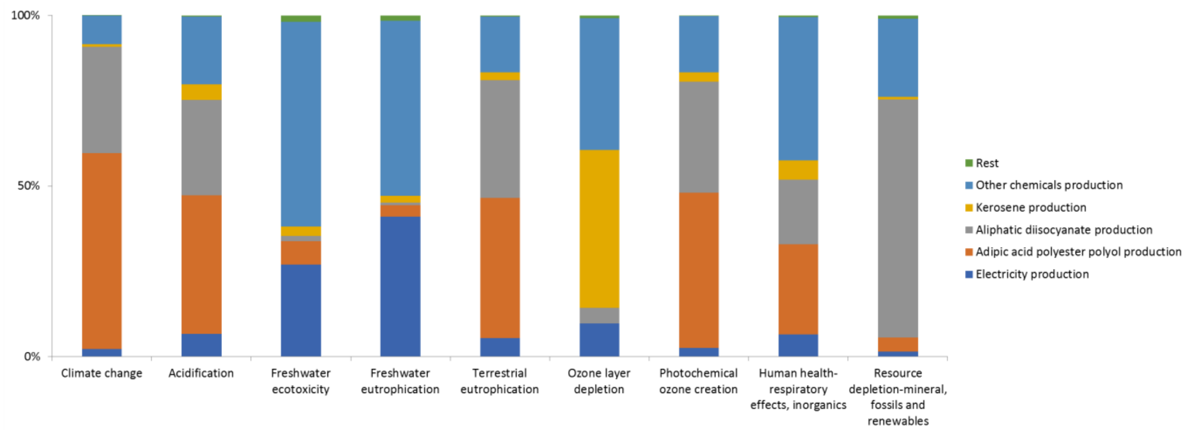

Figure 10: Contribution analysis results for the PUR dispersion process

7. Discussion, conclusions, and outlook

In the Carbon4PUR project, new technologies are being developed that aim at converting steel mill gases from steel production to polyurethane based applications such as insulation panels and wood coatings. The goal of this report was to develop process models that reflect the current state of these technologies (i.e. baseline scenarios for the production and use of steel mill gas in a steel mill and conventional production of insulation panels and wood coatings). The purpose of these baseline scenarios is to have a benchmark against which the technologies developed in the Carbon4PUR project can be compared to in future work with the aim of guiding technology development towards the most environmentally sustainable pathways.

A process model of hot rolled **steel production** of the ArcelorMittal steel mill in Fos-sur-Mer was built in order to have a baseline for the steel mill gas production. The model consists of the four main steelmaking processes, i.e. coke, pig iron, steel production and steel rolling, and includes several processes that describe the production and energetic use of steel mill gas. While steel mill gas itself is not a product of the steel mill at this stage (it is internally used), the environmental contributions within the steel mill are related to a large extent to two driving processes: pig iron production and steel production contribute to 15%-67% and 10%-63%, respectively, to the environmental impacts of the steel mill depending the impact category. These impacts are strongly linked to the inputs to pig iron and steel production, as shown in Fig. A1, and an important share is associated with the required process energy.

A **sensitivity analysis** was conducted for the source of heat and electricity for steel production. It was shown that the internal production of heat and electricity from steel mill gas is associated with substantial impacts, e.g. on climate change, as the steel mill gas derives essentially from the combustion of coal. If heat and electricity were supplied from other sources (as in the model contained in the ecoinvent v3.4 database), their impact would be different (lower for climate change). Obviously, this remains a hypothetical discussion as steel mill gases are co-products of the steel production processes and are used internally for energy purposes in the Fos-sur-Mer plant of ArcelorMittal (which is why we conclude that our models is a more realistic representation than the ecoinvent model, which assumes a supply of heat and electricity from regional markets).

Nevertheless, the sensitivity analysis touches upon a number of issues that need to be considered for a **future use of steel mill gas** in Carbon4PUR technologies: if steel mill gas is not available as an energy source for steel production, another energy source will have to be tapped. Consequently, steel mill gas is not a freely available waste product (due to its energy content). Instead, it must be considered as a co-product of steel production (the reason we built an LCA model for it), which means that it will most likely be associated with environmental impacts. To quantify these environmental impacts is not straightforward, as there is not one objective solution, but a number of techniques within the LCA methodology that can be applied to deal with multi-functional processes, such as allocation and system expansion. This report does not quantify the environmental impacts associated with steel mill gas on purpose, as it is not part of the current system (baseline). Instead, this will be done in our upcoming work on lab and pilot scale models for the Carbon4PUR technologies under development (future scenarios).

Concerning the conventional polyurethane production and its applications, characterisation results for 1m^2 of **insulation panel** were calculated. Contribution analysis showed that MDI production and the production of aluminium used for the preparation of the multi-layer facing are the main contributors for all of the impact categories. The production of phthalic anhydride polyester polyol only contributed to a smaller degree (0-9%) of the overall impacts of insulation panel.

Next, characterisation results for a PUR-based **wood coating** were calculated. The characterisation results showed that the production of the PUR dispersion is the main contributor to most of the characterisation results for the coating production system, accounting for 21%-74% of the results depending on the specific impact category. A contribution analysis of the PUR dispersion process was done to determine the cause of the prominent result for this process. The analysis showed that different process inputs are responsible for high contributions of the PUR dispersion production process depending on the impact category. Adipic acid polyester polyol appeared to be the main cause for climate change, acidification, terrestrial eutrophication, and photochemical ozone creation 41%-58%. Aliphatic diisocyanate showed highest contributions to resource depletion (70%). Kerosene production is the main contributor for ozone layer depletion. The production of other chemicals contributed between 8%-60% depending on the impact category considered.

In our **upcoming work** we will assess the prospective environmental impacts of the technologies developed in the Carbon4PUR project at the lab and pilot scales. The baseline scenarios developed in this deliverable will serve as a reference to evaluate the environmental impacts of these technologies against and to guide technology development from an environmental sustainability perspective. In addition, data for the baseline scenarios for wood coating and insulation panels will be improved to reduce the uncertainties of impact assessment results. In future Carbon4PUR supply chains, different environmental profiles can be expected not only due to the use of the newly developed technologies, but also due to the new carbon source from steel mill gas.

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9. Appendix A

9.1 Assumptions for the calculations

Table A.1: Values used in the calculations performed

	Value	Unit	Source
Steel mill capacity	4,000,000	tonnes/year	ArcelorMittal
Lower heating value COG	18.53	MJ/Nm^3	ArcelorMittal
Lower heating value BFG	3.45	MJ/Nm^3	ArcelorMittal
Lower heating value BOFG	8.9	MJ/Nm^3	ArcelorMittal
Lower heating value NG*	38.75	MJ/Nm^3	ArcelorMittal
Lower heating value NG*	40	MJ/Nm^3	Classen et al., 2009
Calorific value for coke	28.6	MJ/kg	Classen et al., 2009
Calorific value for hard coal	28.6	MJ/kg	Classen et al., 2009
Electrical efficiency for electricity production from steel mill gas	0.36		ArcelorMittal
Thermal efficiency for heat production from steel mill gas	0.85		ArcelorMittal
Efficiency of converting natural gas into heat	0.94		Wernet et al., 2016
Efficiency of converting hard coal into heat	0.79		Wernet et al., 2016

*Note: the lower heating value for NG 38.75 MJ/Nm3 was used in the calculations using ArcelorMittal data, while the lower heating value for NG 40 MJ/Nm3 was used in the calculations using Ecoinvent v3.4 data.

Table A2-A4 show the allocation factors for the production of coke, pig iron and steel. The allocation factors are based on price data calculated by TUB (confidential).

Table A.2: Allocation factors for the production of coke

Functional flow	Allocation factor
Coke (outflow; MJ)	0.828
COG for heat (outflow; MJ)	0.126
COG for electricity (outflow; MJ)	0.046

Table A.3 Allocation factors for the production of pig iron

Functional flow	Allocation factor
Pig iron (outflow; kg)	0.892
BFG for heat (outflow; MJ)	0.067
BFG for electricity (outflow; MJ)	0.041

Table A.4 Allocation factors for the production of steel

Functional flow	Allocation factor
Steel (outflow; kg)	0.994
BOFG for heat (outflow; MJ)	0.005
BOFG for electricity (outflow; MJ)	0.001

9.2 Process contributions for hot rolled steel

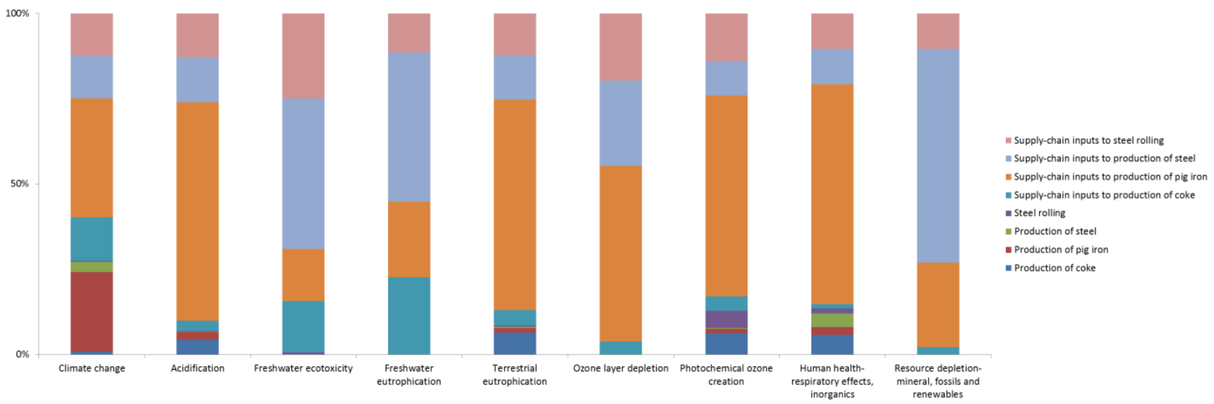

Figure A.1: Process contributions for hot rolled steel

9.3 Process and elementary flow contributions for hot rolled steel

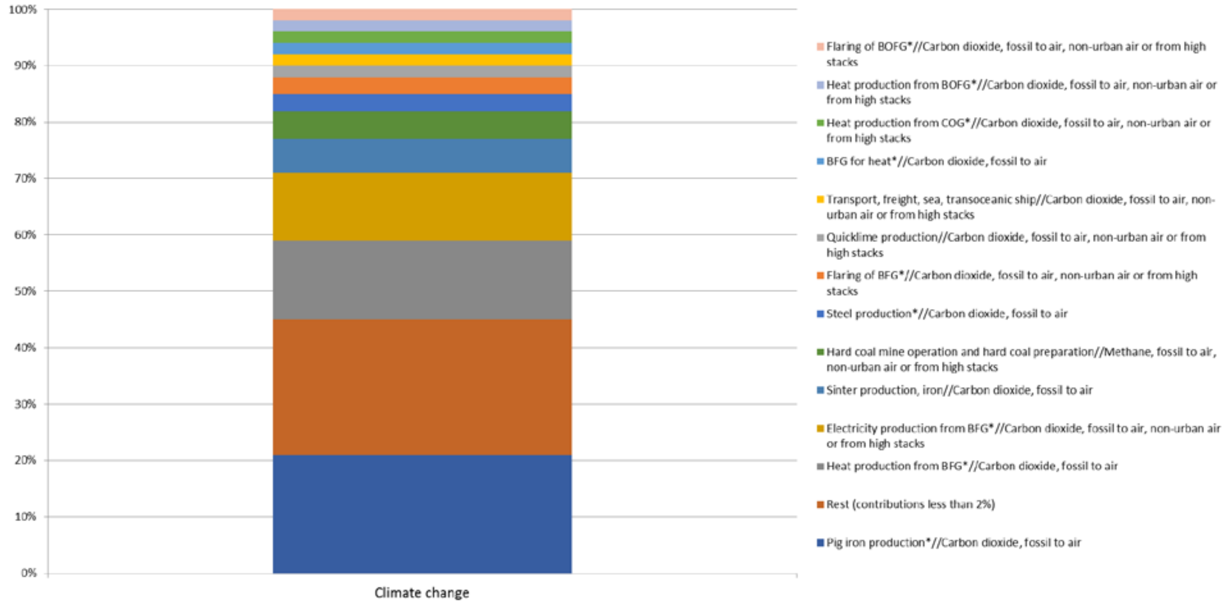

Figure A.2: Process and elementary flow contributions for the baseline system of steelmaking process for climate change

*Foreground process

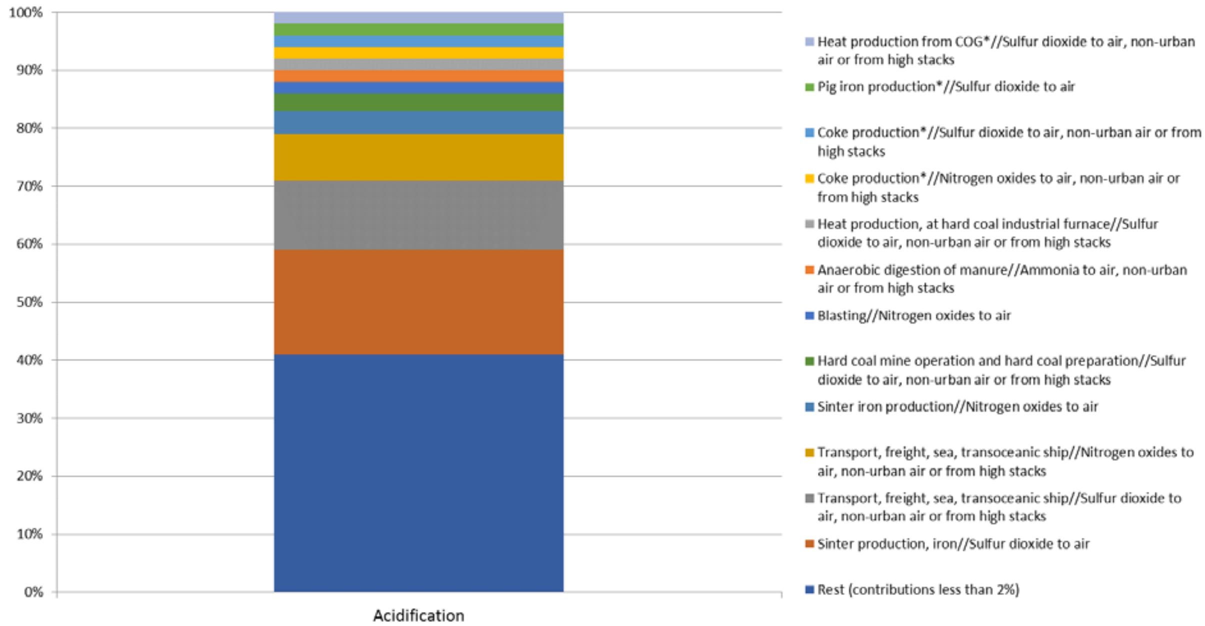

Figure A.3: Process and elementary flow contributions for the baseline system of steelmaking process for acidification

*Foreground process

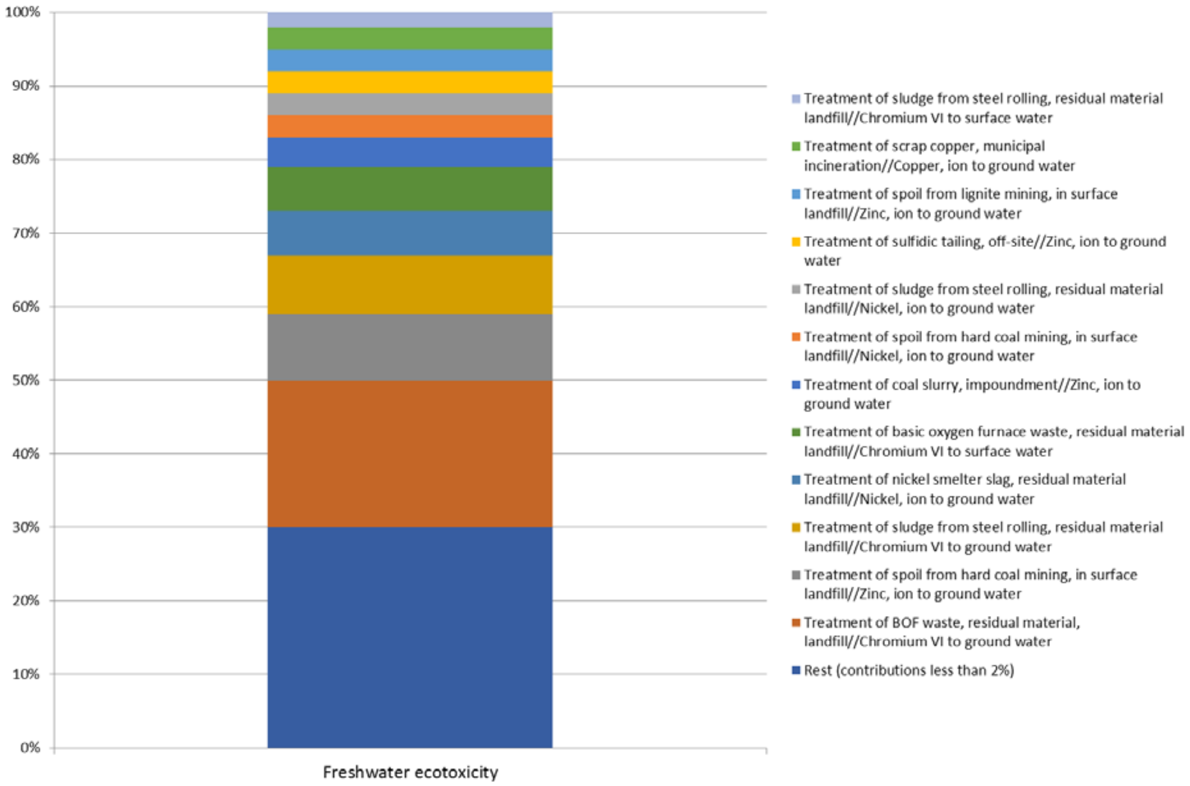

Figure A.4: Process and elementary flow contributions for the baseline system of steelmaking process for freshwater ecotoxicity

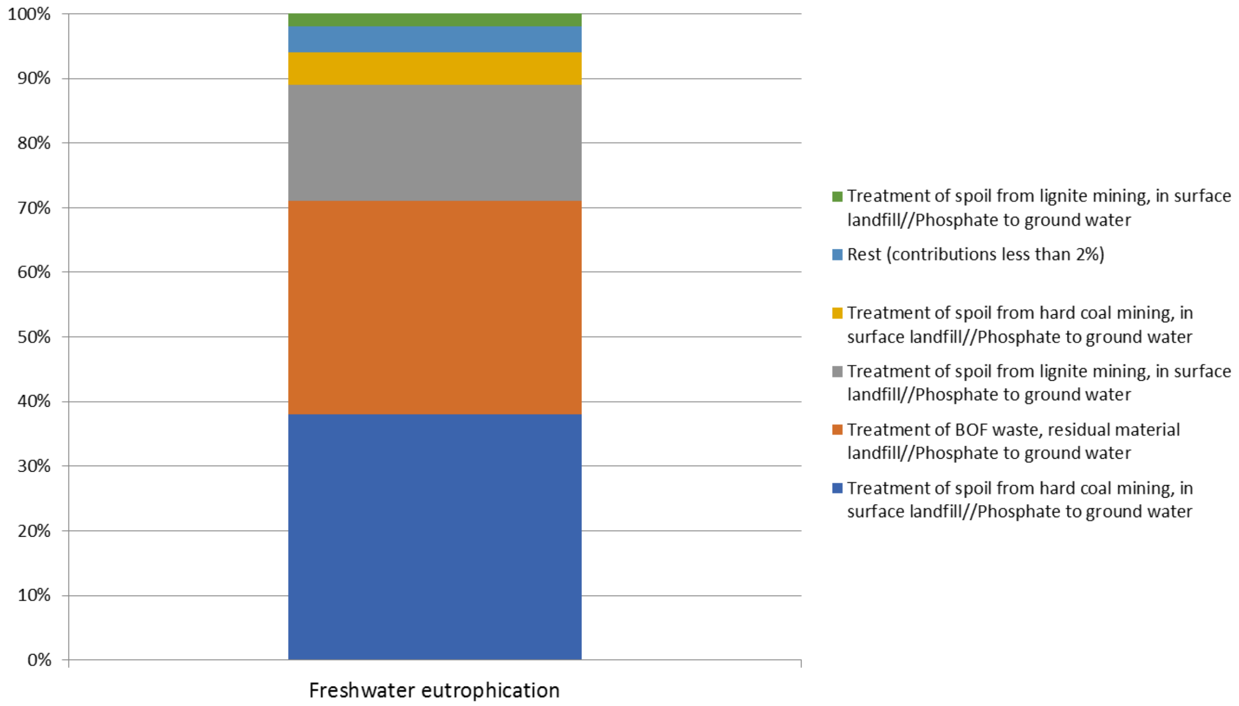

Figure A.5: Process and elementary flow contributions for the baseline system of steelmaking process for freshwater eutrophication

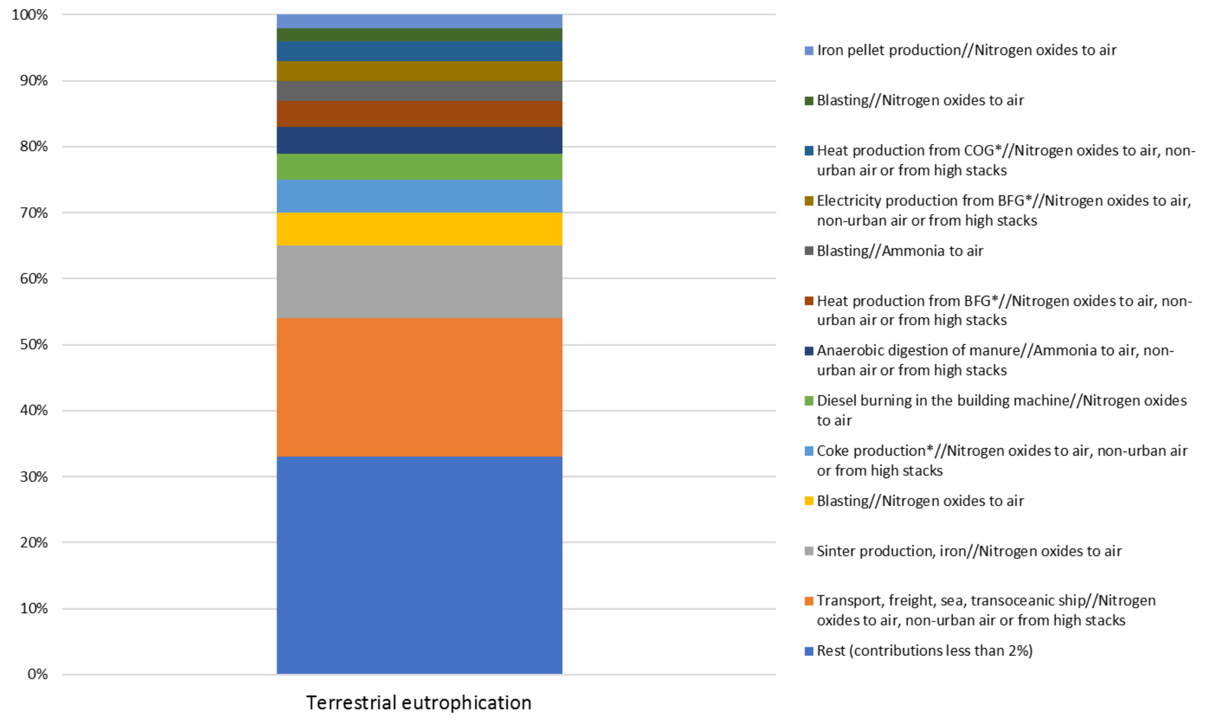

Figure A.6: Process and elementary flow contributions for the baseline system of steelmaking process for terrestrial eutrophication

*Foreground process

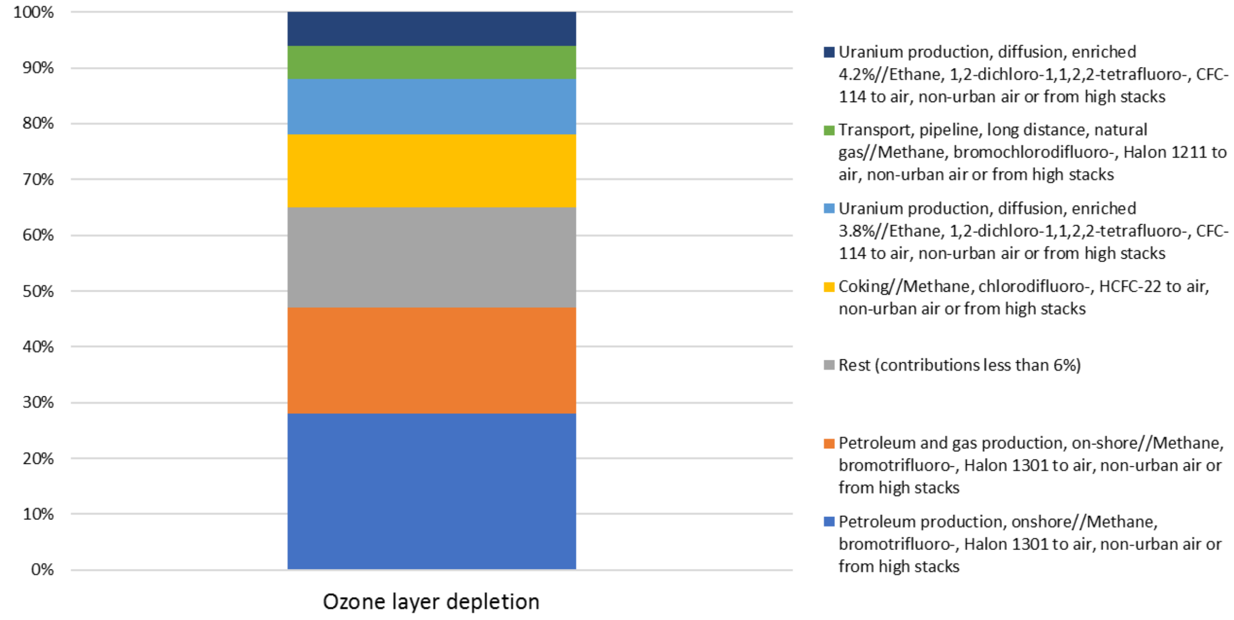

Figure A.7: Process and elementary flow contributions for the baseline system of steelmaking process for ozone layer depletion

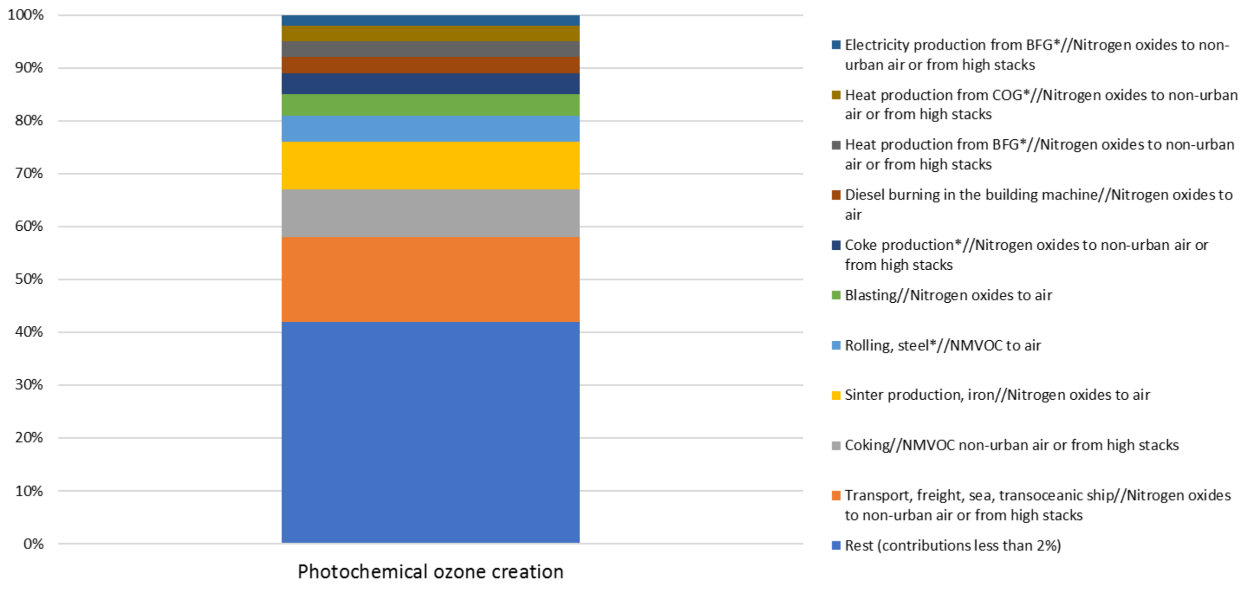

Figure A.8: Process and elementary flow contributions for the baseline system of steelmaking process for photochemical oxidation

*Foreground process

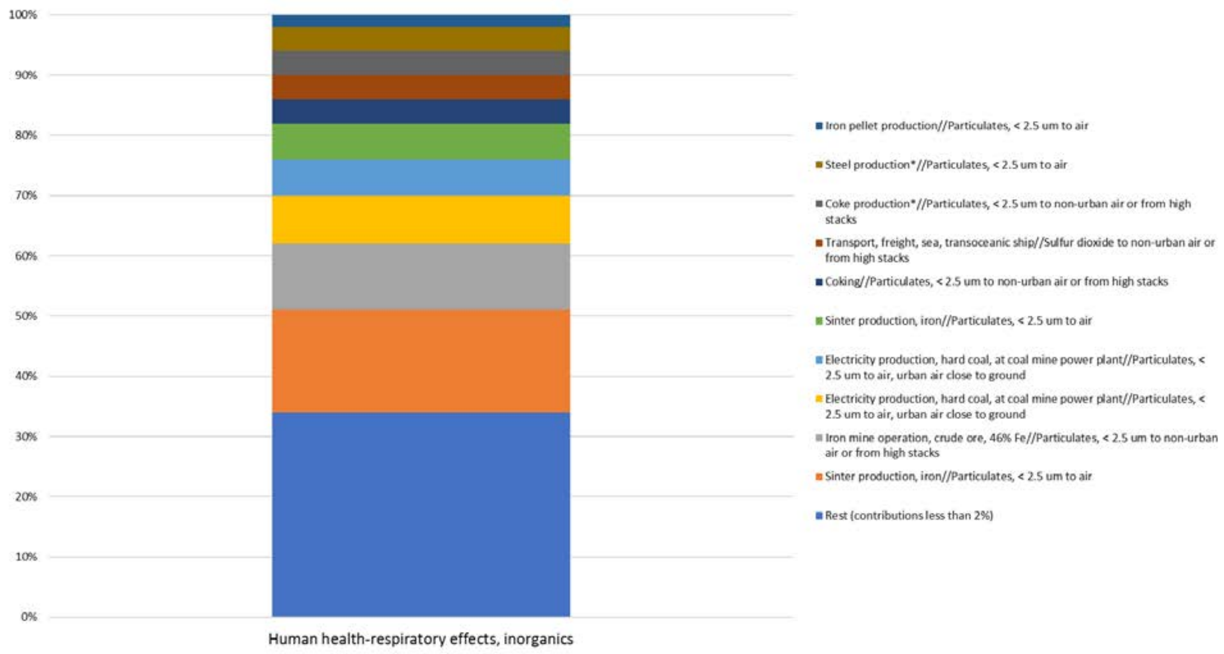

Figure A.9: Process and elementary flow contributions for the baseline system of steelmaking process for human health-respiratory effects, inorganics

*Foreground process

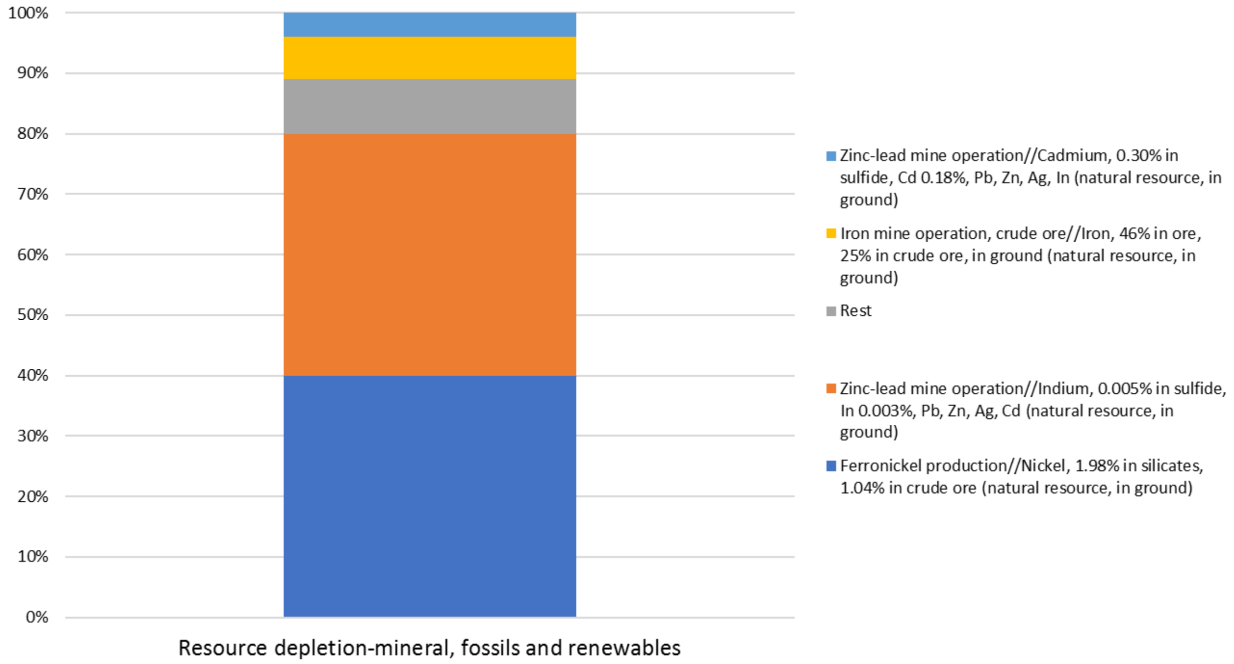

Figure A.10: Process and elementary flow contributions for the baseline system of steelmaking process for resource depletion