Master's thesis

NTNU
Norwegian University of Science and Technology
Faculty of Engineering
Department of Energy and Process Engineering

Leonhard Maxim Bodau

Analyzing the sustainability of the aluminothermic reduction of silicon metal: A combined approach of MFA and spatial LCA.

Master's thesis in Industrial Ecology
Supervisor: Johan Berg Pettersen
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Abstract

Achieving carbon neutrality by 2050 is a multi-disciplinary challenge requiring innovation and transformation in all industrial sectors. The silicon metal production is an energy and carbon intensive process emitting upwards to 12 metric tons of CO_2 per 1 ton of silicon metal produced. The SisAl pilot patented a novel production process using secondary aluminium as a reducing agent and thereby aims to decarbonize the silicon metal production. This thesis uses material flow analysis to quantify the mass flows of the aluminothermic reduction and life cycle assessment to evaluate its sustainability. It uses a spatial approach for transport distances, electricity inputs, and its impact categories to assess the environmental impact of four business cases and a baseline scenario. It compares them with the conventional production and an earlier assessment of the aluminothermic reduction. The assessment shows that taking these parameters into account doubles the overall impact of the aluminothermic reduction compared to earlier assessments and makes them comparable to the conventional production. Especially the consideration of country-specific electricity mixes increases the impact substantially. Additionally, the comparison of regional characterization factors with the global average changes the impact categories ozone formation: ecosystems and freshwater eutrophication by a factor of two, showing that a spatial LCA modifies the outcome of the impact assessment. The assessment shows that a careful consideration of the spatiality in the inventory is key for a comprehensive evaluation of this system. In the upcoming years the silicon metal production needs to be further analysed taking the regional differences into account and improving upon the circularity of the aluminothermic reduction.

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Abbreviations

Abbreviation	**Meaning**
Al	Aluminium
Al2O3	Aluminium oxide or alumina
ALCA	Attributional LCA
AoP	Areas of Protection
AP	acidification potentials
APOS	Allocation at point of substitution
aq	aqua (solved in water)
CaCO3	calcium carbonate or limestone
CaO	calcium oxide or calcia
CCS	Carbon capture and storage
CF	characterization factor

CFC	chlorofluorocarbon
CLCA	Consequential LCA
CO2	Carbon dioxide
CRM	critical raw material
DALY	daily adjusted life years
EC	European Comission
eq.	equivalent
ES	Spain
ET	ecotoxicity
EU	European Union
FEP	freshwater eutrophication potentials
FPMF	Fine particulate matter formation
FRS	Fossil resource scarcity
g	gaseous
Ge	Germanium
GHG	green house gas
GR	Greece
GWP	global warming potential
H2O	water
HP	high purity
HT	Human toxicity
HZDR	Helmholtz zentrum
IEA	international energy agency
ILCD	International Reference Life Cycle Data System
IPCC	Intergovernmental panel on climate change
IR	Ionizing radiation
IRP	ionising radiation potential
IS	Iceland
l	liquid
LCA	life cycle assessment
LCI	Life cycle inventory
LCIA	Life Cycle Impact Assessment
LU	Land use
MFA	Material flow assessment
MG	Metallurgical grade
mPt	milli weighted points
MRS	Mineral resource scarcity
N	Nitrogen
N2O	Nitrous oxide
NDC	Nationally determined contribution
NMVOC	non-methane volatile organic compounds
NO	Norway
O2	Oxygen

OD	ozone depletion
ODP	ozone depletion potential
P	Phosphorus
PDF	potentially disappeared fraction of species
PM	particulate matter
POF	photochemical ozone formation
REE	rare earth elements
RER	Europe (ecoinvent)
RoW	Rest-of-World (ecoinvent)
s	solid
SAF	submerged arc furnace
Si	Silicon
SiO2	silicon dioxide (Silica)
SOx	Sulfur oxides
TA	Terrestrial Acidification
tkm	tonne-kilometre
TWh	tera watt hours
wt%	percentage by weight
WU	water use
yr	year

1 Introduction

In order to keep the global temperature increase to well below 2°C and to aim for 1.5°C above pre-industrial levels 193 entities (192 countries and the European Union (EU)) joined the Paris Agreement in 2015 [1], [2, p. 5]. The legally binding document obliges governments to submit Nationally Determined Contributions (NDC) which they aim to achieve [2, p. 6]. The EU pledged to reduce its Greenhouse Gas emissions by at least 55% by 2030 compared to 1990 and achieve net-zero emissions by 2050 in accordance with the IPCC guidelines and has proposed the European Green Deal to enact the Paris Agreement of 2015 and lead the achievement of the sustainable development goals [3]–[6]. The European Commission (EC) aims to increase the share of renewable energy to 40% of the final energy consumption by 2030 [7]. The EU directive on climate neutrality also establishes aims to ensure an objective assessment of the mitigation measures based on up-to-date scientific findings, such as the reports by the intergovernmental panel on climate change (IPCC) [6, p. 7] which analysed several mitigation pathways aligning with the mitigation goal in the Paris Agreement [8]. The report shows that not only does the primary energy supply need to have an average of 68% of renewable energy by 2050 [8, p. 132], it also shows different mitigation strategies for the industrial sector [8, pp. 138–140]. Industry accounts for 25% of CO_2 emissions, of which material industries such as steel, non-ferrous metals, chemicals, non-metallic minerals, and paper industries account for 72% of its emissions [8, p. 138]. The modelled 1.5°C pathways show that these energy and carbon intensive industries need to decrease their greenhouse gas (GHG) emissions and carbon intensity by 80% and their final energy demand by 30% by 2050 [8, p. 138]. To achieve these mitigation goals, the IPCC placed the strategies into five categories:

1. Reducing Demand
2. Energy efficiency
3. Increasing electrification of energy demand
4. Reducing the carbon content of non-electric fuels
5. Deploying innovative processes and application of carbon capture and storage (CCS)

In order to reduce the general demand end-of-life (EOL) products and industry waste should be recycled, and inter-industry material synergies should be extended [8, p. 140]. Additionally, standard industry processes must be decarbonized, and their energy demand met by renewable energy. Innovative processes can help reform specific industrial sectors and kickstart new synergies.

These changes require a substantial amount of renewable energy and innovation in order to transform entire industries. The EU intends to “play a leading role” in achieving the climate goals [5, p. 1] and has many directives in play to address different issues. Aside from the aforementioned “EU Green Deal” and the NDC of the Paris Agreement, the EU also plans to lead in circular economy [9, p. 22] and recycling and has published various frameworks and action plans to conciliate these efforts [9], [10]. These include among other things the recycling of postconsumer electronics [11], batteries [12], EOL vehicles [13], and plastics [14], but also intends to increase the circularity in production processes [15]. The “New Industrial Strategy” in conjunction with the “European Green Deal” aims to decarbonize energy intensive sectors, establish a sustainable product policy framework, and reinforce Europe’s industrial autonomy [15, pp. 10–13].

The EU plans to invest €260 billion each year until 2030 [3, p. 15], but independent estimates state that an average of €800 billion are needed annually to shift from carbon-intensive to low-carbon technologies [16, p. 11], resulting in a €28 trillion investment cost to decarbonize Europe [16, p. 30]. Global investment in renewable energies reached more than $900 billion by 2020 [17, p. 37] and total renewable power is forecast to grow from 2015 to 2021 by 36% [18, p. 144].

Among the challenges on the way to climate neutrality is the dependence on critical raw materials (CRM) which power renewable energies and decarbonisation efforts [18]. The OECD estimates that the global material demand will double by 2060 to 167 Gt [19, p. 3]. The EU has compiled a list of 30 raw materials that are crucial to Europe’s economy [20, p. 2]. Among them are metals such as Rare Earth Elements (REE), Lithium (Li), or Tungsten (W), metalloids such as Antimony (Sb), Germanium (Ge), or Silicon metal (Si) and non-metal raw materials such as phosphate rock, natural rubber, or coking coal. The CRM and their supply countries are mapped in Figure 1. China supplies 59% of the CRM with the next two biggest suppliers being the USA and South Africa, illustrating the dependence of Europe’s value chain towards third countries [20, p. 14]. Critical metals and metalloids are especially important for renewable energy systems such as solar photovoltaic and wind energy, energy storage facilities, and electric grids and transmission [18, p. 142]. Materials such as REE or Scandium (Sc) are vital for wind turbines, while photovoltaics need Tellurium (Te) and Silicon metal (Si). To address these supply chain issues the EU has started several initiatives such as the CRM action plan, the European Raw material alliance [21], and the CRM Resilience initiative [22] with the aim to reduce Europe's dependency on foreign raw materials and to strengthen the domestic supply.

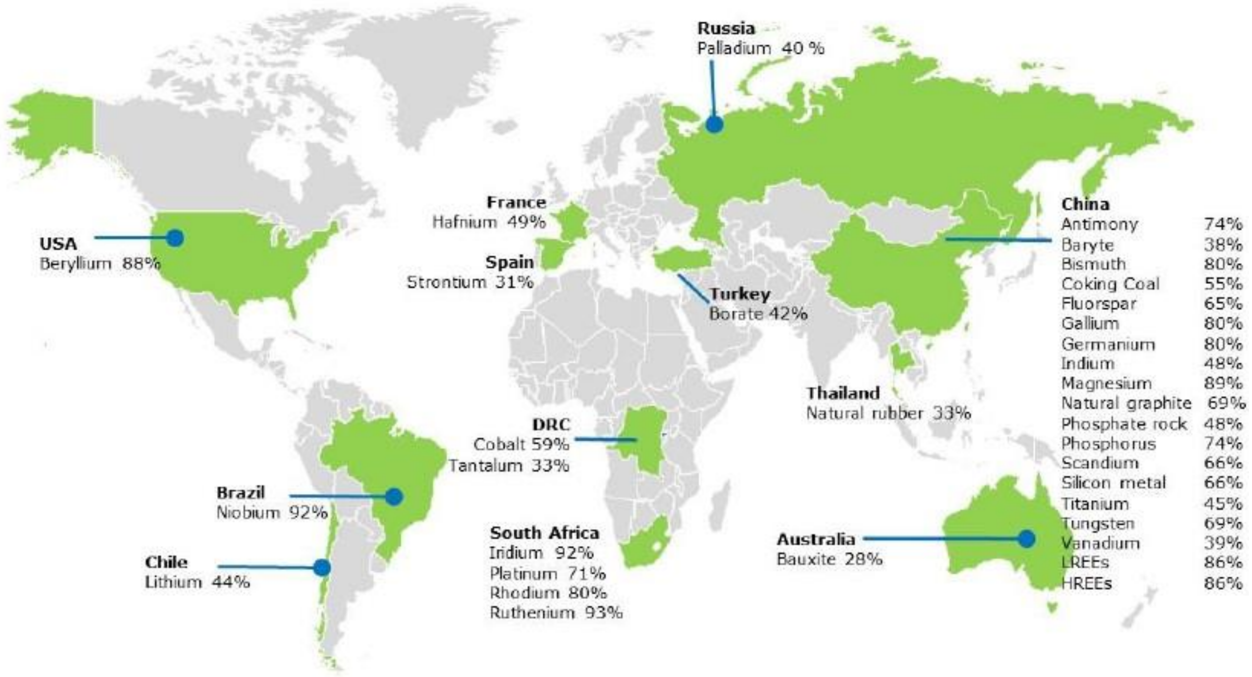

Figure 1: Countries accounting for the largest share of global supply of CRMs [20, Fig. B]

Although a critical raw material, silicon metal is the second most abundant element in the Earth's crust with 29.5 wt% [23, p. 50] and is normally found in its oxidized form as SiO_2 (quartz) or silicates [24, p. 13]. Albeit a metalloid Si is commonly referred to as silicon metal. It has two grades, metallurgical grade (MG) silicon with a 99% purity and polysilicon with a 6N or 11N purity (the N refers to the number of nines after the decimal, a 3N would be 99.999% pure silicon metal) [25, p. 706]. There are four main end uses for silicon metal: aluminium (Al) alloys, chemical, solar, and electronic applications [25, p. 711]:

- **Aluminium alloys:** 38% of MG Si is used to produce aluminium alloys enhancing the mechanical properties of the aluminium. Its primary use is in castings in the automotive industry.
- **Chemical applications:** Has with 54% the highest share of silicon metal end uses. The pure silicon is used to produces silicones and synthetic silica. These are then used as surfactants, lubricants, and adhesives for cosmetics and in industrial processes. Silanes, another common product, are used in the glass, ceramic and painting industry.

- **Solar cell applications:** With only 6% of the entire silicon metal production, solar grade (SoG) silicon needs a purity of at least 6N to be used for photovoltaic applications.
- **Electronics applications:** 2% of the silicon metal is processed for semiconductors, transistors, and circuit boards. It also needs high-purity silicon metal (6N or higher) for its application and is the second biggest use of polysilicon.

Despite its abundance, the classic production of silicon metal is an energy and carbon intensive process [26]. The carbothermic reduction reduces SiO_2 to Si using carbonaceous reductants:

$$SiO_2 + 2\,C \;\rightarrow Si + 2\,CO$$

Equation 1: Carbothermic reduction of silicon dioxide [24, p. 13].

The emerging CO will be further oxidized to carbon dioxide (CO_2). The most commonly used process is a submerged arc furnace (SAF) process with a subsequent combustion and casting step with an average temperature between 1800°C – 2000°C [24, p. 139], [26, Fig. 1]:

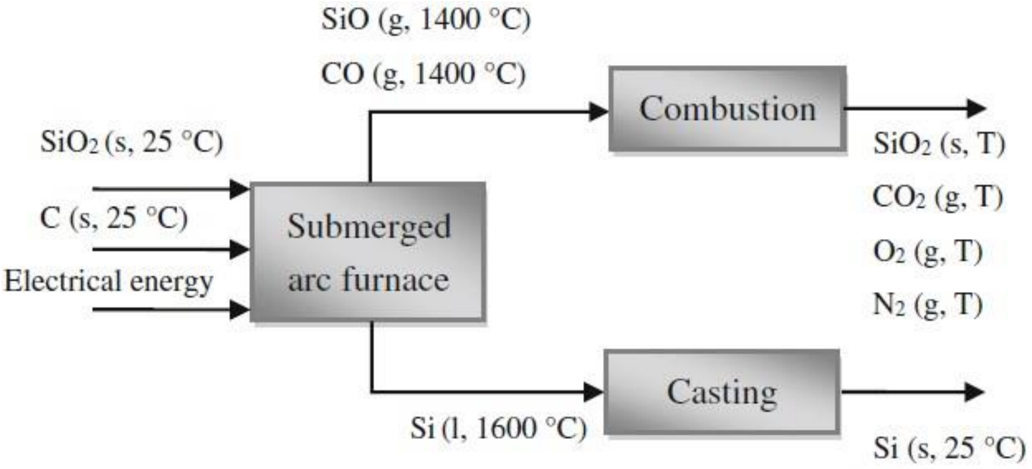

Figure 2: Carbothermic reduction with the three subprocesses submerged arc furnace, combustion, and casting.

The SAF uses electrical current to facilitate the reaction and supply the heat to the carbon-silicate mix. The off-gas (SiO and CO) will be fully oxidized by atmospheric oxygen (O_2) in the combustion step while the molten silicon metal will be cast into its final shape or refined by tapping the molten silicon through a taphole into a refining ladle [27]. The average GHG emissions per ton of MG Si range from 10.2 and 12.6 metric tons CO_2-eq. with around 4.7 tons originating from the carbothermic reduction itself and the remaining emissions resulting from the electric energy mix [28].

A novel silicon metal production process is conceptualized by the SisAl-pilot project, which aims to prove its experimental and commercial feasibility [29], [30]. The project is a collaboration between several companies, universities, and institutes across Europe and aims to inter-connect different industries to improve the sustainability and circularity of the aluminium and silicon metal production.

The patented process is an aluminothermic reduction using aluminium to reduce silicon dioxide to MG silicon and alumina (Al_2O_3) [30, p. 131]:

$$3\ SiO_2 + 4\ Al \ \rightarrow 3\ Si\ (l) + 2\ Al_2O_3 \quad \Delta H_{1550°C} = -174.8\ kJ/mol$$

Equation 2: Chemical reaction of the aluminothermic reduction and its enthalpy [30, p. 131].

The reduction is designed to use secondary or EOL materials for its inputs in order to reduce its environmental footprint:

- **Silicon dioxide:** Main source for MG Si. Sources can range from smaller quartz fines unfit for the SAF to SiO_2 skulls, a slag by-product of the SAF which consists of Al_2O_3-CaO-SiO_2.
- **Aluminium:** Alternative reductant to the process instead of carbon. Al dross, a by-product floating on the liquid aluminium during its electrolysis [30, p. 129] as well as end-of-life Al scrap can be utilized.
- **Calcium oxide:** used as slag during the reduction process. The slag is used to remove impurities, reduce the required temperature [31] and to protect the reactants from oxidation [32]. The used CaO with the not reacted silicon dioxide and the Al_2O_3 will be further processed and reintroduced into the system [33].

After the successful reduction of the silicon dioxide the silicon metal will have a purity of 99% and will therefore be metallurgical grade and can be refined to solar grade [30], [31]. The accrued CaO-SiO_2-Al_2O_3 slag will then be processed in a hydrometallurgical process called the Pedersen-process [30], where the alumina and the CaO will be separated, the calcium oxide refed into the system and the alumina purified as shown in Figure 3 [30, p. 131]:

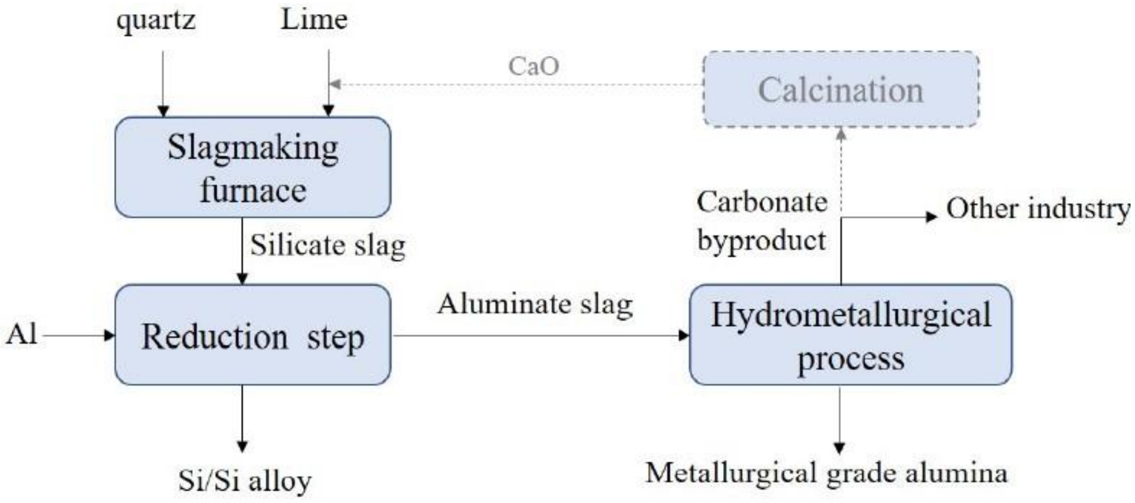

Figure 3: Schematic representation of the SisAl process and the Pedersen process [30, Fig. 1].

According to their findings, the SisAl-projects reports a lower carbon footprint, energy consumption and a higher yield [30]. In addition, nitrous oxide (NOx), polycyclic aromatic hydrocarbon (PAH), and sulfur dioxide (SO_2) emissions are minimal.

To study the environmental impact over the production cycle of the aluminothermic reduction, a life cycle assessment (LCA) has been conducted as part of the master thesis by Pastor-Vallés [34]. It compared the ecological footprint of the carbothermic and the aluminothermic reduction routes in Norway for different impact categories, such as global warming, acidification, and particulate matter formation. It showed that the aluminothermic reduction has a lower carbon footprint, as well

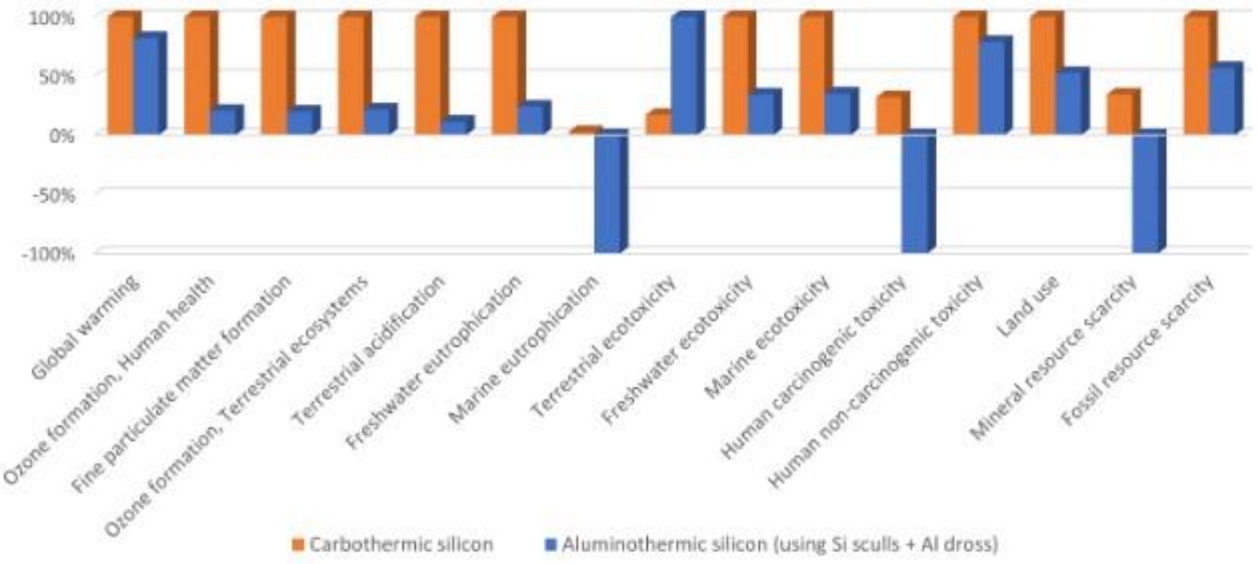

Figure 4: Comparison of the impacts of the carbothermic and aluminothermic reduction[34, Fig. 4.1]

as other impacts, but that the CO_2 reduction are only 20% of the carbothermic reduction despite savings in primary carbon (Figure 4):

It also showed that a change in electricity mix from Norwegian to European or a change in aluminium source from Al dross to EOL aluminium scrap for the aluminothermic reduction increases all footprints drastically [34, pp. 52 and 54] showing several challenges in the novel production process.

Utilizing the knowledge acquired from this research the present work will expand the environmental analysis and focus on other parameters potentially affecting the validity of the LCA and the sustainability of the SisAl pilot.

The previous life cycle assessment by Pastor-Vallés, its data and its findings are the basis for this thesis which aims to answer the following research questions related to the aluminothermic process:

1. How can the use of mass flow analysis improve the accuracy of the inventory in the aluminothermic reduction route and how does it influence the results?
2. How does the life cycle assessment change when considering different contributing parameters, such as processing and resupplying the CaO from the Pedersen process into the aluminothermic reduction, considering regionally different characterisation factors (CF), transporting the materials from and to the different facilities, or using the country-specific electricity mixes?

In order to answer these questions this thesis will use mass flow analysis and life cycle assessment to develop the production systems for the baseline and four different business cases of participating partners. These partners are engaging in industrial symbiosis and plan to use each other’s resources to produce HP alumina and MG silicon in a more cost effective and efficient manner. These partners are located in different countries in the European Economic Area (EEA):

1. **NO-GR 1:** The companies Hydro and Wacker in Norway produce the MG silicon and Mytilineos in Greece produces HP alumina and calcium oxide from the resulting slag, which will be refed into the aluminothermic reduction.

2. **NO-GR 2:** The companies Hydro and Elkem in Norway produce the MG silicon and Mytilineos in Greece produces HP alumina and calcium oxide from the resulting slag, which will be refed into the aluminothermic silicon production.
3. **ES-IS-GR:** The company Erimsa in Spain provides the SiO_2 to Silicor in Iceland which produces the MG silicon and supplies Mytilineos in Greece with the CaO-Al_2O_3 slag. Mytilineos produces HP alumina and CaO which will be refed into the aluminothermic silicon production.
4. **ES-GR:** The companies Befesa and Erimsa (Spain) supply Fundiciones Rey (FRey) in Spain with aluminium and silicon dioxide, which it then uses to produce MG Si and CaO-Al_2O_3 slag. This is shipped to Mytilineos in Greece which produces HP alumina and CaO. The CaO is shipped back to FRey who reuses it in the aluminothermic silicon production

2 Methodology

In this paragraph the underlying methods and tools used in this thesis are presented and explained. The work was split in two sections, the material flow analysis and the life cycle assessment. This work is based on the previous life cycle assessment by Pastor-Vallés [34] and the data assembled from four different business cases. The results in the MFA will be the basis for the LCA inventory These four cases will be evaluated and compared with each other in terms of sustainability in different impact categories.

2.1 Material flow analysis

According to Brunner and Rechberger material or mass flow analysis (MFA) is a systematic assessment of the flows and stocks within a system defined in space and time [35, p. 3]. It delivers a complete set of information about the material flows within the boundaries of the system and the exchange between the anthroposphere and the environment. The anthroposphere is defined as the part of the environment that is made by humans [36], while the natural environment is “driven by nature” [35] These two spheres exchange flows of material, energy, and information. To understand the interaction within a given system its components must be defined and related to each other. A process is defined as a transport, transformation, or storage of materials, while a flow links two processes two each other. A flow across system boundaries is called an import if its flow direction goes from beyond the system into the system and an export if it goes the opposite direction [35, p. 4]. Lastly, a system contains the processes, flows, and stocks within its system boundaries. Mass flow analysis is an iterative process that first defines a problem, then a system, the flows and stocks, and lastly interprets the findings. These redefine and redetermine the system and the problem, which in turn change and determine the interpretation [35, p. 54]. Figure 5 shows the illustration of a typical analysis procedure.

2.1.1 Problem definition

The problem this MFA is trying to solve is the mass balance of the aluminothermic reduction and the alumina production for four business cases. Available sources show the economic development and feasibility of these two processes, but do not account for the balance of in- and outputs within a given time period [34]. The corresponding names for the business cases are shown in

Table 1. This thesis aims for an overall balance of the system. It is assumed that the balance of the elementary flows is achieved when the overall mass of the system is balanced.

2.1.2 System definition

2.1.2.1 System boundaries

The system boundaries for the business cases are defined in space and time. The temporal boundary is the year 2020 for all four cases, and it will be assumed that no accumulation of material is taking place. This eliminates the need for stocks, which classifies this analysis as a stationary model in contrast to a quasi-stationary model which has a change in stock under a time shift. The spatial boundaries include the companies related to the aluminothermic reduction and the alumina production as seen in Figure 5. The boundaries differ slightly from case to case but have the same two processes and input materials. Figure 5 shows the general system boundaries with processes and flows. The data has been extracted from various sources of the SisAl project [34], [37], [38].

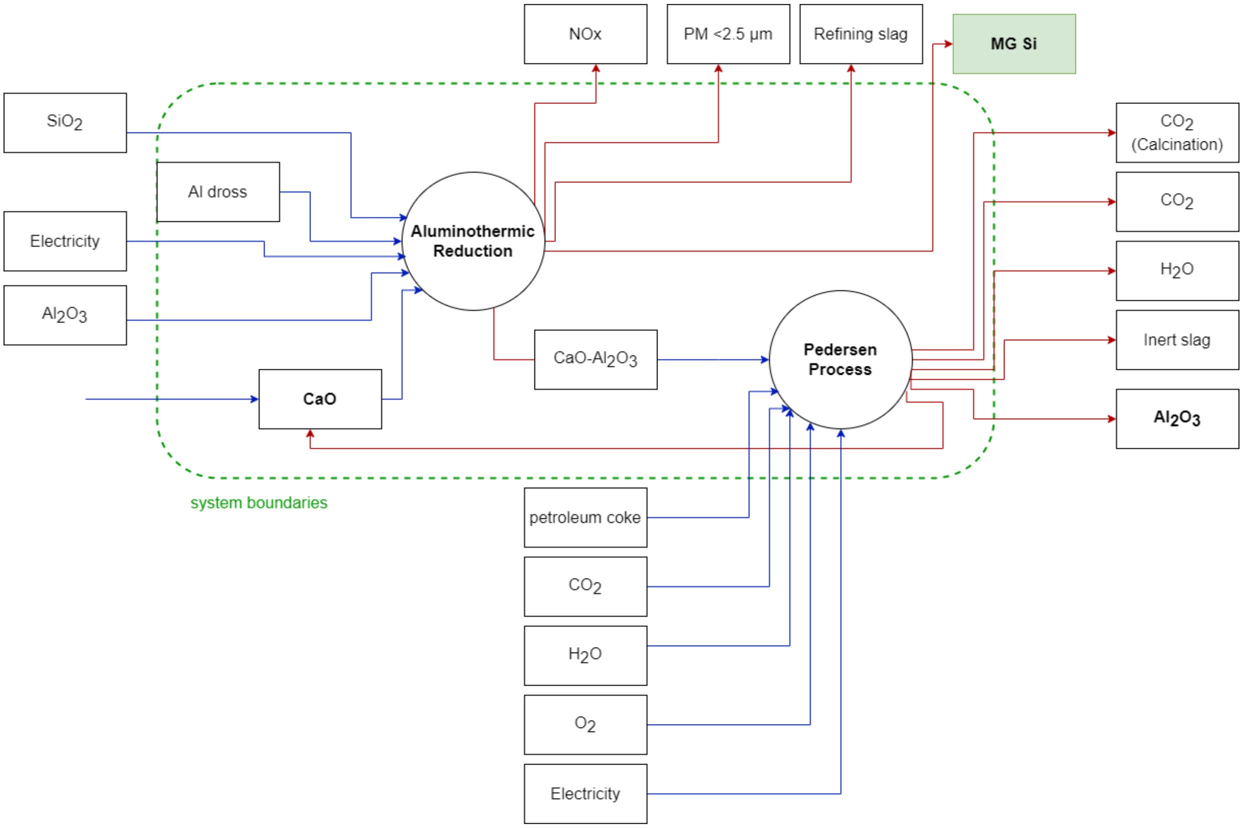

Figure 5: System boundaries of the Aluminothermic production (SisAl process) and the alumina production (Pedersen process). Inputs are marked in blue, outputs in red. The rectangles are the flows, the circles are the processes. The functional unit is the output of metallurgical grade Si (shown in green).

While the alumina production for all cases takes place in Greece, the silicon production differs from business case to business case. The cases Norway-Greece-1 (NO-GR 1) and Norway-Greece-

2 (NO-GR 2) have their production in Norway, the case Spain-Iceland-Greece (ES-IS-GR) has it in Iceland, and the case Spain-Greece (ES-GR) has it in Spain.

Table 1 shows the different locations for the different cases and their role in the system, while Figure 7 shows the locations in Europe. The differentiation between the business cases will be further explained in chapter 23 0 and 2.2.1.2.1 when considering the inventory.

Table 1: Description of the four cases, their location, the corresponding company, and their function in the system.

Case	**Location**	**Function**	**Company**
NO-GR 1	Holla, NO	Aluminothermic reduction	Wacker Holla
	Sunndalsøra, NO	Supply of aluminium dross, processing of MG Si	Hydro Sunndal
NO-GR 2	Kristiansand, NO	Aluminothermic reduction	Elkem Fiskaa
	Håvik, NO	Supply of aluminium scrap	Hydro Karmøy
	Svelgen, NO	Processing of MG Si	Elkem Bremanger
ES-IS-GR	A Coruña, ES	Supply of Silica	Erimsa
	Grundartangi, IS	Aluminothermic reduction	Silicor
ES-GR	A Coruña, ES	Supply of Silica	Erimsa
	Vilagarcía de Arousa, ES	Aluminothermic reduction	Fundiciones Rey
	Erandio, ES	Supply with Al Scrap, processing of MG Si	Befesa
All cases	Distomo (port San Nicolas [GR])	Production of alumina from SisAl production slag	Mytilineos

2.1.2.2 Processes

2.1.2.2.1 SisAl process

The SisAl process, also referred to as the aluminothermic reduction, is a simplification of a complex metallurgical procedure which comprises slag making, aluminothermic reduction, and silicon ladle refining [34]. The companies responsible for the aluminothermic reduction use different sources of materials to produce MG Si, which commonly has a purity of 98% [39]. First the slag will be made from CaO, quartz fines (SiO_2) and Si slag. Al scrap and dross as well as heat will be added to chemically reduce the SiO_2 to Si. The liquid silicon will then be refined to MG Si, while the slag will be prepared for transport and further alkaline leaching. The CaO-Al_2O_3 outflow shown in Figure 5 is a secondary product in the SisAl process and the aluminium source for the Pedersen process.

2.1.2.2.2 Pedersen process

The Pederson process, also known as alumina production, is a simplification of complex metallurgical procedures, too [40]. First, the prepared CaO-Al_2O_3 slag will be shipped to Greece, leached with $Na_2CO_3(aq)$, desilicated with CaO, carbonated with concentrated CO_2 and then separated. The separated $Al(OH)_3$ is then calcinated to Al_2O_3 and cooled. The achieved purity is 99.9% and will then be sold as pure Alumina. The separated slag is $CaCO_3$, and Na_2CO_3. The sodium carbonate is refed to the process, while the calcium carbonate is decomposed under heat to produce CO_2 and CaO. The CaO is then reused for the slag-making in the SisAl process.

The described processes have been simplified for the material flow analysis to focus on the in- and outputs of the system.

2.1.2.3 Materials and goods

The materials and goods are derived from experimental data and model simulations from the Helmholtz centrum Dresden-Rossendorf (HZDR) and was first used in Pastor-Vallés [34]. The companies produce MG-Si and HP- Al_2O_3 from Al slag and spent SiO_2 fines.

2.1.2.3.1 Silicon dioxide

Silicon dioxide, or SiO_2, is derived from different sources for each business case:

- In the case NO-GR 1 the company Wacker uses SiO_2 fines from quartz handling in their aluminothermic reduction process.
- In the case NO-GR 2 the company Elkem uses SiO_2-CaO slag from Si refining for their silicon production
- In the case ES-IS-GR the company Erimsa delivers SiO_2 fines to Silicor in Iceland, which then produces MG Silicon
- In the case ES-GR the company Erimsa delivers SiO_2 fines to Fundiciones Rey, which uses it to produce MG Silicon

2.1.2.3.2 Aluminium

Aluminium is used to convert the silicon dioxide to silicon. Similar to SiO_2 it has different sources for each case:

- The case NO-GR 1 uses Al dross from the primary aluminium production of the company Hydro.
- The case NO-GR 2 uses Al scrap from aluminium recycling in the company Hydro.
- The case ES-IS-GR uses Al-Si dross from Silicon purification at Silicor to purify both the silicon and convert SiO_2 to silicon.
- The case ES-GR uses a variety of aluminium sources, such as Al scrap and dross from Befesa.

2.1.2.3.3 Calcium oxide

Calcium oxide or CaO is used to make the slag used in the aluminothermic reduction. It partly uses spent and refined slag from the alumina production but the CaO is also fed into the process as lime stone. The spent slag is separated into useful $CaCO_3$ which is then calcinated under heat:

$$CaCO_3 + \Delta T \rightarrow CaO + CO_2$$

Equation 3: calcination of calcium carbonate under heat addition

2.1.2.3.4 Alumina

Alumina or Al_2O_3 is used to condition the slag which is then purified by the Pedersen process to alumina and calcia. It is needed to achieve a critical concentration of Al in the slag.

Alumina is the main product in the Pedersen process and achieves high purity of at least 99.5% alumina, which is considered smelter-grade (SG) alumina [41].

2.1.2.3.5 CaO-Al_2O_3 slag

The calcia-alumina slag is a by-product of the aluminothermic reduction. It will be conditioned and then fed into the alumina production, which uses it as its main input to produce HP-CaO and HP-Al_2O_3.

2.1.2.3.6 Petroleum coke

The petroleum coke is used in the calcination reaction of the alkaline leaching process. It transforms the $Al(OH)_3$ to Al_2O_3 by oxidation:

$$2\,Al(OH)_3 + CH_4 \rightarrow Al_2O_3 + H_2O + CO_2$$

Equation 4: Oxidation of Aluminium hydroxide

For simplicity, the oxidation agent in Equation 4 is methane instead of petroleum coke.

2.1.2.3.7 Carbon dioxide

Carbon dioxide (CO_2) is used in the alumina production to carbonate the $NaAl(OH)_4$ solution to $Al(OH)_3$ and $NaHCO_3$:

$$NaAl(OH)_4 + CO_2 \rightarrow\ Al(OH)_3 + NaHCO_3$$

Equation 5: Carbonation of sodium tetrahydroxoaluminate

The sodium hydroxy carbonate then further reacts to sodium carbonate, which is reused in the alkaline leaching.

CO_2 is produced in two ways. One is the burning of unused petroleum coke, since the Equation 4 is an ideal-case scenario. The other is the production of CO_2 during the calcination of $CaCO_3$ (Equation 3). In the baseline scenario it is assumed that the produced CO_2 exits the system into the ecosystem.

2.1.2.3.8 Water

Water, also known as H_2O, is combined with the aforementioned sodium carbonate to produce a alkaline leaching solution.

Water exits the system as hot steam and in the slag during the alkaline leaching.

2.1.2.3.9 Air

Air is used as cooling air in the alkaline route.

2.1.2.3.10 MG Si

Metallurgical grade Silicon is the main product of the aluminothermic reduction with a purity of at least 98%. Even though higher purities can potentially be achieved by some companies, in order to compare them the Si will be assumed to be metallurgical grade. After its production it will either be sold on the open market or further processed by the companies themselves.

2.1.2.3.11 Refining slag

The refining slag is produced during the Ladle refining stage of the aluminothermic reduction. It is inert slag which is landfilled.

2.1.2.3.12 Inert Slag

The residue in the alumina production is separated into $CaCO_3$ and other slag (Equation 3). While the CaO is used for the aluminothermic reduction, the other materials are landfilled as inert slag.

2.1.3 Quantification

The definition of the system, its boundaries, processes, and flows lead to a qualitative model [42, p. 73]. To quantify it the system flows and processes must be measured, estimated, and/or balanced. This coincides with the life cycle inventory for the LCA which, according to the ISO 14040, involves data collection and calculation procedures to quantify relevant inputs and outputs of a product system [43, p. 13].

2.1.3.1 Data quality requirements

To properly quantify the product systems, processes and flows the data quality needs to be defined and examined. Both the MFA and the LCA methodologies consider data quality, but the data quality requirements of the ISO 14044 are more extensive, which is why they are going to be used [42], [44, p. 10]. Normally, the data quality requirements are part of the scope of the LCA, but due to their importance in the quantification of the MFA, they have instead been placed in the quantification. The data used for this thesis should be comprehensive, complete, up to date, consistent and reproducible. The data for the foreground processes should be as precise as possible and should have clearly defined error margins.

2.1.3.2 Inventory

Where possible experimental data from the SisAl project and its partners was used. If not the database ecoinvent 3.6 was used. The software used to build the inventory was Simapro. For the calculation of the distances the website maritimeoptima.com, a website for calculating the shipping distances between ports, impargo.de, a website for calculating transfer distances for trucks, and googlemaps.com, a website with a comprehensive database of world maps, were used. Table 2 shows the foreground processes which are the same for all four business cases and their amount per functional unit of 1 ton of MG Si. For the quantification of the CaO input and the calcination CO2 output the Equation 3 was used. The experimentally determined percentage of $CaCO_3$ in the $CaCO_3$ residue is 65% and the amount of residue per 1 t of MG Si is 4.26 tons. The calculated amount of CO_2 is therefore 1.24 t and the calculated amount of CaO is 1.57 tons. Table 2 shows different results because these calculated and experimentally derived data points were then fed into data reconciliation, which more accurately depicts an overestimated system. This will be explained more thoroughly in 2.1.4.2. The energy needed to perform this reaction was calculated using the enthalpy in Equation 2 and project it on 1 ton.

Table 2: In- and outputs from the foreground process and their denotation in SimaPro

flow	Amount	Unit	comment
outputs to technosphere: products and co-products			
MG Si	1	ton	functional unit of the system
outputs to technosphere: avoided products			
Aluminium oxide, metallurgical {IAI Area, EU27 & EFTA}| market for aluminium oxide, metallurgical | APOS, U	0.9	ton	produced aluminium oxide in the Pedersen process
Inputs from nature			
Air	4.1	ton	Cooling air in the Pedersen process
Water, process, unspecified origin/kg	0.47	ton	Part of the alkaline leaching, the base is refed into the system
Inputs from technosphere: materials/fuels			
Quicklime, in pieces, loose {RoW}| market for quicklime, in pieces, loose | APOS, U	1.16	ton	Input of CaO for the slag making in the aluminothermic reduction
Aluminium oxide, metallurgical {IAI Area, EU27 & EFTA}| market for aluminium oxide, metallurgical | APOS, U	0.3	ton	Input of Al_2O_3 to the slag conditioning. Needed to increase the concentration of the reactant.
Petroleum coke {GLO}| market for | APOS, U	0.0666	ton	Fuel for the calcination of the $Al(OH)_3$ to alumina
Silica sand {GLO}| market for | APOS, U	2.6	ton	Quartz fines were used in this process, but to accurately compare it with the LCA of Pastor-Vallés, the same input was used.
Carbon dioxide, liquid {RER}| production | APOS, U	1.41	ton	In the Pedersen process CO_2 is used to carbonate the slag to separate the aluminium from the base.
Emissions to air			
carbon dioxide	1.25	ton	One of the endproducts of the thermal decomposition of calcium carbonate

carbon dioxide	0.24	ton	Data from HZDR, emitted in the Pedersen process
water	0.49	ton	
nitrogen oxides	2.2	kg	Estimation according to Pastor-Vallés' comparison with the carbothermic reduction [34, p. 35].
particulates, <2.5 µm	9990.33	µg	Estimated from concentration assessments by HZDR
outputs to technosphere: waste and emissions to treatment			
Dross from Al electrolysis {GLO}| market for | APOS, U	-0.89	ton	The Al dross is used as a raw material for the aluminothermic reduction and thus is considered a negative output.
Hazardous waste, for underground deposit {GLO}| market for | APOS, U	0	ton	in contrast to Pastor-Vallés, this waste stream was utilized to CaO and CO_2.
Inert waste {Europe without Switzerland}| market for inert waste | APOS, U	0.98	ton	refining slag from the aluminothermic reduction
Inert waste {Europe without Switzerland}| market for inert waste | APOS, U	2.85	ton	slag from the Pedersen process

Table 3 shows the additional processes modelled in SimaPro to accurately measure the electricity and travel distance of materials in each case.

Table 3: electricity and transport required for the cases NO-GR 1, 2, ES-IS-GR, and ES-GR

NO - GR 1			
flow	**amount**	**unit**	**comment**
Electricity, medium voltage {NO}| market for | APOS, U	2700	kWh	Electricity used for the aluminothermic reduction in Norway
Transport, freight, sea, bulk carrier for dry goods {GLO}| transport, freight, sea, bulk carrier for dry goods | APOS, U	10051,8	tkm	CaO input from Mytilineos to Wacker
Transport, freight, sea, bulk carrier for dry goods {GLO}| transport, freight, sea, bulk carrier for dry goods | APOS, U	183.3	tkm	Al dross input from Hydro Sunndal to Wacker
Transport, freight, sea, bulk carrier for dry goods {GLO}| transport, freight, sea, bulk carrier for dry goods | APOS, U	24160.9	tkm	Alumina-Calcia slag transport from Wacker to Mytilineos
Electricity, medium voltage {GR}| market for | APOS, U	4270	kWh	Electricity used for the alumina production in Greece
NO - GR 2			
Electricity, medium voltage {NO}| market for | APOS, U	2700	kWh	Electricity used for the aluminothermic reduction in Norway
Transport, freight, sea, bulk carrier for dry goods {GLO}| transport, freight, sea, bulk carrier for dry goods | APOS, U	296.7	tkm	Al scrap input from Hydro Karmoy to Elkem Fiskaa

Transport, freight, sea, bulk carrier for dry goods {GLO}| transport, freight, sea, bulk carrier for dry goods | APOS, U	21722.2	tkm	Calcia-Alumina from Elkem Fiskaa to Mytilineos
Transport, freight, sea, bulk carrier for dry goods {GLO}| transport, freight, sea, bulk carrier for dry goods | APOS, U	21722.2	tkm	CaO from Mytilineos to Elkem Fiskaa
Electricity, medium voltage {GR}| market for | APOS, U	4270	kWh	Electricity used for the alumina production in Greece
ES - IS - GR			
Electricity, medium voltage {IS}| market for | APOS, U	2700	kWh	Electricity used for the aluminothermic reduction in Iceland
Transport, freight, sea, bulk carrier for dry goods {GLO}| transport, freight, sea, bulk carrier for dry goods | APOS, U	4423.7	tkm	Calcia from Mytilineos to Silicor
Transport, freight, sea, bulk carrier for dry goods {GLO}| transport, freight, sea, bulk carrier for dry goods | APOS, U	3709.6	tkm	SiO2 from Erimsa to Silicor, freight ship
Transport, freight, lorry >32 metric ton, EURO6 {RER}| transport, freight, lorry >32 metric ton, EURO6 | APOS, U	84	tkm	SiO2 fines from Erimsa to Silicor, truck
Transport, freight, sea, bulk carrier for dry goods {GLO}| transport, freight, sea, bulk carrier for dry goods | APOS, U	19645.8	tkm	Calcia-Alumina from Silicor to Mytilineos
Electricity, medium voltage {GR}| market for | APOS, U	4270	kWh	Electricity used for the alumina production in Greece
ES - GR			
Electricity, medium voltage {ES}| market for | APOS, U	2700	kWh	Electricity used for the aluminothermic reduction in Iceland
Transport, freight, sea, bulk carrier for dry goods {GLO}| transport, freight, sea, bulk carrier for dry goods | APOS, U	811.6	tkm	Al scrap from Befesa to FRey by ship
Transport, freight, lorry >32 metric ton, EURO6 {RER}| transport, freight, lorry >32 metric ton, EURO6 | APOS, U	28.3	tkm	Al scrap from Befesa to FRey by truck
Transport, freight, lorry >32 metric ton, EURO6 {RER}| transport, freight, lorry >32 metric ton, EURO6 | APOS, U	94.5	tkm	SiO2 fines from Erimsa to FRey by truck
Transport, freight, lorry >32 metric ton, EURO6 {RER}| transport, freight, lorry >32 metric ton, EURO6 | APOS, U	9.1	tkm	CaO input from Mytilineos to FRey by truck
Transport, freight, sea, bulk carrier for dry goods {GLO}| transport, freight, sea, bulk carrier for dry goods | APOS, U	4303.8	tkm	CaO input from Mytilineos to FRey by ship
Transport, freight, sea, bulk carrier for dry goods {GLO}| transport, freight, sea, bulk carrier for dry goods | APOS, U	9061.8	tkm	CaO-Al2O3 from FRey to Mytilineos by ship
Transport, freight, lorry >32 metric ton, EURO6 {RER}| transport, freight, lorry >32 metric ton, EURO6 | APOS, U	19.1	tkm	CaO-Al2O3 from FRey to Mytilineos by truck
Electricity, medium voltage {GR}| market for | APOS, U	4270	kWh	Electricity used for the alumina production in Greece

The names used in SimaPro for the described flows will have synonyms for a clearer understanding. The list of flow names and their synonyms can be found in the Appendix, Table 7.

2.1.4 Mass balance

The mass balance of the system is paramount for the accuracy and validity of the MFA. The experimental data obtained from the HZDR and the LCA from Pastor-Vallés accurately depicts the process [34, p. 33], [40]. However, it does not balance the system and certain flows have not been included. To rectify the mass balance, a data reconciliation with an uncertainty analysis was conducted.

2.1.4.1 Uncertainty

The systems accuracy relies on diligent uncertainty assumptions and analysis. Assuming the data and its uncertainty behaves in a normal distribution, also known as Gaussian distribution, the true mean lies with a 68% confidence within the estimated mean ± 1 standard deviation (σ). The standard uncertainty (u) of a given measurement is the standard deviation divided by the number of measurements. To estimate the uncertainty of the data without repeating the measurements the measured values are the *a priori* mean and their uncertainties are the standard deviation with a 68% confidence interval (CI).

To produce reliable data, an uncertainty was assigned to the value of each flow. When available, experimental data was used, otherwise the flows were classified in one of three categories: low, medium, or high uncertainty. the assumed uncertainty for a low uncertainty flow is 5-10%, for a medium uncertainty flow is 10-15%, and for a high uncertainty flow is 15 – 25%.

The in- and outputs of the aluminothermic reduction could be estimated using data from a SisAl-publication [38]. For the Pedersen process experimental data could not be obtained, so the uncertainty had to be assumed.

Table 4 shows the a priori inputs and their assumed uncertainty.

Table 4: mass flow values of the processes aluminothermic reduction and alumina production and their uncertainty

Process	parameter	type	value [t]	uncertainty (%)	uncertainty (+/-)	source
aluminothermic reduction	temperature	input	1650	0.6%	10.00	[33]
	Al dross input	input	0.87	17.0%	0.15	
	SiO2	input	2.58	5.6%	0.14	
	CaO	input	1.14	11%	0.13	
	Al2O3	input	0.3	17%	0.05	
	CaO-Al2O3 slag	output	5.00	9.0%	0.45	
	Refining slag	output	0.99	9%	0.09	
	MG Si	output	1	0%	0.00	FU of the system
	PM <2.5µm	output	9.9903E-09			Assumption
	NOx	output	0.0022			
Alumina production	temperature	input	37.5	20%	7.50	
	CaO-Al2O3 slag	input	5	9%	0.45	
	petroleum coke	input	0.07	10%	0.007	
	CO2	input	1.58	25%	0.40	
	H2O	input	0.48	15%	0.07	
	Air	input	4.1	25%	0.22	
	CaO	output	1.57	9%	0.14	
	CO2	output	0.24	25%	0.06	
	CO2 (Calcination)	output	1.24	7%	0.09	
	H2O	output	0.48	15%	0.07	
	Al2O3	output	0.9	10%	0.09	
	slag	output	2.77	10%	0.28	

2.1.4.2 Data reconciliation

Data reconciliation is a tool used to model the flows in a system more precisely. It uses the Maximum Likelihood Estimate (MLE) to calculate the distribution of the data observed. The *a priori* mean values and their standard deviations are assumed to be in a Gaussian distribution.

Given that, the best estimate of the normal distribution can be calculated using the Lagrange optimisation.

In this work, the computation of the statistically most likely mean and most likely standard uncertainty was done by STAN 2.6.801. The program was produced by the Vienna technical university under the leadership of Oliver Cencic [45]. It uses the least squares minimisation approach on an overdetermined system. This means that it determines the lowest sum of the squares of a residual for each mean. The residual is the difference between the measured mean (x_i) and the best estimate ($\widehat{x_i}$), shown in Equation 6.

$$r_i = \widehat{x_i} - x_i$$

Equation 6: calculation of the residual using the measured and best estimate mean

2.1.4.3 Limitations

Assumptions and limitations of a model and system are inherent to its analysis. In this MFA a variety of limitations have been placed on the system, its data availability, and uncertainty.

The systems data originates from experimental data from pilot projects from singular test runs. The mass flow was generalised from a few data points in a single year. The business cases are theoretical at time of writing and are yet to prove the concept. The mass balance was done on the overall gross weight of the inputs and outputs instead of the balance of the elementary flows. This could mean that even though the total mass is balanced, the mass of singular elements is not. Additionally, the slag flows are assumed to be more uncertain than other flows because their composition is not as well studied. They therefore balance out a lot of imbalances, resulting in potential hidden imbalances in the system. Lastly, the uncertainty of the Pedersen process had to be assumed, because of the lack of available data. These assumptions could over- or underestimate actual uncertainties.

2.2 Life cycle assessment

Life cycle assessment has been classified and standardized under the two standards ISO 14040:2006 and ISO 14044:2006 [43], [44]. They describe it as a systemic analysis of the impact of product, from raw material acquisition to final disposal. The product is modelled as a product system, which is characterised by its function and defined by its boundaries. A life cycle analysis contains four phases: the goal and scope definition, the inventory analysis, the impact assessment, and the interpretation. As shown with the arrows in Figure 6 the analysis is an iterative process where results in each phase influence the other phases.

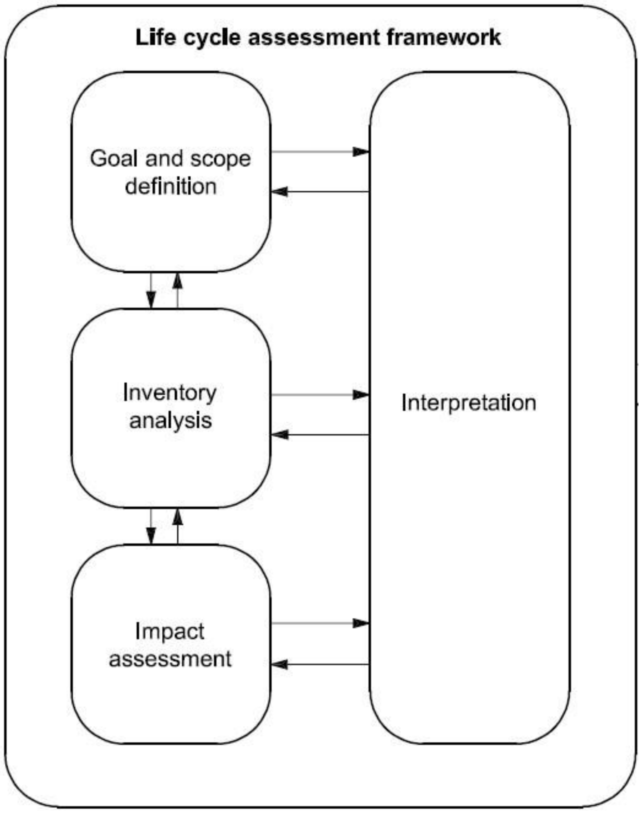

Figure 6: Life cycle assessment framework according to ISO 14040

2.2.1 Goal and Scope

2.2.1.1 Goal

The goal of the study needs to be a well-considered and deliberate definition, which sets the context of the LCA study [46, p. 59]. The goal of this LCA is to analyse the impact of 1 ton of MG Si using the aluminothermic reduction for its production and the production of HP alumina as a means of utilising the produced slag. It hopes to ascertain in what capacity local electricity grids and transport of goods changes the impact of the findings Pastor-Vallés [34]. It therefore uses four different case studies to compare to the study of Pastor-Vallés and with each other. Additionally, it will identify regional impacts on selected impact categories. This thesis intends to further the research of the SisAl-project and to support environmental decision-making for the stakeholders in the aluminium and silicon industry.

2.2.1.2 Scope

The scope of an LCA determines the product system, its functional unit, and the system boundaries [46, p. 75]. It also clarifies how the next steps, the life cycle inventory, the impact assessment, and the interpretation are carried out. This study bases its life cycle inventory and findings on the works of Pastor-Vallés [34]. Its data is used as a baseline and is compared it with data acquired in the MFA. The production of MG Si and its utilization of the slag to produce calcia and alumina as described in the material flow analysis is used as the product system. Since it is a study comparing different production systems the functional unit needs to be applicable to all systems. The four cases represent different companies and value chains in the SisAl project.

Table 1 shows the different cases, their countries, and the involved companies. The functional unit is 1 ton of MG Si produced using the aluminothermic reduction. MG Si is assumed to have a 98% purity [39].

2.2.1.2.1 System boundary

The standard for the system boundary of an LCA defines them as normally from cradle-to-grave, meaning the entirety of a product’s life cycle, from raw material acquisition to final disposal should be considered [43]. This analysis, however, is using a cradle-to-gate approach, meaning that the system boundaries include the processes of raw material acquisition, and production, and the output-treatment. It does not include the use, end-of-life treatment, recycling, or final disposal. This is done to ensure the comparability of the business cases and to limit the uncertainty of the data. The system boundary is shown in Figure 6. It shows that the production and recycling of the aluminium, the aluminothermic reduction, the alumina production, and the recycling of the calcia slag are part of the product system. In addition, the transport from and to each facility is part of the system. The four different cases, the countries, and their respective locations are shown in Figure 8. The raw materials to produce silicon are either present in the facilities producing the silicon or have to be shipped to the production facility.

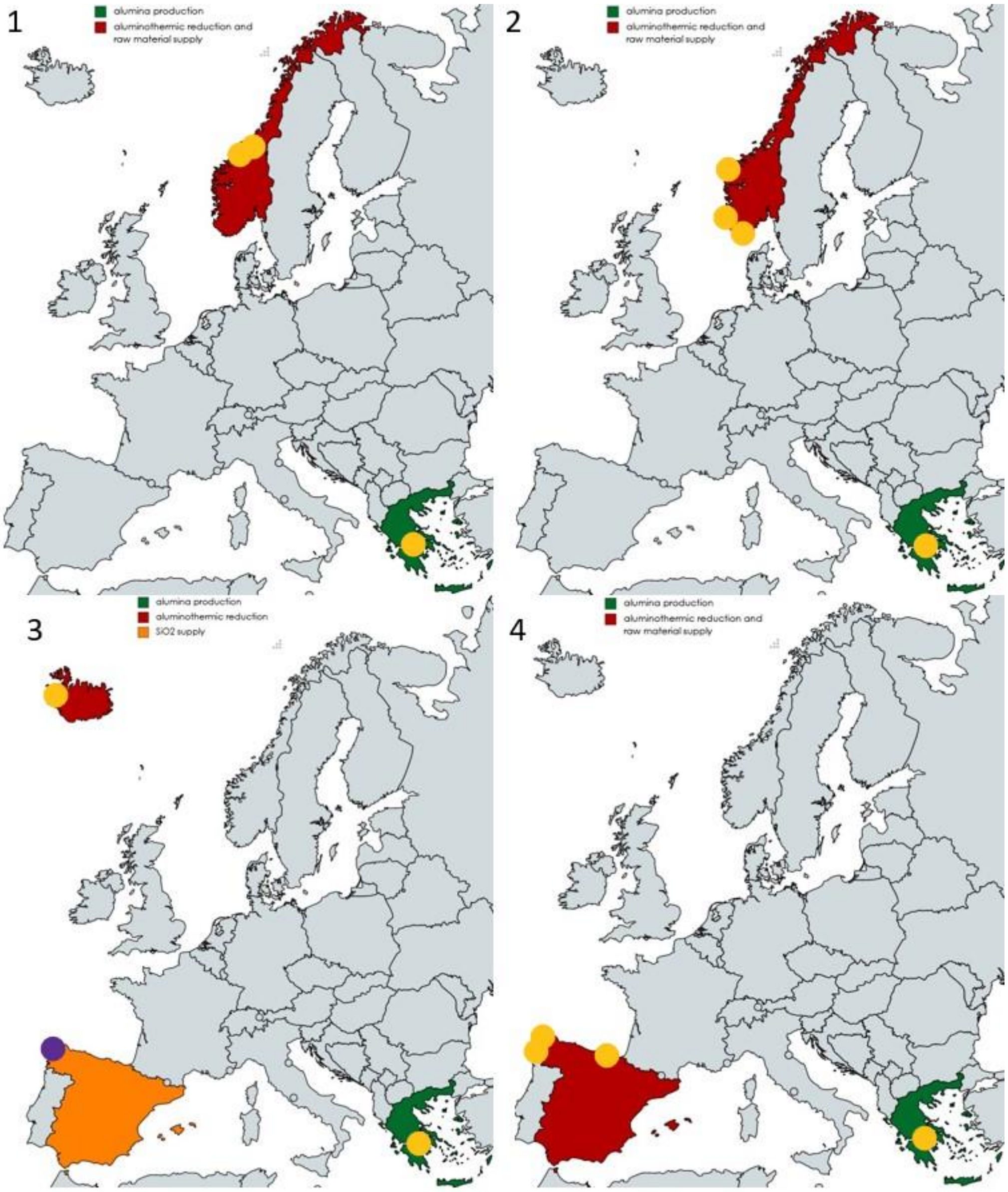

Figure 7: The location for the cases NO-GR 1 (1), NO-GR 2 (2), ES-IS-GR (3), and ES-GR (4). The dots represent the locations of the facilities

The paragraphs 2.1.2.2.1 and 2.1.2.2.2 explain the aluminothermic reduction and the alumina production processes. These and the inputs are the same for all four cases. The difference is in regionalised transport and electricity.

2.2.1.2.2 Multifunctionality and allocation

Multifunctionality of a product depicts the notion that products and their systems can serve more than one function [46, p. 89]. It describes the different functions as either primary or secondary, where the primary function is the desired purpose of the product, while unintended functions have a lesser relevance to the user. They are, however, useful for other systems in the technosphere. A process is multifunctional if it produces a primary product and a secondary product. This poses a challenge for the LCA methodology, which operates under the assumption of the production of an individual function in a system and its associated impacts. To solve this, the ISO 14044 standard has a hierarchy of allocating these processes [44, p. 14]:

1. **Subdivision of Unit process:** The multifunctionality should be avoided by dividing the unit process in question into sub-processes where the multifunctionality is divided into different functions that can be examined separately
2. **System expansion:** The product system is expanded to include the additional functions provided by the secondary product. It can be done in 2 ways: By expanding the product system that does not have an additional function or by crediting, and therefore subtracting, the additional function from the product system that has it. This leads to an avoided product instead of a multifunctionality.
3. **Allocation:** If the first two methods cannot resolve a multifunctionality the in- and outputs of the system should be divided by the different products. This should be done by relating the physical relationships between them or, if that does not work, by other relationships, such as economic evaluation.

Figure 5 shows that the aluminothermic reduction does produce CaO-Al_2O_3 slag in addition to the functional unit. This slag has an additional use as a baseline for the alumina production and the Calcium oxide production. This multifunctionality was solved by crediting the silicon production 2 avoided products, the alumina and calcium oxide. In addition, these have been refed into the system avoiding the production of raw materials.

2.2.1.2.3 Attributional and consequential LCA

The definition of a LCA comes with a need for a precise definition of the many parts in it. A correct definition of a life cycle system can be performed with two approaches, attributional or consequential. The International Reference Life Cycle Data System (ILCD) handbook has a different description of the two models [47, p. 71]:

- **Attributional:** In attributional modelling the system is modelled as it is or was. Average or generic data is typically used. It is also considered as a “descriptive” or accounting procedure.

- **Consequential:** In consequential modelling the aim is to identify the consequences that a decision in the foreground system has for other processes and systems in the economy. In contrast to attributional modelling, it uses marginal data and processes.

To bring it into context for the system described in the aluminothermic reduction, an attributional LCA would only describe the environmental impacts and benefits in contrast to the comparison. Hauschild et al. presents it as describing a product system in isolation [46, p. 94]. The use of the inputs like alumina and aluminium dross will not affect other industries. Consequential LCA, on the other hand, would include the ramifications for introducing the new market for aluminium and silicon oxide. While the SisAl project is using mostly secondary raw materials it still uses materials that can be used as a substitute for other production routes. Aluminium dross has several prospective applications, from its use in concrete to multi-based ceramics [48], [49]. Aluminium, like other commodities, saw a significant increase in value from 2020 [50], which increases efforts to utilise as much aluminium as possible. This could lead to a competition of recycling efforts. In addition, Pastor-Vallés shows that the utilisation of silicon skulls could prevent its use in the silicomanganese industry, which only has an energy and carbon intensive alternative [34, p. 20]. The joint utilisation of secondary raw materials from different countries in Europe also increases the demand for shipment to and from the facilities.

However, the SisAl-project is in its experimental stages and the amount of alumina stock is large enough that changes will not have a negative impact [51], while silicon oxide sources are not only limited to silicon skulls, but also include quartz fines, and foundry sand [52]. Erimsa already uses smaller silicon dioxide fines in its test-stages. This shows that the consequences of the SisAl-project can be considered negligible, resulting in the implementation of the attributional modelling for this thesis.

Attributional modelling and the use of system expansion therein, as well as the definitions by the ILCD resulted in fundamental discussions and debates. These concerns have to be at least mentioned to contextualize the decisions in this thesis. Different authors have highlighted problems with the ILCD handbook and particularly its inconsistencies [53], [54]. They also show that attributional and consequential LCA have different definitions, depending on the authors. According to the Shonan Guidance Principles the two approaches can be defined as [55, pp. 134–136]:

- **Attributional (ALCA):** A system modelling approach in which in- and outputs are attributed to the functional unit of a product system by linking and/or partitioning the unit processes of the system according to a normative rule.
- **Consequential (CLCA):** A system modelling approach in which activities in a product system are linked so that activities are included in the product system to the extent that they are expected to change as a consequence of a change in demand for the functional unit.

While other authors have different definitions still [56]–[58], the definition and the discussion about the implementation of the modelling approaches has evolved over the years [53], [57]–[59]. It also shows that marginal data is a defining factor for the use of a consequential LCA, but the ILCD handbook recommends average data for small changes, contradicting its own definition. Ekvall et al. argues that the handbook, as a guideline for policy-making, is outdated and should be revised, showing that the proper use of methodology changes with advances in said field [53].

2.2.1.2.4 LCIA methodology, types of impacts and software

Life cycle impact assessment (LCIA) transforms the vast amounts of elementary flows in the life cycle inventory into a small, but comprehensive list of environmental impact scores [60, p. 1]. According to ISO 14040 it can be categorized in five steps, as illustrated in the Figure 8.

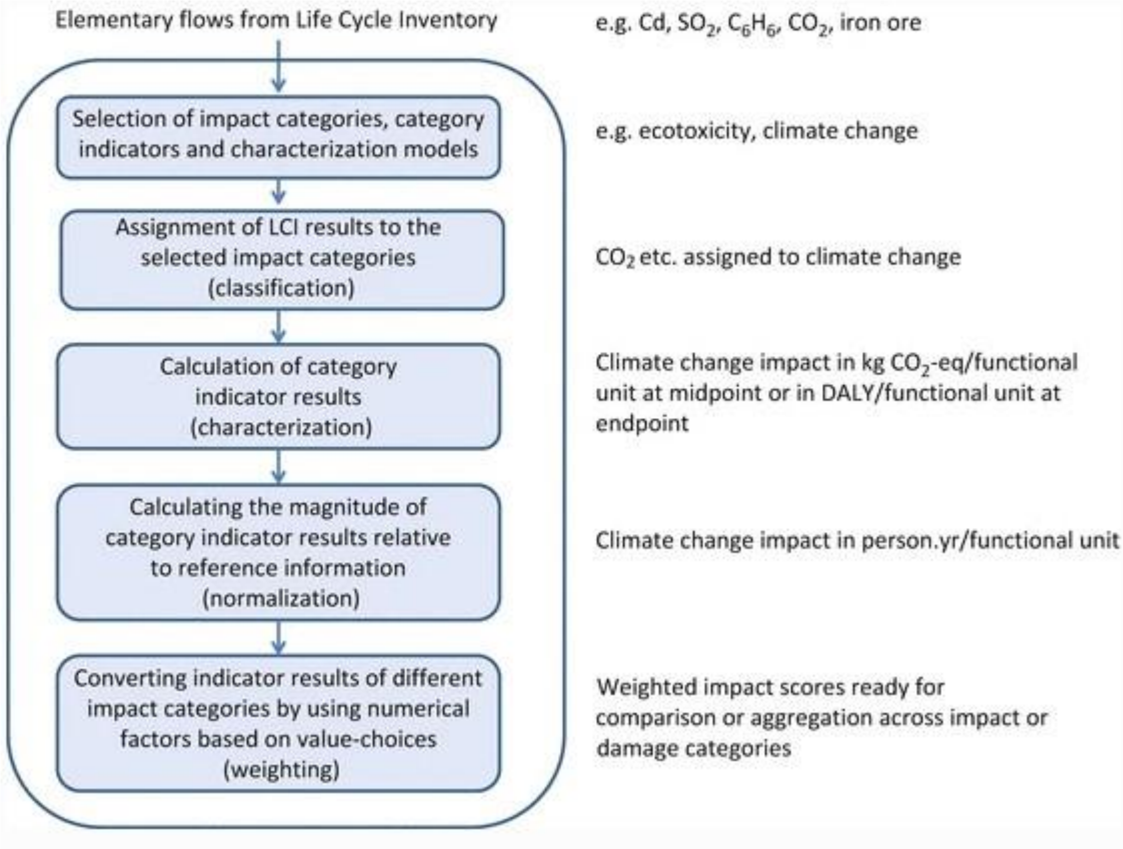

Figure 8: The five steps of a LCIA from the elementary flows to the impact categories, according to [60].

The selection of categories should, according to the ISO 14044, be consistent with the goal and scope of the LCA, the selection of impact categories should reflect a comprehensive set of environmental issues, should not disguise significant impacts, should allow traceability, and not lead to double counting [44, p. 17], [46, p. 172]. Additionally, the categories, category indicators and characterisation models should be internationally accepted. Over the years there has been a plethora of emerging LCIA methods with different application area, normalisation factors, weighting, and impact categories. This makes the selection of a specific category vital for the next steps. Various sources have extensive lists comparing the different categories, such as Impact world, TRACI, or ReCiPe2016 [46, p. 1152], [61].

The chosen LCA software coincides with the choice of the database and the impact method. The software chosen for this thesis is Simapro 9.3.0.3 with the ecoinvent 3.6 database and the ReCiPe 2016 (H) impact categories for mid- and endpoint level [62].

The Hierarchist (H) perspective is one of three potential cultural perspectives, Individualist (I), Hierarchist (H), and Egalitarian (E) which can influence the characterization factors (CF) [63]. The

ReCiPe methodology uses these three perspectives to handle uncertainty, especially in the endpoint category. While the individualist perspective assumes humans are capable of strong adaptations, therefore short timeframes are used for the CF, the egalitarian perspective assumes the opposite. The Hierarchist perspective is a middle ground and is commonly used as the default [60, p. 46]. While characterisation factors at the endpoint level have a higher degree of understandability, they also have a higher degree of uncertainty [62]. According to [62] the CF at endpoint level usually reflect one of three areas of protection, namely human health, ecosystem quality, and resource scarcity:

- **Human health:** The endpoint category examines the damage to human health in disability adjusted life years (DALY), representing the years that are lost for a person due to death or disability. The unit is DALY
- **Ecosystem quality:** The endpoint category examines the damage to the ecosystem quality in local relative species loss in terrestrial, freshwater, and marine ecosystems integrated over space and time. The unit is PDF × yr, with PDF = potentially disappeared fraction of species
- **Resource scarcity:** The endpoint category examines the damage to resource availability in monetary values, which represent the extra cost in mineral and fossil resource extraction. The unit is $.

The midpoint levels have a lower uncertainty, since they are closer to the elemental flows they represent. However, they are also harder to communicate to stakeholders and policy makers, which makes both levels complementary to each other. Endpoint level characterisation factors (*CFe*) are translated from midpoint level characterisation factors (*CFm*) using mid-to-endpoint factor ($F_{M\text{-}>E,a}$) per category:

$$CFe_{x,a} = CFm_x \times F_{M\rightarrow E,a}$$

Equation 7: Translation equation from mid- to endpoint level [62].

ReCiPe 2016 uses damage pathways as a link between the midpoint categories and the endpoint areas of protection, as seen in Figure 9.

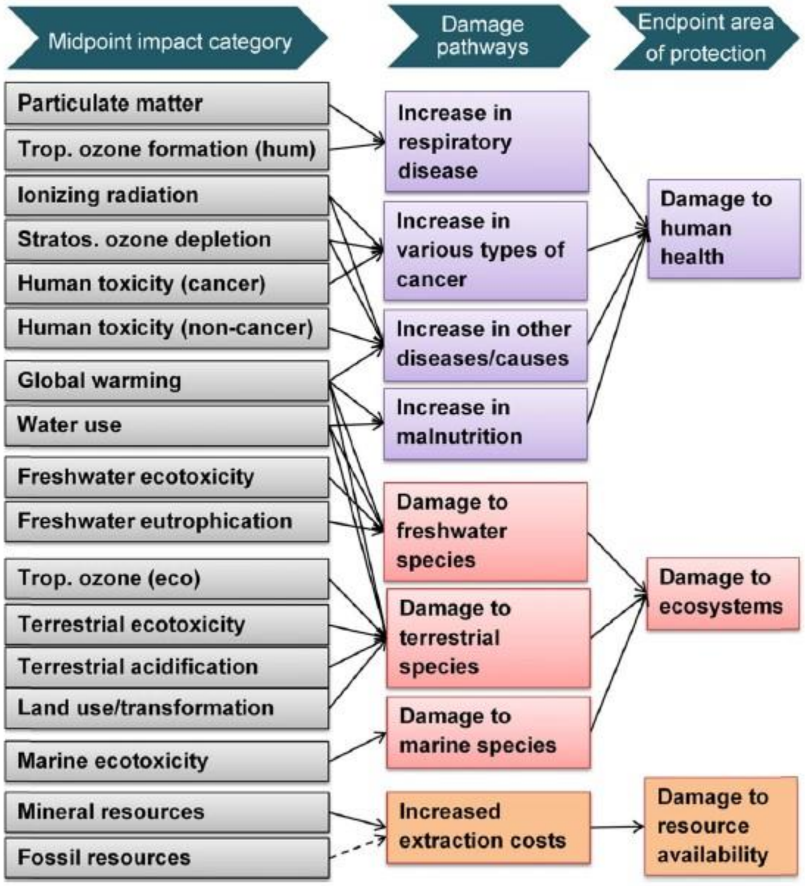

Figure 9: Midpoint impact categories in ReCiPe 2016 and their translation to AoP.[62]

The impact categories at midpoint level for ReCiPe 2016 are Climate change, stratospheric ozone depletion, ionising radiation, fine particulate matter formation, photochemical ozone formation, terrestrial acidification, freshwater eutrophication, marine eutrophication, toxicity, water use, land use, mineral resource scarcity, and fossil resource scarcity [64]. In the following list all midpoint categories for the hierarchist timeframe are presented and explained according to the ReCiPe 2016 framework [62], [64], [65]:

- **Climate Change (CC):** The impact category climate change uses global warming potential (GWP) as a characterisation factor, which quantifies the radiative forcing increase of a greenhouse gas (GHG) over 100 years. It was developed by the IPCC. The unit is kg CO_2 -eq. to air and the associated endpoint levels are damage to human health, disappeared terrestrial species, and disappeared freshwater fish.

- **Stratospheric ozone depletion (OD):** It uses the ozone depletion potential (ODP), which quantifies the decrease of stratospheric ozone concentration over 100 years. The unit is kg of CFC (chlorofluorocarbon) -11 eq. to air and the associated endpoint level is the damage to human health.
- **Ionizing radiation (IR):** it uses the ionising radiation potential (IRP), which quantifies the radionuclide emissions over 100 years. The unit is kBq Co-60 to eq./kBq (kilo Becquerel) to air and the associated endpoint level is the damage to human health.
- **Fine particulate matter formation (FPMF):** It uses the Particulate matter formation potential (PMFP), which quantifies the intake of $PM_{2.5}$ equivalents. The hierarchist perspective considers primary aerosols and secondary aerosols from SO_2. The unit is $PM_{2.5}$ eq. to air and the associated endpoint level is the damage to human health.
- **Photochemical ozone formation (POF):** It uses human health ozone formation potential (HOFP) which quantifies the increase of tropospheric ozone. There is no difference in the three cultural perspectives for this category. The unit is 1 kg of NOx-eq. to air and the associated endpoint levels are damage to human health and damage to terrestrial ecosystems.
- **Terrestrial acidification (TA):** It uses acidification potentials (AP) to quantify the proton increase in natural soils. There is no difference in the three cultural perspectives for this category. The unit is 1 kg of SO_2 -eq. to air and the associated endpoint level is the damage to terrestrial ecosystems.
- **Freshwater eutrophication (FE):** It uses freshwater eutrophication potentials (FEP) to quantify the phosphorous increase in freshwater. There is no difference in the three cultural perspectives for this category. The unit is 1 kg of P-eq. to fresh water and the associated endpoint level is the damage to freshwater ecosystems.
- **Toxicity:** To accurately model toxicity levels the midpoint categories are divided into human and ecotoxicity. They are then further divided into cancer and non-cancer human toxicity and terrestrial, marine, and freshwater ecotoxicity. The human toxicity (HT) uses human toxicity potential cancer or non-cancer (HTPc and HTPnc) to quantify the increase

of either cancer or non-cancer disease incidences over 100 years. The ecotoxicity (ET) uses the terrestrial, marine, or freshwater ecotoxicity potential (TETP, METP, FETP) to quantify the hazard-weighted increase in natural soils, marine water, or freshwaters over 100 years respectively. The unit is 1 kg 1,4-DCB-eq. (1,4-dichlorobenzene) and the associated endpoint levels are damage to human health for the human toxicity and damage to the ecosystem for the ecotoxicity.

- **Water use (WU):** It uses the water consumption potential (WCP) to quantify the increase in water consumed. The hierarchist perspective examines a standard regulation of stream flow and a standard management for food production. The unit is 1 m^3 of water-eq. consumed and the associated endpoint levels are damage to human health, $\text{PDF}_{\text{terrestrial}}$, and potentially disappeared freshwater fish species.
- **Land use (LU):** It uses the agricultural land occupation potential (LOP) to quantify the occupation and time-integrated land transformation. The cultural perspective has no influence on the land use CF. The unit is 1 $m^2 \times yr$ annual cropland-eq. and the associated endpoint level is the damage to the ecosystem by PDF.
- **Mineral Resource scarcity (MRS):** It uses the surplus ore potential (SOP) to quantify the increase of ore extracted per 1 kg of mineral resource extracted. The hierarchist perspective estimates the reserves at ultimate recoverable resource (URR) at the earth’s crust. The unit is 1 kg of Cu-eq. and its associated endpoint level is the resource scarcity.
- **Fossil resource scarcity (FRS):** It uses the fossil fuel potential to quantify the increase in surplus cost to extract future fossil fuels. The unit is 1 kg oil-eq., and its corresponding endpoint level is the resource scarcity.

These midpoint categories normally have global characterisation factors, but there exist country-specific CF for the five impact categories photochemical ozone formation: human health and ecosystems, particulate matter formation, Terrestrial acidification, and freshwater eutrophication [64, pp. 121–158]. These have been used for the case NO-GR 1 to compare the midpoint and endpoint impacts of these categories with their global counterpart. The local CF was calculated using the following formula:

$$IP_{country} = CF_{country} \times Substance$$

Equation 8: $IP_{country}$ (country-level impact potential) is equal to the $CF_{country}$(country level characterisation factor) times the amount of the particular substance.

The $IP_{country}$ (country-level impact potential) is equal to the $CF_{country}$(country level characterisation factor) times the amount of the particular substance. In Table 5 the corresponding country-level Midpoint impact factors are shown, while Table 6 shows the corresponding endpoint characterisation factors.

Table 5: Country-level MidPoint impact factors for Norway, Greece, and the global average with the corresponding substances.

Country factors impact categories, MIDPOINT					
impact category	**region**	**Substance**	**CF amount**	**CF unit**	**emitted to**
Photochemical ozone formation: Human health	World	NOx	1.00E+00	(kg NOx-eq·kg-1)	
		NMVOC	1.80E-01		
	Norway	NOx	1.03E+00		
		NMVOC	2.00E-01		
	Greece	NOx	9.50E-01		
		NMVOC	4.20E-01		
Ozone Formation Potential: Ecosystem	World	NOx	1.00E+00	(kg NOx-eq·kg-1)	
		NMVOC	2.90E-01		
	Norway	NOx	3.24E+00		
		NMVOC	5.10E-01		
	Greece	NOx	3.27E+00		
		NMVOC	1.39E+00		
Particulate Matter Formation Potential (PMFP)	World	PM2.5	1.00E+00	kg primary PM2.5-equivalents/kg	
		NH_3	2.40E-01		
		NO_x	1.10E-01		
		SO_2	2.90E-01		
	Norway	PM2.5	3.39E-01		
		NH_3	4.82E-02		
		NO_x	5.79E-02		
		SO_2	5.30E-02		
	Greece	PM2.5	8.28E-01		
		NH_3	1.87E-01		
		NO_x	1.60E-01		
		SO_2	2.67E-01		
Acidification potentials (AP)	World	NO_x	3.60E-01	kg SO2-eq·kg-1	
		NH_3	1.96E+00		
		SO_2	1.00E+00		
	Norway	NO_x	7.30E-01		
		NH_3	5.52E+00		
		SO_2	2.28E+00		

	Greece	NO_x	4.20E-01		
		NH_3	1.50E+00		
		SO_2	7.80E-01		
Freshwater Eutrophication potentials (EP)	World	P	1.00E+00	kg P to freshwater-equivalents/kg	Freshwater
		PO_4^{3-}	3.30E-01		
		P	1.00E-01		Soil
		PO_4^{3-}	3.30E-02		
	Norway	P	6.00E-01		Freshwater
		PO_4^{3-}	1.96E-01		
		P	6.00E-02		Soil
		PO_4^{3-}	1.96E-02		
	Greece	P	5.00E-01		Freshwater
		PO_4^{3-}	1.63E-01		
		P	5.00E-02		Soil
		PO_4^{3-}	1.63E-02		

Table 6: Country-level Endpoint impact factors for Norway, Greece, and the global average with the corresponding substances.

Country factors impact categories, ENDPOINT					
impact category	**region**	**Substance**	**CF amount**	**CF unit**	**emitted to**
Photochemical ozone formation: Human health	World	NOx	9.10E-01	yr·kton-1	
		NMVOC	1.60E-01		
	Norway	NOx	4.50E-01		
		NMVOC	1.20E-01		
	Greece	NOx	4.40E-01		
		NMVOC	2.30E-01		
Ozone Formation Potential: Ecosystem	World	NOx	1.29E-01	species·yr·kton-1	
		NMVOC	3.68E-02		
	Norway	NOx	3.37E-01		
		NMVOC	5.01E-02		
	Greece	NOx	2.71E-01		
		NMVOC	1.07E-01		
Particulate Matter Formation Potential (PMFP)	World	PM2.5	6.29E+02	species·yr·kton-1	
		NH_3	1.49E+02		
		NO_x	7.01E+01		
		SO_2	1.83E+02		
	Norway	PM2.5	2.50E+02	yr·kton-1	

		NH_3	3.90E+01		
		NO_x	4.80E+01		
		SO_2	4.80E+01		
	Greece	PM2.5	6.50E+02	yr·kton-1	
		NH_3	1.60E+02		
		NO_x	1.40E+02		
		SO_2	1.70E+02		
Terrestrial Acidification potentials (AP)	World	NO_x	7.70E-08	species·yr/kg	
		NH_3	4.14E-07		
		SO_2	2.12E-07		
	Norway	NO_x	1.15E-07	species·yr/kg	
		NH_3	7.01E-07		
		SO_2	3.54E-07		
	Greece	NO_x	1.07E-07	species·yr/kg	
		NH_3	3.95E-07		
		SO_2	2.57E-07		
Freshwater Eutrophication potentials (EP)	World	P	6.10E-07	species·yr/kg	Freshwater
		PO_4^{3-}	2.01E-07		
		P	6.10E-08		Soil
		PO_4^{3-}	2.01E-08		
	Norway	P	1.42E-06	species·yr/kg	Freshwater
		PO_4^{3-}	4.63E-07		
		P	1.42E-07		Soil
		PO_4^{3-}	4.63E-08		
	Greece	P	2.96E-07	species·yr/kg	Freshwater
		PO_4^{3-}	9.65E-08		
		P	2.96E-08		Soil
		PO_4^{3-}	9.65E-09		

2.2.2 Inventory

The second step in setting up a life cycle assessment is the assembly of a life cycle inventory. The most important step of the life cycle inventory is the data collection. It can be divided in foreground and background system data. A foreground system consists of processes under the control of the decision maker, while they have little or no influence on the background system [66]. In this project the majority of the foreground data was collected using data from the HZDR and the master thesis of Pastor-Vallés [34]. For the background data the ecoinvent 3.6 database was used. For the electricity the ecoinvent 3.6 database was used, and for the distance the websites maritimeoptima.com, impargo.de, and googlemaps.com were used. For the Calcination process of the $CaCO_3$ residue, the Equation 3 was used. Table 2 shows the complete inventory with in- and outputs and their denotation in SimaPro.

There are various mass flows not considered, because their input equals their output. This means that even though they are technically in the process, they will not be transmitted into the techno- or ecosphere and their impact in the system will be assumed to be negligible. The following processes were not considered:

- **CaO output from Calcination:** This process is the result of the calcination of the $CaCO_3$ residue. It will be reintegrated into the system, and therefore does not leave the system. The only repeated burden to the environment is the transport and the energy, while the rest was subtracted from the CaO input to the system.
- **Na_2CO_3 solution:** The solution is used in the alkaline leaching but is completely retrieved and reused. Its burden to the environment is negligible.

2.2.3 Impact assessment

The impact assessment is the third step of a LCA and uses methodologies previously described in the scope to assess the environmental impacts of the fore- and background processes [44, p. 24]. The methodology ReCiPe 2016, explained in 2.2.1.2.4 will serve as the midpoint and endpoint characterisation for the different impact categories. However, for available impact categories (Table 5) at mid- and endpoint level there will be a comparison between their global characterisation factor and the country characterisation factor for the foreground processes.

2.2.4 Interpretation

The fourth and last step of a LCA is the interpretation in which the findings of the inventory analysis and the impact assessment are considered and based on these conclusions are reached and recommendations are made [43, p. 16] It is an iterative process, meaning that the interpretation influences further inventory and impact assessment and goal and scope definitions. The present work uses a contribution analysis to evaluate the impact contribution of different foreground processes to the system. Since this thesis compares the impact of different changes to the system with the baseline scenario, it also does a sensitivity analysis for the electricity and transport parameters.

3 Results

3.1 Mass balance

The data reconciliation and uncertainty analysis described in 2.1.4.1 is visualised in Figure 10. It shows that most processes have only minor changes, such as SiO_2 which changed from 2.6 tons *a priori* to 2.58 tons. However, the CaO-Al_2O_3 slag changed from 5 +/- 0.5 tons *a priori* to 4.58 +/- 0.2 tons and the inert slag changed from 2.77 +/- 0.3 tons *a priori* to 2.85 +/- 0.2 tons, showing that the increased uncertainty and mass in those flows have a profound impact on these flows.

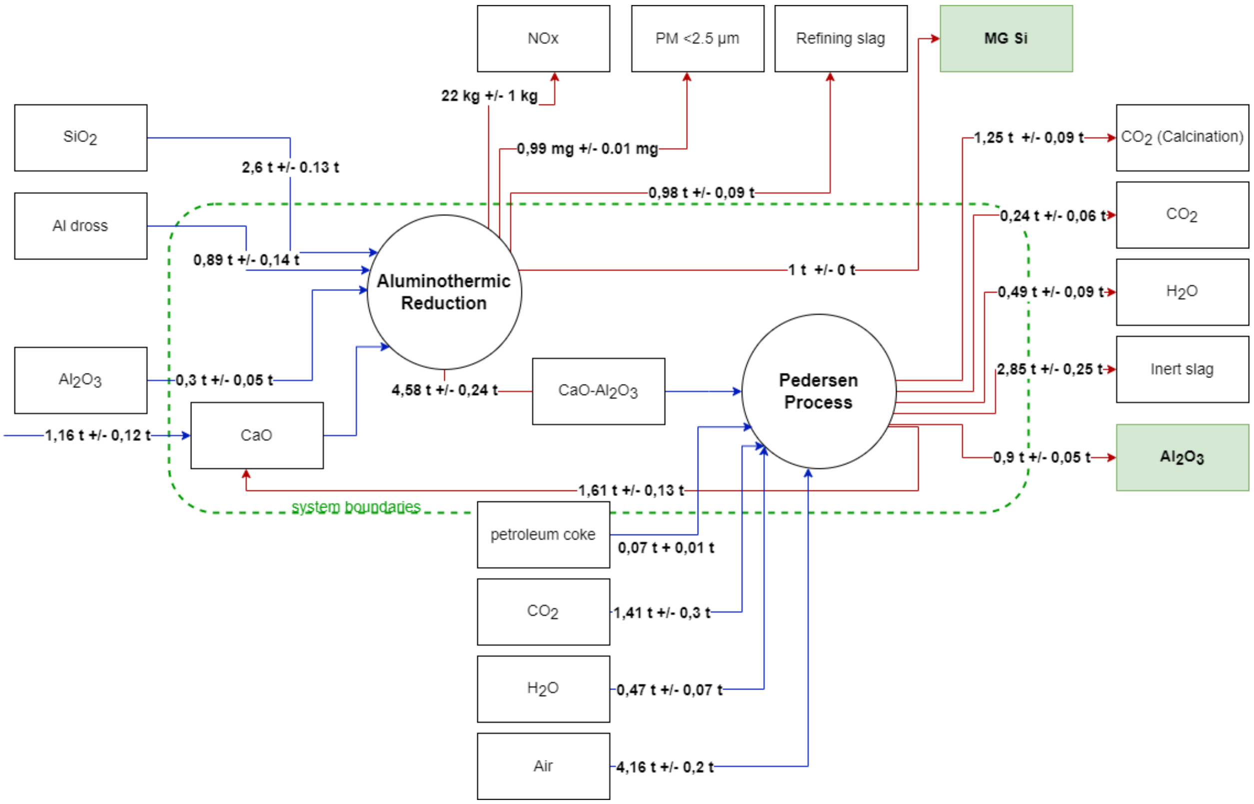

Figure 10: Mass flow of the system with calculated values.

3.2 Life cycle assessment

The life cycle assessment interpretations will be structured as followed. First, the impact assessment of the general system without transport will be analysed at the mid- and endpoint level. This will be the baseline scenario. The country-specific electricity will be set to Norway according to the assumptions made by [34] Afterwards, the cases will be compared with each other in two scenarios: First, the case-specific transport will be included, and the cases compared, second the country-specific electricity for each case will be compared. These will be compared at the midpoint level to illustrate differences in the impact categories. Lastly, the four cases and the baseline scenario, as well as the aluminothermic and carbothermic reduction modelled in [34] will be compared to each other at both mid- and endpoint level.

After the comparison of the impact at mid- and endpoint level, the assessment of the regional CF and their difference to the global CF at mid- and endpoint level will be conducted.

3.2.1 Contribution analysis of the baseline scenario

The baseline scenario shows the impact of 18 midpoint categories and 3 endpoint categories for the system without transport and with Norwegian electricity. It entails, in contrast to the aluminothermic reduction process by Pastor-Vallés, the division of calcium carbonate into carbon dioxide and calcium oxide and its subsequent use as an input for the aluminothermic reduction.

Figure 11 shows that the biggest process contribution to the impacts varies from category to category. While the categories terrestrial, freshwater, and marine ecotoxicity, as well as ionizing radiation, land use and freshwater eutrophication have the CO_2 input as their biggest contributor, the water consumption has the Norwegian electricity consumption as its biggest contributor. SiO_2 input has its main contributions in global warming and ozone formation: human health, and ecosystems. The direct emissions of MG Si account for a third of the global warming, and ozone formation: human health and ecosystems emissions.

The Figure 11 shows, that the process accounting for a majority of the impacts contributions is the CO_2 input in the alumina production. Other processes, disregarding a few, are equally distributed among the emitters. There are, however, some processes which are reducing the impacts across different impact categories. While the Al_2O_3 input reduces only the marine eutrophication, the alumina output reduces the impact of all other categories. The impacts of the categories human carcinogenic toxicity and mineral resource scarcity are completely negated by the negative emissions of the HP Alumina production. Other categories, such as fossil resource scarcity or fine particulate matter formation also have a significant reduction in their impact due to the negative

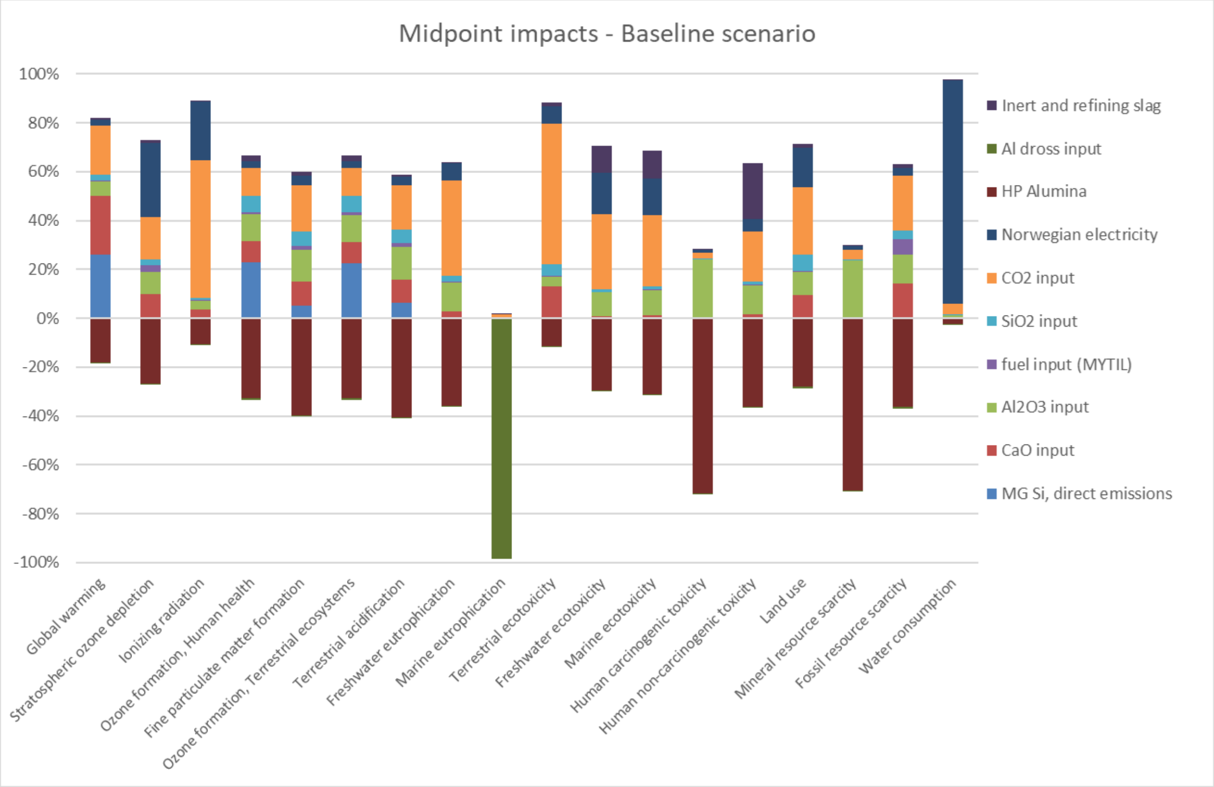

Figure 11: Life cycle impacts of the baseline scenario, Midpoint level ReCiPe 2016 (H)

emissions of HP Alumina. The endpoint impact assessment visualises a more distinct picture of the contributions of different production processes. It shows in Figure 12 that the positive impacts for Human health are divided between CaO input, CO_2 input, Al_2O_3 input, and the direct emissions in the aluminothermic reduction. Similarly, the damage to ecosystems are largely dominated by the CaO input, CO_2 input, and the direct emissions. However, the Al_2O_3 input emissions have smaller percentage impact than in the human health damage. Lastly, the Al_2O_3, CaO and CO_2 inputs have the biggest contribution to the resource damage, but direct emissions from the aluminothermic reduction play only a little role in these impacts. These emissions, however, are to a large extent offset by the negative emissions of the HP Alumina output. In the Human health and resource damage assessment they negate more than two thirds of the positive emissions, while they counteract 25% of the ecosystems damage, showing a clear reduction in environmental damage. The hierarchist perspective has a weighting choice of 40% Human Health, 40% Ecosystems, and

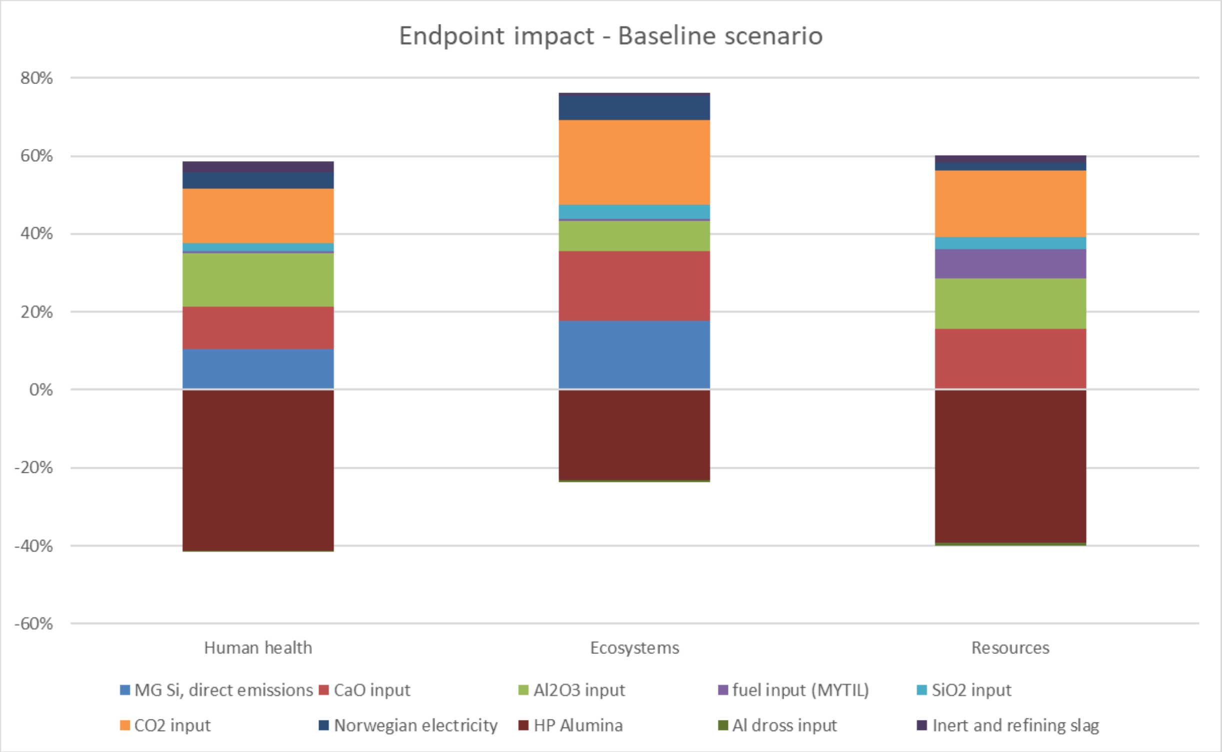

Figure 12: Endpoint impact assessment of the damage categories human health, ecosystems, and resources

20% Resources, meaning that the impacts of Human health and ecosystems are doubled in comparison to the resource depletion.

When normalising and weighting the impacts (Figure 13), the results show a strong contribution towards human health with over 100 mPt (milli weighted endpoints), which is however offset by the large negative impact of the production of HP Alumina with -75 mPt, so that the result is 32 mPt. In contrast, the impact of the ecosystem damage is much lower with only 10 mPt, while its offsets are only -3.5 mPt resulting in an impact of 7.7 mPt or more than four times lower than the human health damage. The resource depletion has the lowest damage score of a total of 0.74, which can be partially attributed to the lower weighting, showing that majority of the endpoint damage is accumulated in the human health category.

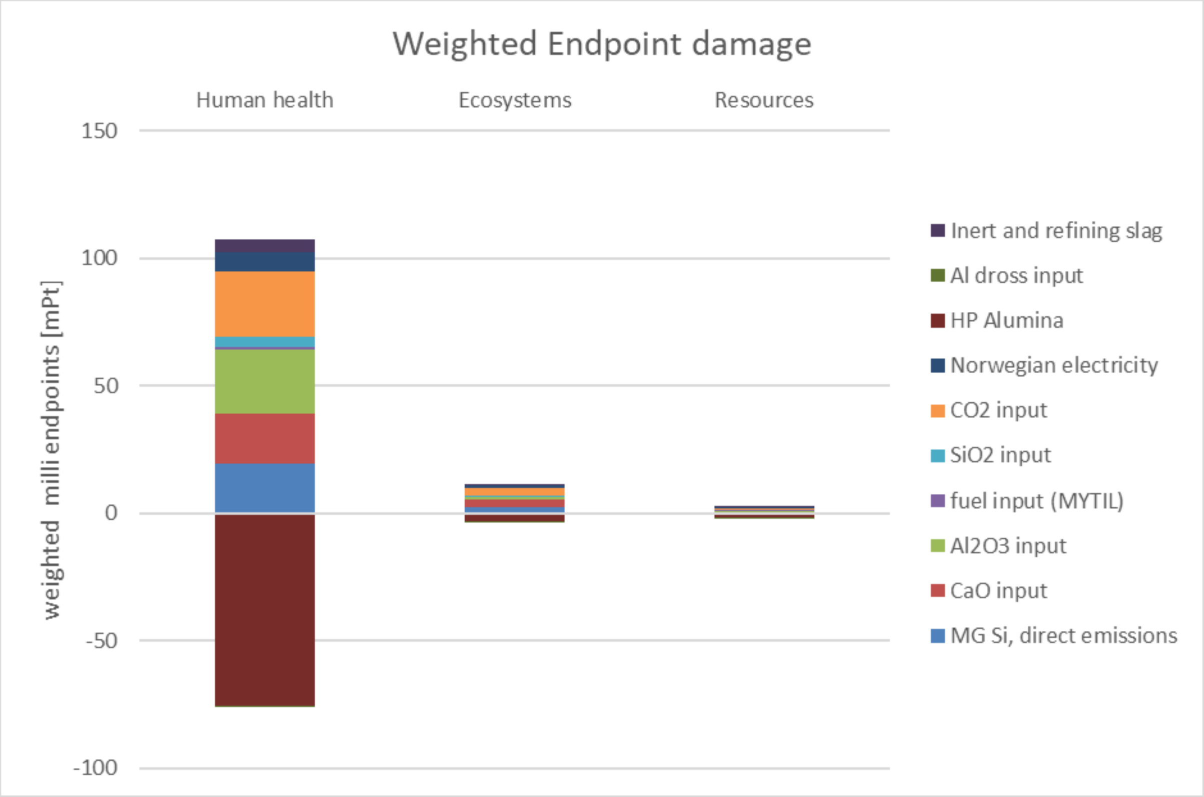

Figure 13: Weighted Endpoint damage in mPt (milli weighted endpoints)

3.2.2 Transport

To compare the different cases, the baseline and the cases NO-GR 1, NO-GR 2, ES-IS-GR, and ES-GR have been compared in different parameters. The first parameter whose impacts will be compared is the additional transport needed to ship the materials between the facilities (Table 3).

The hypothesis is that the higher the amount of transported material the higher the impact. The unit is tonne-kilometre (tkm), which represents the shipped mass times the shipping distance. Since the case NO-GR 2 has the highest amount of tkm, it is assumed that it also has the highest impact. Figure 14 visualises the midpoint impact for the 18 different categories available in ReCiPe 2016 by normalising the highest contributor of each impact category to 100% and the other as a fraction of it. It shows the baseline scenario in dark green, case NO-GR 1 in light green, NO-GR 2 in orange, case ES-IS-GR in yellow, and case ES-GR in blue. It shows that the baseline scenario has the lowest positive impact and the highest negative impact in all categories. Considering it has no additional transportation in its life cycle, this makes sense. The highest impact among the majority of categories has the case NO-GR 2, showing a significant increase in the categories Ozone formation, particulate matter formation, and terrestrial acidification. Additionally, all but the categories marine eutrophication and water consumption have the highest impact in this case, which makes sense since it is the case with the highest tkm in its transport sector. However, apart from the first mentioned categories and the fossil resource scarcity and ozone depletion, the impact difference between the cases is not substantial, only ranging 0 – 10% difference. This reveals the biggest contribution of the ship transport to the impact categories as photochemical ozone

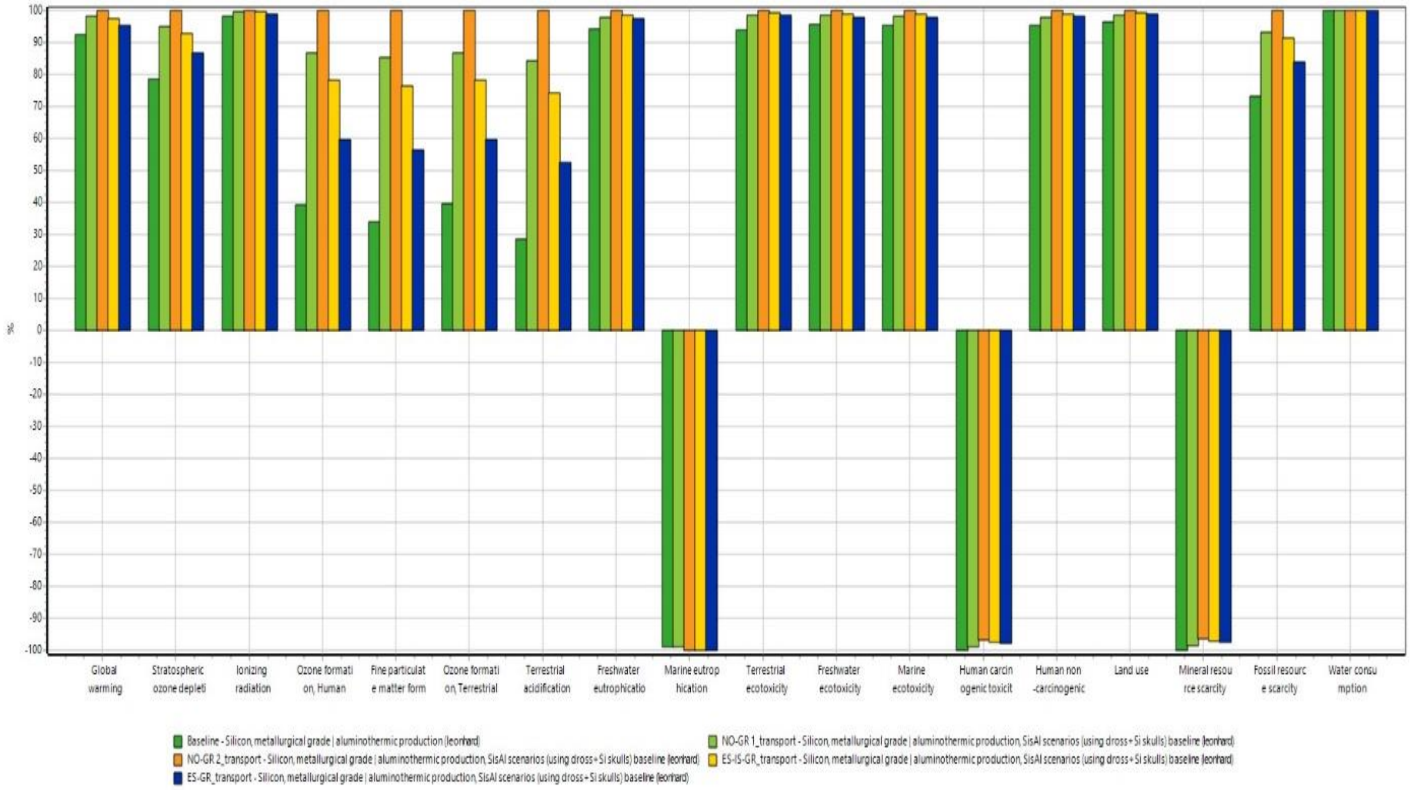

Figure 14: Comparison midpoint impact for the different cases by only adding the additional transport needed.

formation, both human health and terrestrial ecosystems, fine particulate matter formation, and terrestrial acidification with minor contributions to ozone depletion and fossil resource scarcity. This can be explained by considering that the main input to ship transport in ecoinvent is heavy fuel oil. This fuel has high SOx, NOx and NMVOC emissions [67], [68] which are the main contributors to the impact categories POF, FPMF, TA, OD, and FRS [64].

3.2.3 Electricity

After the impact assessment of the transport, the regional electricity mix for each case will be assessed. All cases and the baseline have the same 6970 kWh needed to produce 1 ton of MG Si. The baseline has a completely Norwegian energy mix, while all business cases have their alumina production in Greece which need 4270 kWh per FU. The aluminothermic production needs 2700 kWh per FU and is situated in Norway for the case NO-GR 1 and 2, in Iceland for the case ES-IS-GR and in Spain for the case ES-GR. The hypothesis is that all cases have a significantly higher impact than the baseline scenario and that the case ES-GR will have a higher impact than the other cases, since the Spanish electricity mix, in contrast to the Icelandic and Norwegian electricity mix, has a substantial share of fossil fuels [69]–[72].

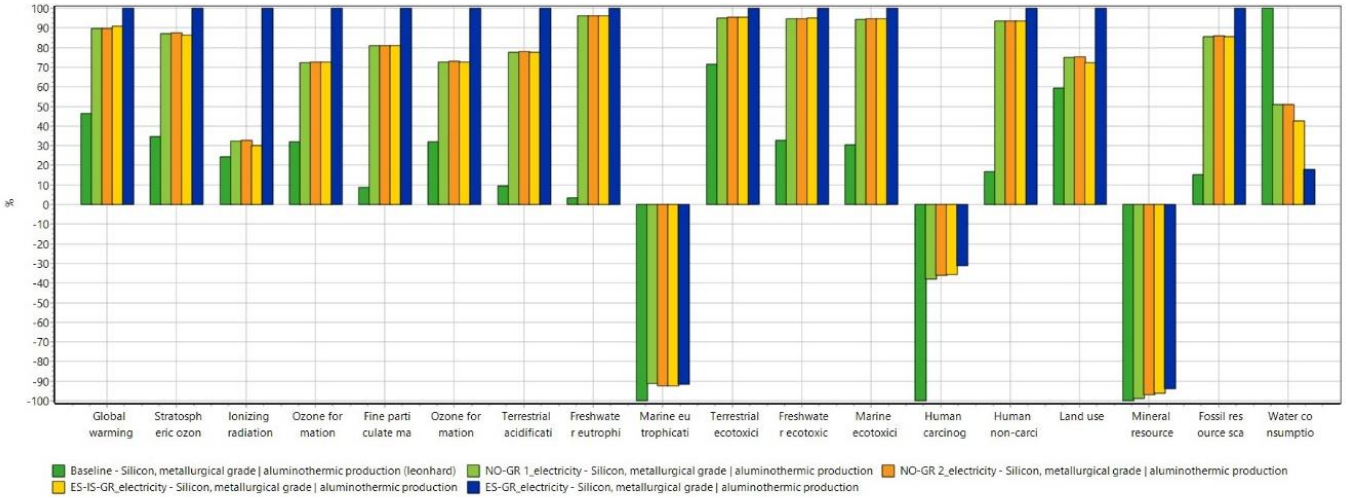

Figure 15: Midpoint comparison of the electricity mix of the baseline scenario and the four cases

The Figure 15 visualises the impact of the 18 impact categories by normalising the highest contributor of each impact category to 100% and the other as a fraction of it. It shows that in accordance with the hypothesis the impact of the baseline scenario is significantly less than the impact of the other cases in most categories. Especially the categories Freshwater eutrophication, fine particulate matter formation, terrestrial acidification, human non-carcinogenic toxicity and fossil resource scarcity show a substantial difference between the baseline and the business cases. In these cases the baseline scenario has less than 20% of the impact the highest contributor has. Additionally, the other impact categories still show a large increase when considering regional electricity. In the category global warming the baseline scenario emits 50% less CO_2-eq. compared to the next case, showing that the electricity mix is main contributor to the system in most categories. And comparing the cases NO-GR 1 and 2 to the baseline scenario it shows that the Greek electricity mix in particular has a large contribution to the systems impacts. When looking at the Greek electricity mix, that makes sense, since their electricity is mostly derived from fossil fuels, with less than 20% share of renewable energies [70].

There are, however, exceptions to this. First, the impact of the electricity mix in the categories marine eutrophication and mineral resource scarcity is not as high as compared to the aforementioned categories. This can be explained by looking at the main contributor to those negative emissions, which is the production of alumina, which dominates these impact categories.

Second, the impact categories ionizing radiation, land use, and to a lesser extent ozone formation: human health and ecotoxicity, terrestrial acidification, and fine particulate matter formation show a distinction between the cases NO-GR 1, 2, ES-IS-GR and the case ES-GR, where ES-GR shows a substantial increase in the emissions compared to the others. This can be explained by the electricity mix of Spain, which in contrast to the other countries has a high share of nuclear energy and natural gas.

3.3 Lastly, the one impact category where the baseline scenario has the highest impact is the water use, which is a result of the large percentage of hydropower in Norway. The case ES-GR shows a substantially lower impact there as well, showing that in comparison to the other cases the Spanish and Greek electricity mix does not use as much water.

Table of midpoint impact data for electricity

Table 8 in the appendix shows the data of the midpoint impacts per impact category.

3.3.1 Impact comparison to previous work

The last two chapters showed the impacts of transportation and electricity at the midpoint level. Next their combined impact will be analysed and compared to the baseline scenario and the impact of the aluminothermic and carbothermic reduction of the work of Pastor-Vallés at both mid- and endpoint level [34]. The hypothesis hereby is that the baseline scenario has a lower impact than both the carbothermic and aluminothermic reduction, but the combined impact of the electricity and transportation will increase the impacts of the cases so that they will be higher than the impacts of the aluminothermic reduction and potentially of the carbothermic reduction as well.

3.3.1.1 Midpoint impacts

Figure 16 visualises the midpoint impact categories for the aforementioned cases by normalising the highest contributor of each impact category to 100% and the other as a fraction of it. It shows that, in accordance with the hypothesis the baseline scenario (without transport or electricity changes) has a lower impact than the aluminothermic reduction in all categories, revealing that the further utilization of the calcium carbonate residue and the associated reuse of the calcium oxide in the aluminothermic reduction has a significant consequence on the impact of the system. For example the impact of global warming was reduced by 33%, while the terrestrial acidification was reduced by 40% and the impact of the fine particulate matter formation was even reduced by 70% (for further information Table 9 in the appendix).

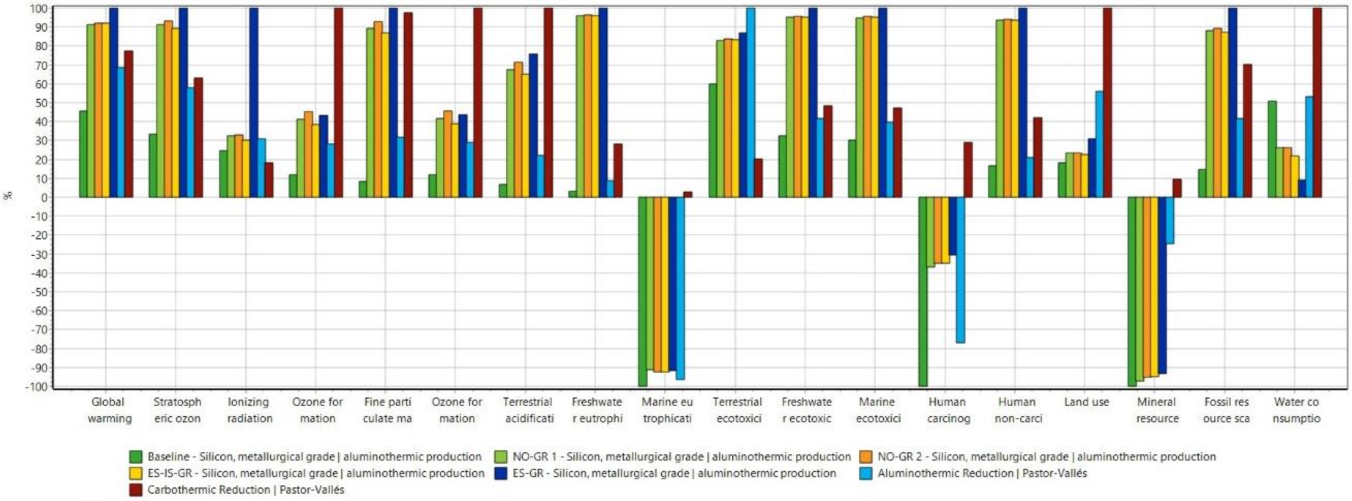

Figure 16: Comparison of the baseline scenario with the four business cases and the aluminothermic and the carbothermic reduction of Pastor-Vallés [34].

It also has a lower impact than the carbothermic reduction in most impact categories, except for ionizing radiation and terrestrial ecotoxicity. These results are in line with the in Pastor-Vallés described differences between the carbothermic and aluminothermic reduction, which indicates that the aluminothermic reduction generally has a lower impact than the carbothermic reduction. It also shows that the terrestrial ecotoxicity and ionizing radiation impact higher attributing the difference to the input of carbon dioxide in the alumina production (Figure 11), which is not part of the conventional production [34, p. 43].

The consequence of considering regional electricity mixes and the transport between the facilities observed in paragraph 423.2.2 and 3.2.3 is also present here. The associated impacts for the four business cases are substantially higher than both the aluminothermic and the carbothermic reduction in a variety of categories: Global warming, ozone depletion, freshwater eutrophication, marine and freshwater ecotoxicity, and fossil resource scarcity. In the following categories the impact of the business cases is higher than the aluminothermic reduction but not the carbothermic reduction: ozone formation human health and ecotoxicity, fine particulate matter formation and terrestrial acidification showing that impact of the transport, which mostly impacted these categories is not as high as the impact of the electricity mix. This is further visualised by the Figure 23 and Figure 24 in the appendix, comparing the additional impact of the transport and the electricity mix. This shows an overall increase in the impacts, but the significance is better evaluated when comparing the endpoint impacts:

3.3.1.2 Endpoint impacts

To better visualise the impact of the different cases, the endpoint impact of human health in DALY, ecosystem damage in PDF*yr and resource depletion in $ are calculated. Figure 17 shows the damage assessment in these three categories.

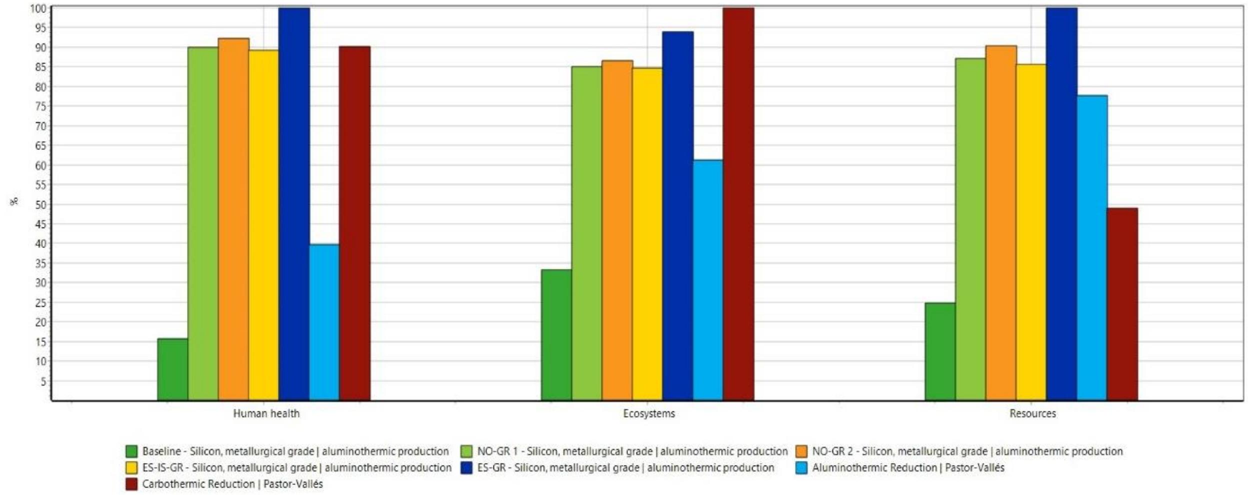

Figure 17: Damage assessment of the baseline scenario, the four business cases, and the aluminothermic and carbothermic reduction according to

Addressing the human health damage, the figure shows that the baseline scenario and the aluminothermic reduction have a substantially lower impact than the other cases and that the business cases have a similar impact as the carbothermic reduction. However, the case ES-GR has the highest impact which is 10% higher than the impact of the carbothermic reduction. This indicates a high degree of impact from the electricity mix and the transport which negates the emission savings made by the utilisation of the $CaCO_3$ residue.

The ecosystems damage analysis shows a similar picture where the two scenarios with the lowest impact are the baseline scenario and the aluminothermic reduction of Pastor-Vallés with them having a 20% reduced impact to the next scenario. The four business cases and the carbothermic reduction have a similar impact, with the carbothermic reduction having the highest impact by a slight margin of 6%, also offsetting the savings made in the baseline scenario.

Lastly, the damage to resource availability is highest with the case ES-GR and lowest with the baseline scenario. Interestingly, the second-lowest impact has the carbothermic reduction revealing that the fossil resource scarcity has a high impact in this category, because the mineral resource scarcity visualised in Figure 16 shows a significantly lower impact of all non-carbothermic scenarios. The main contributor to the fossil resource scarcity is the CO_2 input.

In the ReCiPe (H) endpoint factors the endpoint categories are weighted: 40% human health damage, 40% ecosystem damages, and 20% damages to fossil resource availability. With that and the addition of weighted points (Pt) the scenarios can be compared in single scores, as seen in Figure 18. It shows that in total the baseline scenario, with 50 Pt, has the lowest impact followed by the aluminothermic reduction depicted by Pastor-Vallés. The next impact scores are relatively close with NO-GR 1 and 2, ES-IS-GR, ES-GR and the carbothermic reduction ranging between 260 to 290 Pt, showing that the overall impact of the electricity mix and the transportation is high enough to negate the improvement made in the aluminothermic reduction or the utilisation of the slag.

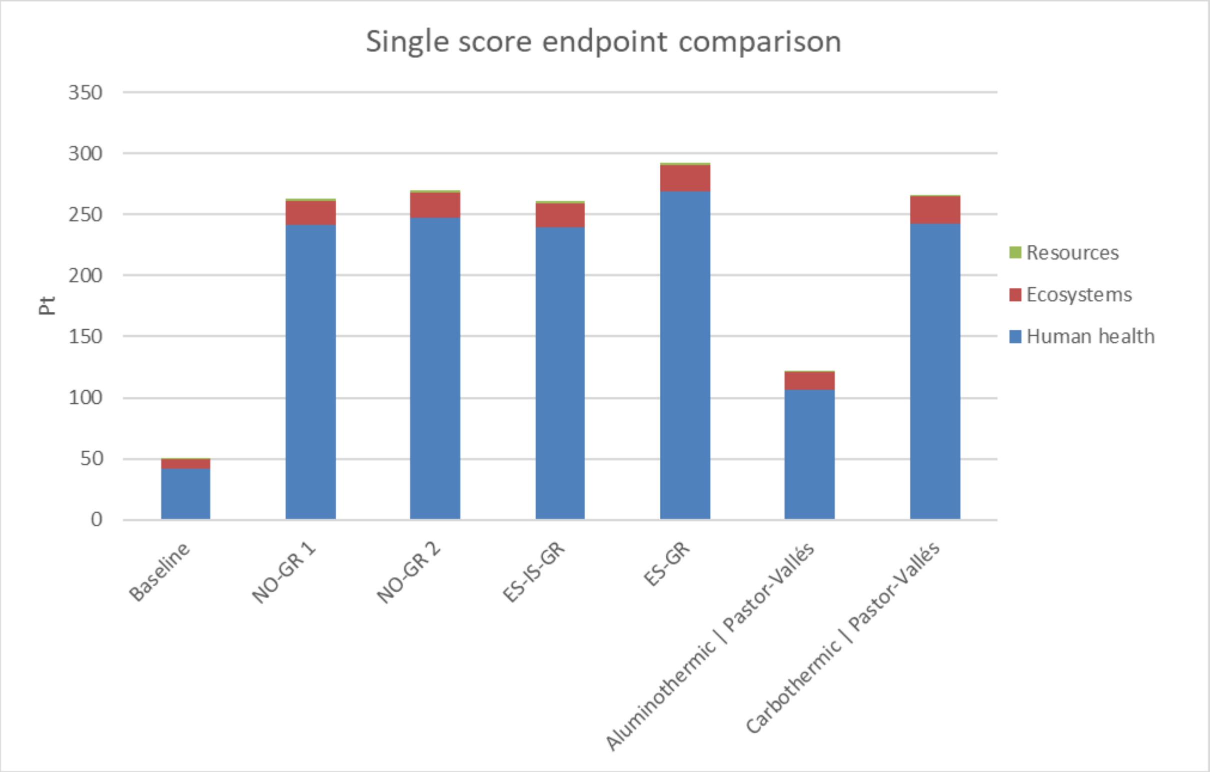

Figure 18: Single score comparison endpoint impact of the baseline scenario, the four business cases and alumino- and carbothermic reduction according to Pastor-Vallés[34]

3.3.2 Regional Characterisation factors

To fully understand the ramifications of regional emissions, the ReCiPe methodology has developed country-specific characterisation factors for the impact categories Ozone formation, human health and ecosystem, particulate matter formation, Terrestrial acidification, and freshwater eutrophication [64]. The associated substances NOx, NMVOC. PM2.5, NH_3, SO_2, P, and PO_4^{3-} have regionally different characterisation factors, indicating different impact severities for different countries. For this thesis the business case NO-GR 1 was used as an example of identifying the regional mid- and endpoint impacts for these substances. Table 5 and Table 6 show the country specific characterisation factors for Greece and Norway, as well as the global average. For each process the substance was multiplied with either the local or the global CF to obtain the associated impact.

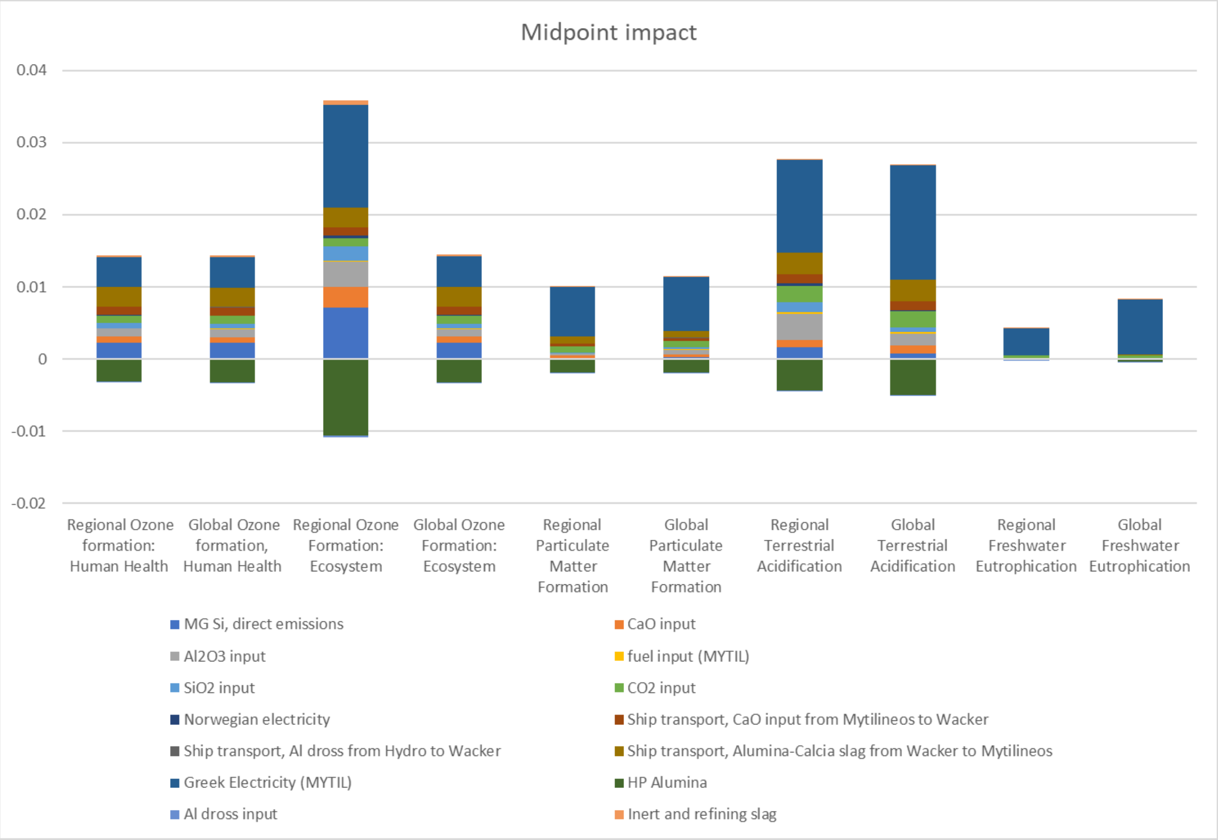

Figure 19: Midpoint comparison between localised impacts and their global counterparts for each process

Figure 19 shows the comparison of the localised impact and their global counterpart, which were retrieved from SimaPro. It shows that the localisation of the impacts has different consequences depending on the category. While the country-specific impact for ozone formation: terrestrial ecosystem is more than twice as high as original, the regional freshwater eutrophication impact is only 50% of its global counterpart. The impact categories ozone formation: human health, particulate matter formation, and terrestrial acidification, however, have only minor differences with 1%, 15% and 7% respectively (the raw data is shown in the in the appendix). This means that the main differences between the regional impacts and the global impacts for this case are the ozone formation: ecosystems and the freshwater eutrophication. These results were compared to the regional CF:

- **Ozone formation: ecosystems:** When comparing these results with the CF, it shows that CF of Norway and Greece for NOx is 3 times the global average, while the Norwegian CF for NMVOC is nearly twice as big as its global counterpart, confirming the impact results. This means that the ecosystems in Greece and Norway are three times more likely to take up the substances, as their CF are determined by their fate factors (FF), which represent the overall persistence in a given ecosystem [64, p. 54], [73].
- **Freshwater eutrophication:** The Norwegian and Greek CF for phosphorous in both Freshwater and soil are roughly half the amount of the global average, with 0.6 and 0.5 kg

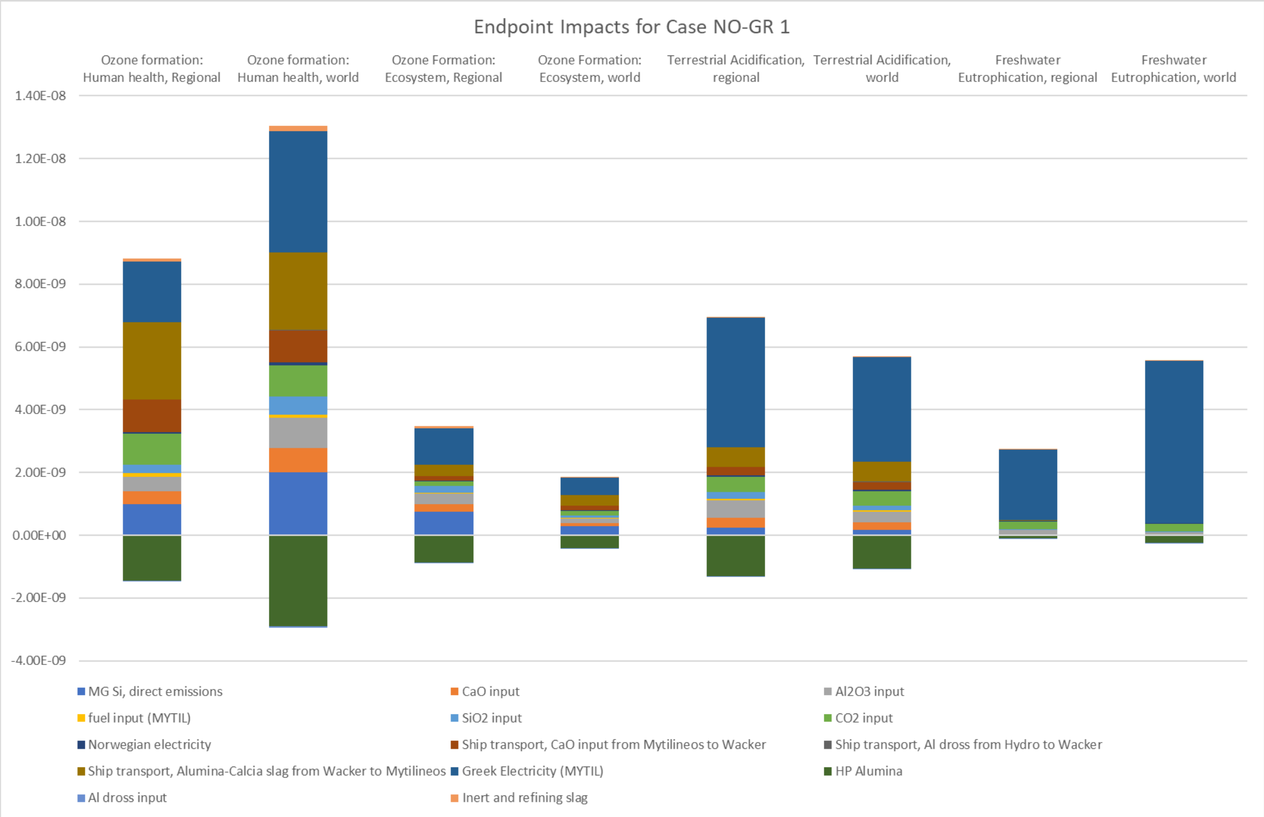

Figure 20: Comparison between regional and global endpoint impacts for case NO-GR 1 without particulate matter formation.

P to freshwater eq. to 1 kg of global average. The country-specific CF for the Phosphate is similar, affirming the observed difference of the calculated impact. Similar to the explanation for the ozone formation, the CF of Freshwater eutrophication is determined by their FF which is divided by the world average FF, indicating that the persistence of phosphorous and phosphate are half as strong in Greece and Norway as they are in the world.

Additionally, the impacts have been analysed with the endpoint CF from Table 6. In the Figure 20 and Figure 21 it shows that the differences between the regional and the global impact are similar to the observed differences at midpoint level. It shows that the differences between the regional and global CF for the categories particulate matter formation, ozone formation: human health, and terrestrial acidification ranges between 10% - 25% and that the regional impact of the ozone formation: ecosystems is approximately twice as high as the global impact, while the regional impact for freshwater eutrophication is half the global impact. The particulate matter formation was separated from the other impacts because their impact was 600x bigger than the second highest

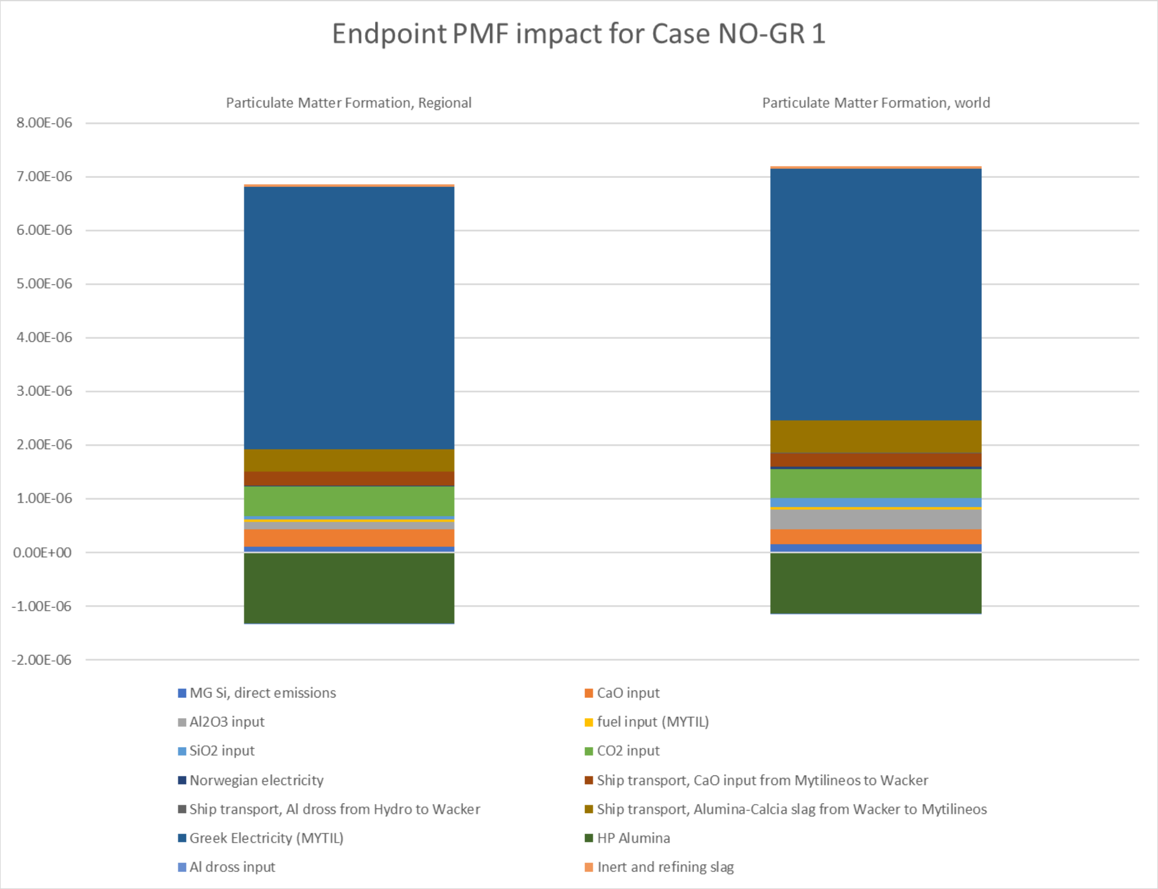

Figure 21: Comparison of the regional and global endpoint impacts for particulate matter formation

impact for both the global and the regional impact category. However, the figures also show that smaller differences in the midpoint are now larger, while the more profound differences have balanced themselves. This illustrates the importance of regionally distinct LCA, even with similar midpoint impacts.

Figure 25 in the appendix shows the cumulative endpoint damages in DALY and PDF*yr for all impact categories combined, which shows a significant environmental burden by the particulate matter formation.

4 Discussion

4.1 Key findings

Aiming to evaluate the aluminothermic system and process, this thesis tried to answer the following two research questions:

1. How can mass flow analysis (MFA) be used to balance the process system of the aluminothermic reduction?
2. How does the life cycle analysis changes when considering different contributing parameters, such as processing and resupplying the CaO from the Pedersen process into the aluminothermic reduction, considering regionally different characterisation factors (CF), transporting the materials from and to the different facilities, or using the country-specific electricity mixes?

The in- and outputs of the aluminothermic system were previously experimentally quantified but not mass balanced or analysed statistically. This thesis examined the existing in- and outputs to the SisAl and Pedersen process both qualitative and quantitative, identified the uncertainties of the flows and based on that calculated the MLE for a more precise mass distribution of the system. These values were then visualized in a flowchart (Figure 10). It shows that the experimentally derived values of the important flows such as MG silicon metal, HP alumina or the reactants were accurately measured, but the waste streams such as the Pedersen-process slag and the CaO-Al_2O_3 slag were wrongly determined, and the data reconciliation could more accurately identify these streams impacting the resulting LCA.

The second research question can be separated into several subsections. First, which processes contribute the most to the impacts of the baseline scenario? Figure 11 shows the process contributions to the midpoint categories, while Figure 12 and Figure 13 show the endpoint impacts. Both the mid- and endpoint level show that the main contributors are the CO_2 input to the alumina production, the Norwegian electricity mix, and the SiO_2 input to the aluminothermic reduction, while the production of HP alumina has a substantial negative impact, especially in categories such as human carcinogenic toxicity or mineral resource scarcity. In contrast to the baseline scenario in Pastor-Vallés, the impact of the CaO input is reduced by 50% e.g., the global warming impact is reduced from 3.15 t CO_2-eq. to 1.35 t CO_2-eq. confirming that introducing the circularity of the

CaO flow reduces its impact. Many of the impacts of SiO_2 and CO_2 can be traced to the electricity mix and heat of their production. Ecoinvent assumes the European electricity mix which has a large share of coal and other fossil fuels, increasing the footprints of these inputs [74]. The Norwegian energy mix consists of 94% hydropower [69] which, although a renewable energy source, produces impacts during the dam construction and its use phase.

Second, how sensitive is the system to changes in electricity and transportation? Four real-life business cases were quantified and compared to the baseline scenario. Figure 14 shows the midpoint impacts of the comparison and illustrates that the addition of transport between the facilities shows a significant increase in ozone formation, particulate matter formation, and terrestrial acidification. The greater the distance, the bigger the impact, with the case NO-GR 2 having the greatest impact in these categories. The explanation for that is the use of heavy fuel oil, which has a lot of impurities and emits substantially NOx, SO_2 and NMVOCs compared to gasoline or natural gas [68]. The impacts of the regionally distinct electricity mixes for the business cases in comparison to the baseline scenario are shown in Figure 15. They visualize how much a change in electricity increases the impacts. While the differences in mineral resource scarcity are less than 10%, the differences in freshwater eutrophication exceed 3000%, and the impact global warming is more than doubled. Most impactful is the Greek electricity mix which consists of mostly coal, natural gas and oil, with only 20% of renewable energies [70]. The addition of the Spanish or Icelandic electricity mix changes the impacts only slightly, apart from ionizing radiation, which can be explained by their larger share in renewables and nuclear energy [71], [72].

Third, how do the previously discussed changes in the process system compare to the assessment by Pastor-Vallés? Figure 16 shows the comparison between the midpoint impacts of the baseline, the four business cases, and the previous assessment of the aluminothermic and carbothermic reductions by Pastor-Vallés [34]. It visualises that the emission savings by the recirculation of the CaO in the baseline scenario significantly reduces the impacts, such as a 40% reduction in Global warming compared to the carbothermic reduction (Table 9). However, it also shows that the introduction of transport and especially regional electricity mixes places a substantial environmental burden on the system resulting in a higher impact in most categories, such as an average increase of 22% in CO_2-eq. emissions compared to the carbothermic production (Table 9). The single score endpoint impact (Figure 17 and Figure 18) illustrates that the addition of these two processes has a profound impact on the sustainability of the entire system. While the baseline scenario has an impact score of 50 Pt the average impact of the business cases is 500% higher than that and as high as the carbothermic reduction showing that this energy intensive system is very sensitive to changes in the electricity mix.

Fourth and lastly, does the consideration of different regional CF change the assessment of the environmental impacts of the case NO-GR 1? Figure 19 shows the comparison between the regional and global CF in the relevant impact categories. It shows that two categories have a profound difference comparing the regional and global CF: Ozone formation: Ecosystems and Freshwater eutrophication, showing an increase of 200% and a decrease by 50% respectively. This shows that regional CF can have a significant impact on the assessment of spatial impact categories and should be considered. The single score in Figure 25, however, shows that certain impact categories, in this case FPMF, can have a much higher impact on the damage to ecosystems and human health than others, negating the impact of regional CF entirely.

4.2 Limitations and outlook

The life cycle assessment is highly dependent on the choices of the methodology and assumptions. This is illustrated by the fact that the choice of subprocesses such as electricity, CaO input or transport can substantially change the outcome of the sustainability of the process. Especially the assumption of a country-specific electricity mix can alter the outcome of an LCA significantly. This study, however, has assumed the country-specific electricity mix of the ecoinvent 3.6 database, which uses electricity data from 2016 [74]. This data does not accurately depict the electricity mixes, since Greece and Spain have undergone substantial efforts to change their electricity sources [70], [72]. While Greece had a share of coal of 18.9 TWh in 2016 it fell to 6 TWh in 2020 [70]. It also increased its share of renewable energy by 16% in four years. Spain’s development is similar, with a drop of coal energy from 37 TWh in 2016 to 6 TWh in 2020 and an increase in renewable energy by 6% in the same time span, showing that high-carbon energy sources are being replaced by low-carbon alternatives, reducing the environmental footprint of their electricity mix.

Additionally, it was assumed that the energy-intensive carbothermic reduction will be implemented in Norway, whose electricity mix is 98% renewable [69]. When using the European energy mix, the carbon footprint of the conventional production is twice as high and other categories have a similar increase [34, Fig. 4.11]. This shows that the aluminothermic and carbothermic processes are very sensitive to the selection of the location of the facilities and their electricity mixes.

Another assumption was the choice of the carbon source, choosing 65% fossil fuel carbon for the carbothermic reduction and external CO_2 for the Pedersen process [34, pp. 30–31]. According to Pastor-Vallés the use of 100% biogenic carbon will reduce CO_2-eq. emissions by 50% but will leave other impacts such as FPMF or TA unchanged [34, Fig. 4.15]. Other sources have concluded that the choice of the carbon reactant could even have a more profound impact [75], [76], showing a reduction in CO_2 emissions by 97% [75, p. 8] or 67% [76, Fig. 4] respectively. However, the carbon footprint analysis of both articles does not report on the overall impact of the production of 1 ton of silicon but instead compare the CO_2-eq. emissions of the different carbon reductants with each other. Additionally, the recirculation of the emitted CO_2 in the Pedersen process (Figure 10) could reduce the impact of the aluminothermic reduction, as the thermal decomposition of calcium carbonate could be used to produce high-purity CO_2 for the Pedersen process [77]–[79]. These studies have shown that CO_2 capture in the cement industry is feasible because the CO_2 waste stream in the clinker production can purified for the CCS [78], [79]. The decomposition of the residual calcium carbonate from the Pedersen process is essentially the same reaction as the clinker production (Equation 3). A elimination of the emission of the CO_2 input process would theoretically reduce the CO_2-eq. emissions of the baseline scenario by over 30%, while the impact of categories such as TA or IR would be negative (Figure 11). Since the energy needed for the decomposition of $CaCO_3$ is already in the baseline scenario the only additional impact would be the purification of the CO_2 stream. Future studies in the SisAl pilot could improve the circularity of the system by reintroducing the captured CO_2 into the Pedersen process. Since both the thermal decomposition and the alumina production will be at the same facility, the industrial symbiosis is not bound by spatial challenges.

To put the sustainability of the aluminothermic reduction into context the SisAl pilot must be compared to other alternatives to the conventional production. Other reducing agents have been proposed, such as silicon carbide (SiC) [80], EOL plastics [81], [82], hydrogen [83, p. 4], or magnesium (Mg) [83, p. 6]. These proposals, however, are either in early stages of development, such as Mg or SiC, or have several challenges accompanying them. Hydrogen, a potential alternative for steel production [84], [85] has only a limited use for SiO_2 since it has unfavourable thermodynamics, requiring temperatures above 4500°C making it too energy intensive [84]. The use of SiC needs a largescale SiC supply, which is rarely found naturally [86] making it a processed reducing agent, increasing the environmental impact. Magnesium, on the other hand, could be used as a reductant it faces challenges with scalability and low yield [87]. The use of EOL plastics has mostly been studied as carbon substitute in the SAF in the steelmaking process [81], [82] and has yet to be tested in the carbothermic reduction of silicon dioxide. It would also be another fossil resource, as the source of the plastics will not be biogenic. These examples show that alternatives to the aluminothermic or the conventional production are not ready for large scale production if at all.

Further studies on the sustainability of the aluminothermic reduction need to be conducted. Additional assessments should entail up-to-date electricity mixes from the participating companies, consider the circularity improvements, and analyse the carbothermic production in other countries. Because the electricity mix has such a high impact on the environmental burden of the process, electricity country mixes need to be up-to-date. The system described in Figure 10 shows improvement for circularity, which first needs to be experimentally evaluated and then assessed with an LCA. The utilization of the emerging CO_2 and the produced slag could further improve the sustainability of the system. The produced slag has a low environmental burden because it is inert, but the extraction of useable materials could have a similar impact to that of the utilization of the CaO. The carbothermic production of silicon metal is the environmental benchmark which the aluminothermic reduction is compared against. The thesis compared its Norwegian production route with the Norwegian electricity mix to different aluminothermic scenarios while the transport and regional CF of the carbothermic reduction were not considered. The majority of the global and 11% of European silicon comes from China [25, p. 707], whose electricity mix has a share of over 60% coal [88] increasing its impact substantially.

5 Conclusion

The novel aluminothermic reaction patented by the SisAl pilot aims to decarbonize the silicon metal production by using secondary aluminium sources instead of coal. This thesis explored its sustainability by using MFA and LCA. It aimed to answer two sets of questions: First, is the aluminothermic reduction system mass balanced and second, how do the environmental impacts change when adding different parameters such as calcium oxide recirculation, transport distances, country-specific electricity mixes, and spatial CF to the LCA?

To answer these questions this work employed two methods, the MFA and the LCA. Mass flow analysis is a systematic assessment of the flows of materials within a system of processes [35, p. 3]. It was herein used to quantify the in- and outflows of the system and to balance the streams of materials within. The life cycle assessment addressed the environmental impacts throughout the silicon's life cycle from raw material acquisition to production (cradle-to-gate). This thesis did a comparative study on the environmental impact of four business cases and a baseline scenario by changing certain parameters of the system. It showed that the inclusion of transport and especially electricity had a profound impact on the sustainability of the system. It visualised that the average impact of the business cases is five times higher than the baseline impact. Comparing these findings with previous LCA showed that the added environmental impacts of the business cases is high enough to offset the emission savings by the aluminothermic reduction compared to the carbothermic reduction. It, however, also showed that reintroducing calcium oxide into the system while not changing other parameters (baseline scenario) can decrease overall impact by 50% compared to previous assessments of the aluminothermic reduction. Lastly, the impact of the case NO-GR 1 was spatially analysed by comparing regional CF with their global averages, showing that certain impact categories have a significant sensitivity towards regional CF, therefore substantially changing their impact. These findings show that the sustainability of the energy-intensive aluminothermic reduction is dependent on the electricity mix and that a conventional production has a lower environmental impact if it is powered by renewable energy.

To improve the validity of the system further research should address the reintroduction of the CO_2 into the system, the topicality of the electricity source, and the robustness of the carbothermic reduction as a benchmark. Alternatives to the aluminothermic reduction could be the substitution of the reductant in the carbothermic production with biogenic carbon, which would reduce the CO_2

emissions by 50%, however it would increase its land use. Other alternatives such as hydrogen, magnesium or silicon carbide are less viable or matured options, showing that the aluminothermic reduction could be a sustainable alternative to the conventional production if its employed in a country with a green electricity mix.

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7 Appendix

7.1 Simapro denotations and synonyms

Table 7: Simapro denotation for the flows and their used synonyms in the thesis

SimaPro denotation	**Used Synonym**
Silicon, metallurgical grade | aluminothermic production, SisAl scenarios (using dross+Si skulls) baseline (leonhard)	MG Si
Aluminium oxide, metallurgical {IAI Area, EU27 & EFTA}| market for aluminium oxide, metallurgical | APOS, U	HP Alumina
Air	Air input
Water, process, unspecified origin/kg	Water input
Quicklime, in pieces, loose {RoW}| market for quicklime, in pieces, loose | APOS, U	CaO input
Aluminium oxide, metallurgical {IAI Area, EU27 & EFTA}| market for aluminium oxide, metallurgical | APOS, U	Al2O3 input
Petroleum coke {GLO}| market for | APOS, U	fuel input
Silica sand {GLO}| market for | APOS, U	SiO2 input
Carbon dioxide, liquid {RER}| production | APOS, U	CO2 input
Electricity, medium voltage {NO}| market for | APOS, U	Norwegian electricity
carbon dioxide	CO2 output, calcination
carbon dioxide	CO2 output, emission
water	Water output
nitrogen oxides	NOx
particulates, <2.5 µm	PM2.5
Dross from Al electrolysis {GLO}| market for | APOS, U	Al dross input
Hazardous waste, for underground deposit {GLO}| market for | APOS, U	hazardous waste
Inert waste {Europe without Switzerland}| market for inert waste | APOS, U	refining slag
Inert waste {Europe without Switzerland}| market for inert waste | APOS, U	inert slag

Electricity, medium voltage {IS}| market for | APOS, U	Icelandic Electricity input
Electricity, medium voltage {ES}| market for | APOS, U	Spanish Electricity input
Electricity, medium voltage {GR}| market for | APOS, U	Greek Electricity input
Transport, freight, sea, bulk carrier for dry goods {GLO}| transport, freight, sea, bulk carrier for dry goods | APOS, U	Ship transport, from (…) to (…)
Transport, freight, lorry >32 metric ton, EURO6 {RER}| transport, freight, lorry >32 metric ton, EURO6 | APOS, U	Truck transport, from (…) to (...)

7.2 Comparison Baseline and former LCA

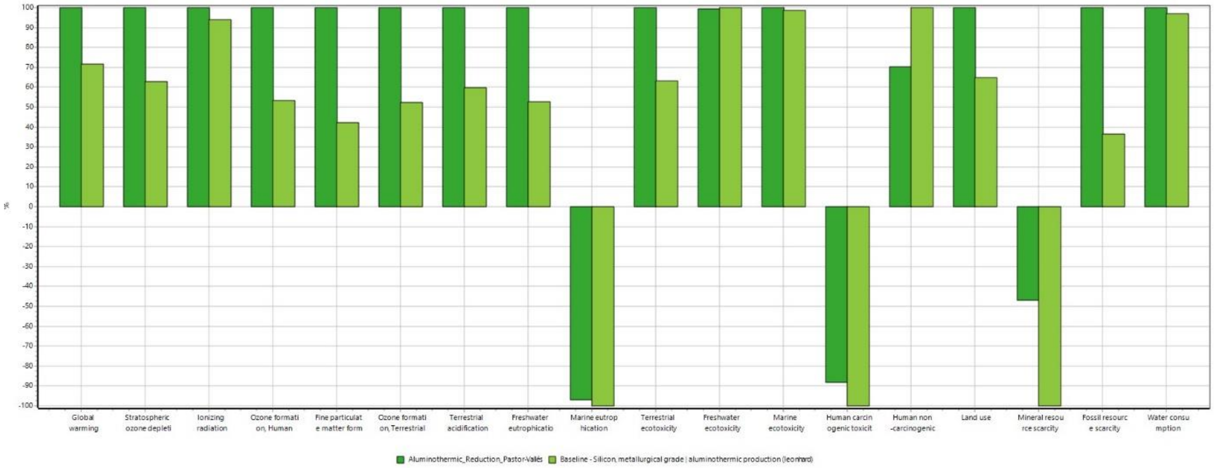


Figure 22: Comparison Baseline and aluminothermic reduction according to Pastor-Vallés [34].

7.3 Table of midpoint impact data for electricity

Table 8: Midpoint comparison for the addition of regional electricity mix for the baseline scenario and the four business cases.

Midpoint comparison - Electricity mix						
Impact category	**Unit**	**Baseline**	**NO-GR 1**	**NO-GR 2**	**ES-IS-GR**	**ES-GR**
Global warming	kg CO2 eq	3.62E+03	7.01E+03	7.02E+03	7.11E+03	7.83E+03
Stratospheric ozone depletion	kg CFC11 eq	7.46E-04	1.88E-03	1.88E-03	1.86E-03	2.15E-03
Ionizing radiation	kBq Co-60 eq	1.94E+02	2.57E+02	2.57E+02	2.37E+02	7.91E+02
Ozone formation, Human health	kg NOx eq	3.19E+00	7.27E+00	7.30E+00	7.28E+00	1.00E+01
Fine particulate matter formation	kg PM2.5 eq	8.95E-01	8.26E+00	8.28E+00	8.28E+00	1.02E+01
Ozone formation, Terrestrial ecosystems	kg NOx eq	3.23E+00	7.36E+00	7.39E+00	7.37E+00	1.01E+01
Terrestrial acidification	kg SO2 eq	2.17E+00	1.77E+01	1.78E+01	1.77E+01	2.28E+01
Freshwater eutrophication	kg P eq	2.71E-01	7.93E+00	7.94E+00	7.93E+00	8.25E+00
Marine eutrophication	kg N eq	-5.34E+00	-4.87E+00	-4.93E+00	-4.93E+00	-4.90E+00
Terrestrial ecotoxicity	kg 1,4-DCB	1.29E+04	1.72E+04	1.72E+04	1.72E+04	1.80E+04
Freshwater ecotoxicity	kg 1,4-DCB	1.07E+02	3.08E+02	3.09E+02	3.09E+02	3.25E+02
Marine ecotoxicity	kg 1,4-DCB	1.32E+02	4.10E+02	4.11E+02	4.11E+02	4.34E+02
Human carcinogenic toxicity	kg 1,4-DCB	-6.17E+02	-2.33E+02	-2.22E+02	-2.20E+02	-1.92E+02
Human non-carcinogenic toxicity	kg 1,4-DCB	1.71E+03	9.66E+03	9.68E+03	9.68E+03	1.03E+04
Land use	m2a crop eq	2.34E+02	2.95E+02	2.97E+02	2.85E+02	3.95E+02
Mineral resource scarcity	kg Cu eq	-4.99E+01	-4.92E+01	-4.83E+01	-4.79E+01	-4.68E+01
Fossil resource scarcity	kg oil eq	2.36E+02	1.34E+03	1.35E+03	1.34E+03	1.57E+03
Water consumption	m3	2.12E+02	1.08E+02	1.08E+02	9.02E+01	3.81E+01

7.4 Table of midpoint impact data for all compared scenarios

Table 9: Data points for the midpoint impact categories for the baseline scenario, the four business cases and the carbothermic and aluminothermic reduction

Midpoint Impacts for all cases and the carbothermic and aluminothermic reduction								
Impact category	**Unit**	**Baseline**	**NO-GR 1**	**NO-GR 2**	**ES-IS-GR**	**ES-GR**	**Aluminothermic**	**Carbothermic**
Global warming	kg CO2 eq	3.62E+03	7.23E+03	7.31E+03	7.30E+03	7.93E+03	5.43E+03	6.12E+03
Stratospheric ozone depletion	kg CFC11 eq	7.46E-04	2.03E-03	2.08E-03	1.99E-03	2.23E-03	1.29E-03	1.41E-03
Ionizing radiation	kBq Co-60 eq	1.94E+02	2.59E+02	2.60E+02	2.39E+02	7.93E+02	2.44E+02	1.44E+02
Ozone formation, Human health	kg NOx eq	3.19E+00	1.11E+01	1.22E+01	1.04E+01	1.16E+01	7.59E+00	2.69E+01
Fine particulate	kg PM2.5 eq	8.95E-01	9.62E+00	1.00E+01	9.38E+00	1.08E+01	3.41E+00	1.05E+01

matter formation								
Ozone formation, Terrestrial ecosystems	kg NOx eq	3.23E+00	1.12E+01	1.23E+01	1.05E+01	1.18E+01	7.80E+00	2.69E+01
Terrestrial acidification	kg SO2 eq	2.17E+00	2.19E+01	2.31E+01	2.12E+01	2.46E+01	7.16E+00	3.25E+01
Freshwater eutrophication	kg P eq	2.71E-01	7.94E+00	7.95E+00	7.94E+00	8.26E+00	7.24E-01	2.32E+00
Marine eutrophication	kg N eq	-5.34E+00	-4.87E+00	-4.93E+00	-4.93E+00	-4.90E+00	-5.16E+00	1.48E-01
Terrestrial ecotoxicity	kg 1,4-DCB	1.29E+04	1.78E+04	1.80E+04	1.79E+04	1.86E+04	2.15E+04	4.32E+03
Freshwater ecotoxicity	kg 1,4-DCB	1.07E+02	3.11E+02	3.12E+02	3.11E+02	3.27E+02	1.36E+02	1.58E+02
Marine ecotoxicity	kg 1,4-DCB	1.32E+02	4.14E+02	4.16E+02	4.15E+02	4.36E+02	1.74E+02	2.06E+02
Human carcinogenic toxicity	kg 1,4-DCB	-6.17E+02	-2.28E+02	-2.15E+02	-2.15E+02	-1.90E+02	-4.76E+02	1.80E+02
Human non-carcinogenic toxicity	kg 1,4-DCB	1.71E+03	9.70E+03	9.74E+03	9.72E+03	1.04E+04	2.16E+03	4.34E+03
Land use	m2a crop eq	2.34E+02	3.01E+02	3.04E+02	2.91E+02	3.99E+02	7.21E+02	1.29E+03
Mineral resource scarcity	kg Cu eq	-4.99E+01	-4.86E+01	-4.74E+01	-4.74E+01	-4.65E+01	-1.24E+01	4.79E+00
Fossil resource scarcity	kg oil eq	2.36E+02	1.41E+03	1.43E+03	1.40E+03	1.60E+03	6.64E+02	1.12E+03
Water consumption	m3	2.12E+02	1.08E+02	1.08E+02	9.03E+01	3.82E+01	2.21E+02	4.15E+02

7.5 Midpoint comparison all scenarios for transport

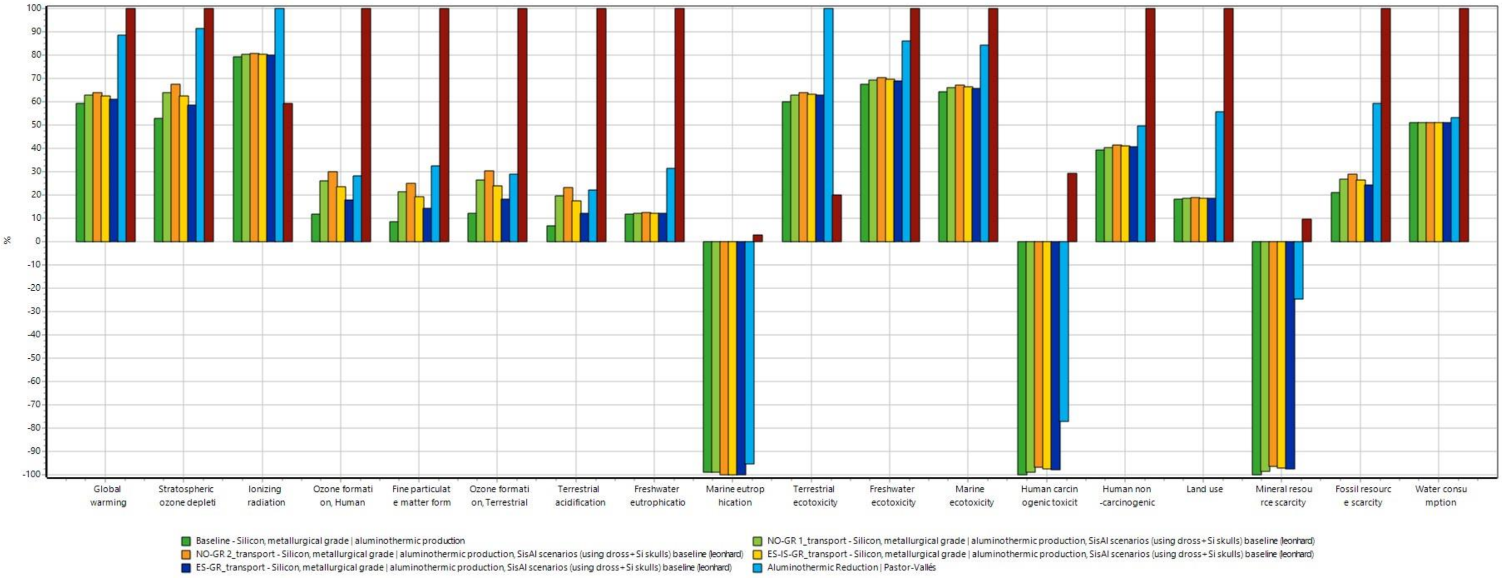


Figure 23: Midpoint comparison of the transportation impact with aluminothermic and carbothermic reduction of Pastor-Vallés [34]

7.6 Midpoint comparison for all scenarios for electricity

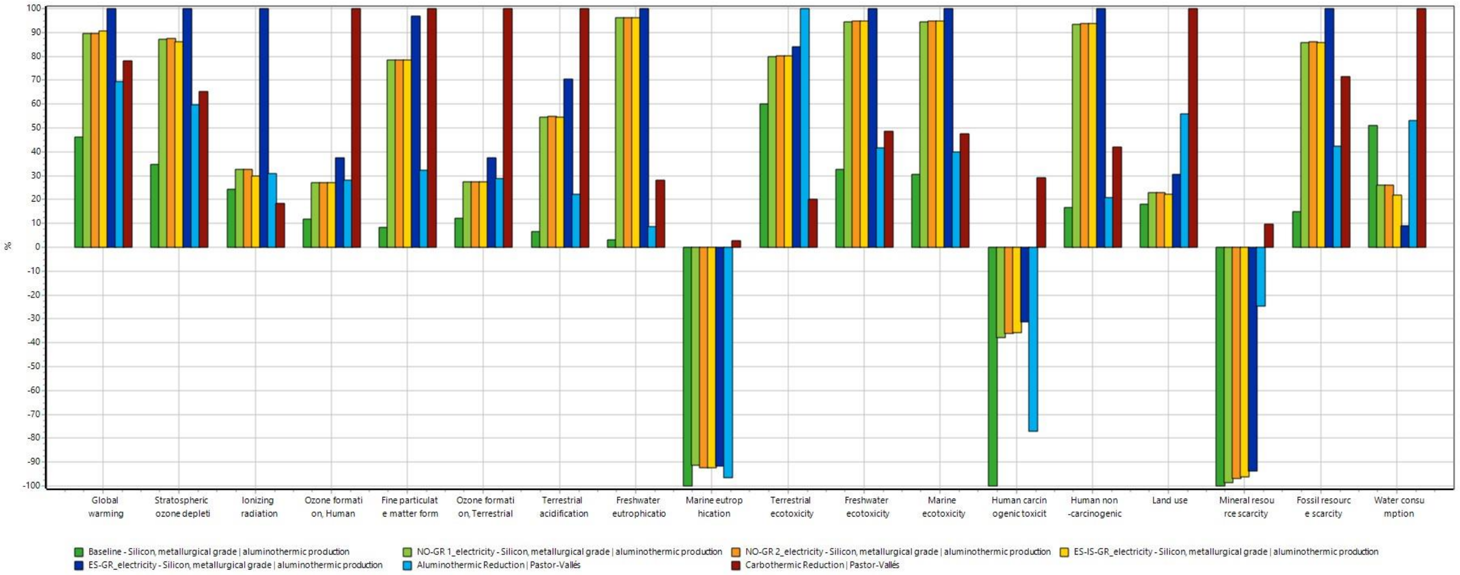


Figure 24: Midpoint comparison of the impact of country-specific electricity with the aluminothermic and carbothermic reduction of Pastor-Vallés [34].

7.7 Single score endpoint impact of regional and global CF

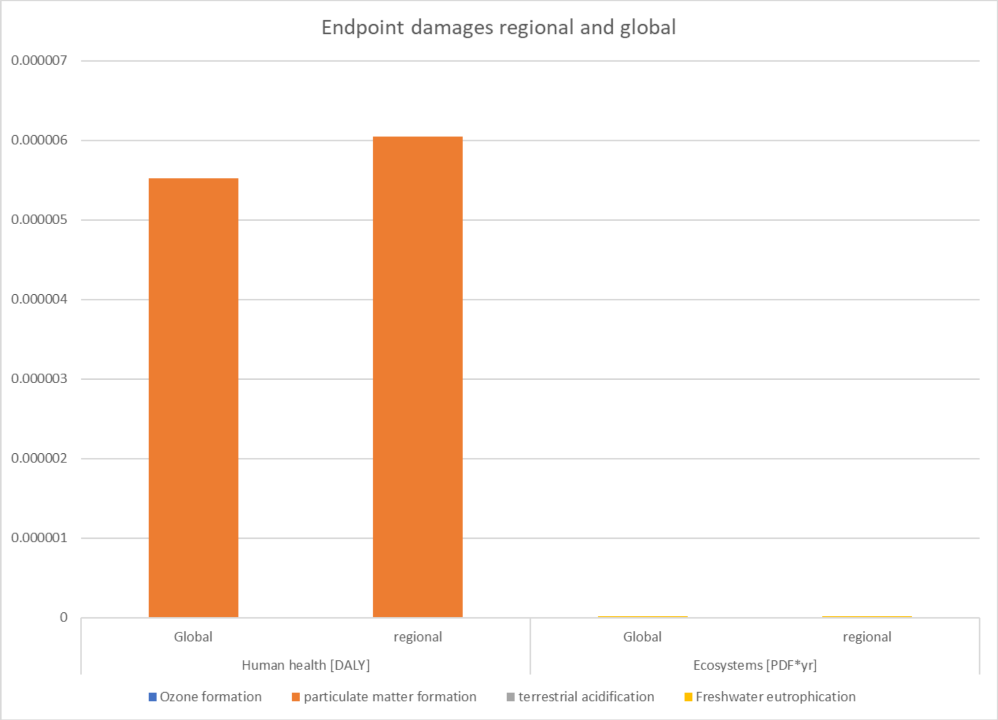
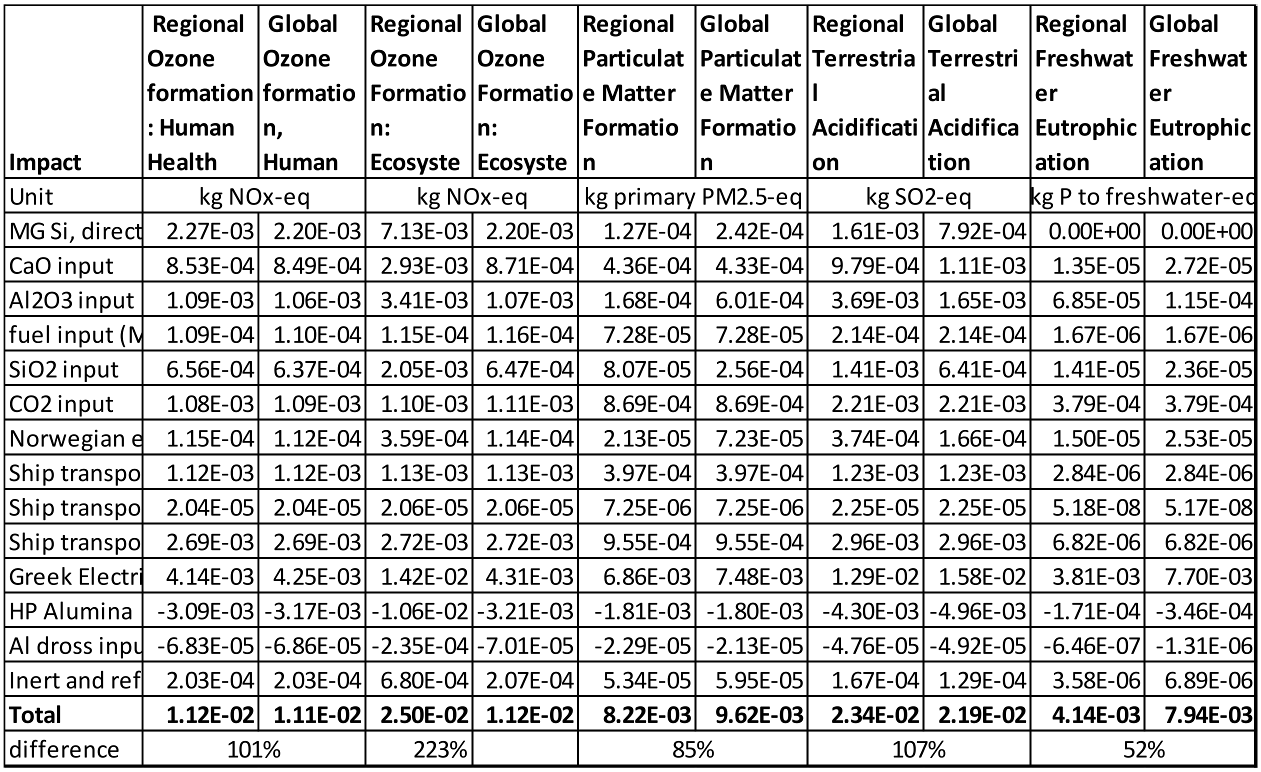


*Figure 25: Cumulative endpoint damages in DALY or PDF*yr for both global and regional CF. Damage to the ecosystems is 500 times lower than to human health, which is why it seems to be empty.*

Table 10:Data showing the impact of the regional and global impact categories.



Impact	**Regional Ozone formation: Human Health**	**Global Ozone formation, Human**	**Regional Ozone Formation: Ecosyste**	**Global Ozone Formation: Ecosyste**	**Regional Particulate Matter Formation**	**Global Particulate Matter Formation**	**Regional Terrestrial Acidification**	**Global Terrestrial Acidification**	**Regional Freshwater Eutrophication**	**Global Freshwater Eutrophication**
Unit	kg NOx-eq		kg NOx-eq		kg primary PM2.5-eq		kg SO2-eq		kg P to freshwater-ec	
MG Si, direct	2.27E-03	2.20E-03	7.13E-03	2.20E-03	1.27E-04	2.42E-04	1.61E-03	7.92E-04	0.00E+00	0.00E+00
CaO input	8.53E-04	8.49E-04	2.93E-03	8.71E-04	4.36E-04	4.33E-04	9.79E-04	1.11E-03	1.35E-05	2.72E-05
Al2O3 input	1.09E-03	1.06E-03	3.41E-03	1.07E-03	1.68E-04	6.01E-04	3.69E-03	1.65E-03	6.85E-05	1.15E-04
fuel input (M	1.09E-04	1.10E-04	1.15E-04	1.16E-04	7.28E-05	7.28E-05	2.14E-04	2.14E-04	1.67E-06	1.67E-06
SiO2 input	6.56E-04	6.37E-04	2.05E-03	6.47E-04	8.07E-05	2.56E-04	1.41E-03	6.41E-04	1.41E-05	2.36E-05
CO2 input	1.08E-03	1.09E-03	1.10E-03	1.11E-03	8.69E-04	8.69E-04	2.21E-03	2.21E-03	3.79E-04	3.79E-04
Norwegian e	1.15E-04	1.12E-04	3.59E-04	1.14E-04	2.13E-05	7.23E-05	3.74E-04	1.66E-04	1.50E-05	2.53E-05
Ship transpo	1.12E-03	1.12E-03	1.13E-03	1.13E-03	3.97E-04	3.97E-04	1.23E-03	1.23E-03	2.84E-06	2.84E-06
Ship transpo	2.04E-05	2.04E-05	2.06E-05	2.06E-05	7.25E-06	7.25E-06	2.25E-05	2.25E-05	5.18E-08	5.17E-08
Ship transpo	2.69E-03	2.69E-03	2.72E-03	2.72E-03	9.55E-04	9.55E-04	2.96E-03	2.96E-03	6.82E-06	6.82E-06
Greek Electri	4.14E-03	4.25E-03	1.42E-02	4.31E-03	6.86E-03	7.48E-03	1.29E-02	1.58E-02	3.81E-03	7.70E-03
HP Alumina	-3.09E-03	-3.17E-03	-1.06E-02	-3.21E-03	-1.81E-03	-1.80E-03	-4.30E-03	-4.96E-03	-1.71E-04	-3.46E-04
Al dross inpu	-6.83E-05	-6.86E-05	-2.35E-04	-7.01E-05	-2.29E-05	-2.13E-05	-4.76E-05	-4.92E-05	-6.46E-07	-1.31E-06
Inert and ref	2.03E-04	2.03E-04	6.80E-04	2.07E-04	5.34E-05	5.95E-05	1.67E-04	1.29E-04	3.58E-06	6.89E-06
Total	**1.12E-02**	**1.11E-02**	**2.50E-02**	**1.12E-02**	**8.22E-03**	**9.62E-03**	**2.34E-02**	**2.19E-02**	**4.14E-03**	**7.94E-03**
difference	101%		223%		85%		107%		52%	

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