Contributions to *Contribution Analysis*

Structuring and extension of approaches to understanding contributions to impacts in Life Cycle Assessment

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Contributions to Contribution Analysis: Improving our understanding of contributions to impacts in Life Cycle Assessment

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Summary

Life Cycle Assessment (LCA) is the primary method for evaluating environmental performance across a product's life cycle, with the interpretation phase being critical for identifying significant issues and guiding improvements. Contribution Analysis (CA) is the main tool for understanding how processes and flows contribute to overall impacts, yet despite its importance, CA is not well standardized.

CA is widely used in LCA interpretation to identify key contributors to impacts, detect data quality issues, and select parameters for sensitivity analysis. However, CA lacks an overarching definition and structured methodology, leading to inconsistent and sometimes irreproducible results and a lower credibility of LCA studies. Various approaches to CA exist and can assess two different sides: Direct contributions (e.g. CO_2 emitted from electricity production) and Indirect contributions (e.g. CH_4 emitted during coal mining for the production of electricity from coal). Each approach can assess one or both of these sides from a different perspective.

For large groups of processes however, combined Direct and Indirect CA cannot be easily applied. However, the Hypothetical Extraction Method (HEM), used in the field of Input Output Analysis, in principle is capable of providing such a perspective on CA. It was however unclear if that approach could be adapted to LCA and what insights it could provide.

CA is especially important in the context of prospective LCA (pLCA), where scenario-driven change in the data makes it harder to interpret results. In pLCA, the most used tool currently is *Premise* to generate future versions of background databases based on scenario storylines. To learn about the specific challenges that different approaches to CA pose and learn how they could be overcome, this thesis applied CA in three pLCA cases. These cases were chosen for the following reasons: 1) cobalt production given its low production scale but high expected change in demand; 2) sand and gravel production, given concrete demand and the vastly larger production scale relative to cobalt; and 3) evaluation of the pLCA tool *Premise* via analysis of nine commonly used industrial products to clarify drivers of future impacts.

In this way, this thesis aimed to realize the following main objective: to structure and -where necessary- formalize CA and to learn from practical cases so that this toolbox of approaches becomes more useful to LCA practitioners.

Chapter 2 provides an overarching definition of Contribution Analysis that covers current uses of the term and structures different approaches. A distinction is made between Direct and Indirect contributions, The different approaches are demonstrated using an example case study and the differences between approaches are discussed. Each of these approaches provides a unique insight into results in LCA. Five direct and three combined Direct and Indirect approaches are described.

The five Direct approaches are:

- **Individual Elementary Flow (EF) CA** from specific individual EFs from single processes (Individual EF CA), e.g. the contribution from CH_4 emission from a single process 'coal mining'.
- **EF CA**, from one EF across all processes, e.g. the contribution from all CO_2 flows from all processes in the system.
- **Process CA**, from all EFs per process, e.g. the contribution from all EF (CO_2, CH_4 etc.) from the process 'electricity production from coal' to Climate Change impact.
- **EF group CA**, from groups of EF, e.g. the contribution from a group of all carbon containing flows.
- **Process group CA**, from groups of processes, e.g. the contribution from all 'electricity production' processes.

Three combined Direct+Indirect approaches have also been introduced:

- **First-Tier CA**, measuring the Direct contribution from the Functional Unit (FU) process and Direct+Indirect contribution from each intermediate flow of the FU, e.g. the contribution from 'aluminium production' and contribution from all intermediate flows needed for 'aluminium production' like 'electricity' and 'bauxite'.
- **Life Cycle Stage CA**, from life cycle stages, e.g. the contribution from life cycle stages like 'production', 'use' and 'end of life'.
- **Path CA**, contributions from a path (e.g. value chain) of processes, often visualized in Sankey diagrams, e.g. the contribution from intermediate flows throughout the product system lead to the final LCA score, showing the 'path' of contributions.

Guidance was formalized for practitioners on how to report and present their CA methodologies and results, such that LCA studies could become more replicable and interpretable. Primarily, when CA is used, it should be described as contributing *from* something (e.g. a process or EF) *to* something (e.g. LCI or a characterized result). The work in Chapter 2 should contribute to a higher quality and more reproducible body of LCA literature and more well-founded conclusions.

Chapter 3 introduces the HEM to LCA through outlining a four step process including a mathematical framework. HEM is demonstrated as a CA approach using a small example case study and a larger example using ecoinvent. Making use of HEM provides insights in cases where an Indirect perspective is required and for groups of processes such as industry sectors or regions. While other existing approaches have their own advantages, they could not provide this perspective effectively. The work in Chapter 3 shows how and when HEM can be a useful approach for CA in cases where current CA approaches may be lacking, such as assessing the Direct and Indirect contributions from groups of processes, providing an additional CA approach to the LCA practitioner in understanding impacts from their systems.

Next, Chapters 4, 5 and 6 are three case studies that make use of CA with the intent of learning from applying CA in practical cases. Chapter 4 is a case study demonstrating pLCA on the production of cobalt. Process group CA was used to assess what the main contributing process groups were in each of these variable-scenario combinations. The processes were grouped based on the products they produce (e.g. all electricity production). This case study provided the main learning that led to the structuring of CA in Chapter 2. Chapter 5 is a case study demonstrating pLCA on the production of sand and gravel. Process group and First-Tier contributions (contribution of intermediate products to concrete production) were assessed. These CA approaches were used to assess how conventional production and production from recycling lead to different impacts and to show the contributions from sand, gravel and cement to concrete production. This case study provided as a main learning that current combined Direct+Indirect approaches cannot effectively be applied to large groups of processes, HEM as introduced in Chapter 3 helps provide this perspective in LCA. Chapter 6 is a study where nine important industrial products from the *Premise* database are assessed. CA via process group CA and HEM were used to assess the effect from fifteen large product groups representing industry sectors producing similar products. The CA approaches were used to assess the Direct and combined Direct+Indirect contribution of these groups to the nine products. Process group CA is essential in this assessment to show where contributions (or changes in contribution) originate. HEM allowed the finding that some sectors play an important role as 'connecting' sectors. These connecting sectors/processes don't necessarily have high contributions themselves, but 'connect' to other processes in the product-system that have high contributions. This analysis of Indirect contributions from large process groups was possible through adapting HEM from IOA into LCA in Chapter 3. Together, the learnings from all three cases show it is important to define clear categories of CA approaches and develop a new approach to analyze new perspectives when relevant, such as HEM.

To conclude, through dividing CA approaches into two groups of perspectives, Direct and Indirect and clearly describing how these approaches should be applied from some entity to another entity CA has been better structured. Furthermore, other approaches may in the future be added into this framework, such as HEM. This structure gives practitioners a common language to discuss CA approaches with and helps practitioners choose which approaches they need for their work.

It is important for a practitioner to understand how CA may fit in the goal and scope of their LCA study, to describe the methodological approach of CA used in a study and finally to clearly interpret and describe their results. While CA is a large toolbox of approaches, the various approaches all come with limitations of their own, which practitioners should be mindful of when they make use of CA. Finally, it also becomes clear from this thesis that the use of multiple approaches to CA in studies makes sense in many cases, as this can provide multiple perspectives and deeper insights on the same results.

It should be noted that in this thesis only CA approaches in literature were studied. LCA is an applied field, and many LCA software alternatives exist, each with their own features. These software options should be better studied as well. LCA software is the 'lab equipment' of LCA practitioners and the ability to verify the functioning of this equipment is essential for trust in the findings generated in this field. Furthermore, this thesis has a focus on CA is applied to characterized results (e.g. after the conversion from CO_2 and CH_4 emissions to 'climate change impact'). While most studies currently are concerned with characterized results, making use of CA for the inventory, normalized or weighted results can also provide useful insights and should not be forgotten in LCA.

Samenvatting

Levenscyclusanalyse (LCA) is de primaire methode voor het evalueren van milieuprestaties gedurende de levenscyclus van een product, waarbij de interpretatiefase cruciaal is voor het identificeren van significante kwesties en het sturen van verbeteringen. Zwaartepuntsanalyse (ZA) (Engels: Contribution Analysis) is het belangrijkste instrument om te begrijpen hoe processen en stromen bijdragen aan de totale effecten, maar ondanks het belang ervan is ZA niet goed gestandaardiseerd.

ZA wordt veel gebruikt in de interpretatie van LCA om de belangrijkste bijdragers aan milieueffecten te identificeren, problemen met datakwaliteit op te sporen en parameters voor gevoeligheidsanalyse te selecteren. ZA mist echter een overkoepelende definitie en gestructureerde methodologie, wat leidt tot inconsistente en soms niet-reproduceerbare resultaten en een lagere geloofwaardigheid van LCA-studies. Er bestaan verschillende benaderingen voor ZA die twee verschillende kanten kunnen beoordelen: directe bijdragen (bijv. CO_2-uitstoot door elektriciteitsproductie) en indirecte bijdragen (bijv. CH_4-uitstoot tijdens kolenwinning voor de productie van elektriciteit met kolen). Elke benadering kan een of beide van deze kanten vanuit een ander perspectief evalueren.

Voor grote groepen processen is een gecombineerde Directe en Indirecte ZA echter niet eenvoudig toe te passen. De ‘Hypothetical Extraction Method’ (HEM), gebruikt binnen het vakgebied Input-Outputanalyse, is in principe wel in staat om een dergelijk perspectief op ZA te bieden. Het was echter onduidelijk of deze benadering kon worden toegepast in LCA en welke nieuwe inzichten dit zou kunnen opleveren.

ZA wordt nog belangrijker in de context van prospectieve LCA (pLCA), waarbij scenario-gestuurde veranderingen in de data het moeilijker maken om resultaten te interpreteren. In pLCA is *Premise* momenteel het meest gebruikte instrument, waarmee toekomstige versies van achtergrond-databases worden gegenereerd op basis van scenario-verhaallijnen. Om inzicht te krijgen in de specifieke uitdagingen die verschillende benaderingen van ZA met zich meebrengen en hoe deze kunnen worden overwonnen, heeft deze thesis ZA toegepast in drie pLCA-casussen. Deze casussen zijn gekozen om de volgende redenen: 1) kobaltproductie vanwege de beperkte productieschaal maar de

sterk verwachte toename in vraag; 2) zand- en grindproductie, gezien de vraag naar beton en de aanzienlijk grotere productieschaal in vergelijking met kobalt; en 3) evaluatie van de pLCA-tool *Premise* via analyse van negen veelgebruikte industriële producten om de oorzaken achter toekomstige milieueffecten te verduidelijken.

Op deze manier was het hoofddoel van deze thesis om ZA te structureren en, waar nodig, te formaliseren, en om te leren van praktische casussen zodat deze toolbox van benaderingen nuttiger wordt voor LCA gebruikers.

Hoofdstuk 2 biedt een overkoepelende definitie van Zwaartepuntsanalyse die de huidige toepassingen van de term omvat en verschillende benaderingen structureert. Er wordt onderscheid gemaakt tussen benaderingen voor directe en indirecte bijdragen. De verschillende benaderingen worden geïllustreerd aan de hand van een voorbeeldcasus en de verschillen tussen de benaderingen worden besproken. Elke van deze benaderingen biedt een uniek inzicht in LCA resultaten. Vijf directe en drie gecombineerde directe en indirecte benaderingen worden beschreven.

De vijf directe benaderingen zijn:
- **Individuele elementaire stroom (ES)** ZA van specifieke individuele ESen uit afzonderlijke processen (Individuele ES ZA), bijv. de bijdrage van CH_4 emissies uit één specifiek proces 'kolenwinning'.
- **ES ZA**, van één ES over alle processen, bijv. de bijdrage van alle CO_2 stromen uit alle processen in het systeem.
- **Proces ZA**, van alle ESen per proces, bijv. de bijdrage van alle ESen (CO_2, CH_4 enz.) van het proces 'elektriciteitsproductie met kolen' aan de effectcategorie klimaatverandering.
- **ES groep ZA**, van groepen ESen, bijv. de bijdrage van een groep van alle koolstofhoudende elementaire stromen.
- **Procesgroep ZA**, van groepen processen, bijv. de bijdrage van alle processen voor 'elektriciteitsproductie'.

Er zijn ook drie gecombineerde Directe + Indirecte benaderingen geïntroduceerd:
- **Eerste-Orde (Engels: First-Tier) ZA**, die de directe bijdrage van het proces van de functionele eenheid (FE) en de directe + indirecte bijdrage van elke productstroom van de FE meet, bijv. de bijdrage van 'aluminiumproductie' en de bijdrage van alle productstromen

die nodig zijn voor ‘aluminiumproductie’, zoals ‘elektriciteit’ en ‘bauxiet’.
- **Levenscyclusstadium ZA**, gebaseerd op levenscyclusstadia, bijv. de bijdrage van levenscyclusstadia zoals ‘productie’, ‘gebruik’ en ‘einde levensduur’.
- **Pad-CA**, bijdragen vanuit een pad (bijv. waardeketen) van processen, vaak gevisualiseerd in Sankey-diagrammen, bijv. de bijdrage van productstromen door het gehele productsysteem die leiden tot de uiteindelijke LCA-score, waarbij het ‘pad’ van bijdragen wordt weergegeven.

Richtlijnen werden geformaliseerd voor praktijkgebruikers over hoe zij hun ZA-methodologieën en resultaten kunnen rapporteren en presenteren, zodat LCA-studies beter reproduceerbaar en interpreteerbaar worden. In de eerste plaats moet, wanneer ZA wordt toegepast, worden beschreven dat iets bijdraagt *van* een entiteit (bijv. een proces of ES) *aan* een andere entiteit (bijv. LCI of een gekarakteriseerd resultaat). Het werk in Hoofdstuk 2 beoogt bij te dragen aan een kwalitatief hoger en beter reproduceerbaar corpus van LCA-literatuur en meer goed onderbouwde conclusies.

Hoofdstuk 3 introduceert de HEM in LCA door het uiteenzetten van een vierstappenplan en biedt daarbij een wiskundig kader om deze stappen toe te passen. HEM wordt gedemonstreerd als een ZA benadering aan de hand van een kleine voorbeeldcasus en een groter voorbeeld met gebruik van ecoinvent. Het toepassen van HEM biedt inzichten in situaties waarin een indirect perspectief vereist is, en voor groepen processen zoals industriële sectoren of regio’s. Hoewel andere bestaande benaderingen hun eigen voordelen hebben, kunnen zij dit perspectief niet effectief bieden. Het werk in Hoofdstuk 3 laat zien hoe en wanneer HEM een nuttige benadering kan zijn voor ZA in gevallen waarin huidige ZA benaderingen tekortschieten, zoals bij het beoordelen van de directe en indirecte bijdragen van groepen processen, en biedt daarmee een aanvullende ZA benadering voor de LCA praktijkgebruiker om milieueffecten van hun productsystemen beter te begrijpen.

Vervolgens zijn Hoofdstukken 4, 5 en 6 drie casussen die gebruikmaken van ZA met als doel te leren van de toepassing van ZA in praktische situaties. Hoofdstuk 4 is een casus waarin pLCA wordt toegepast op de productie van kobalt. Procesgroep ZA werd gebruikt om te beoordelen welke procesgroepen de belangrijkste bijdragen leverden in elk van deze variabele scenario combinaties. De processen werden gegroepeerd op basis van de producten die zij produceren (bijv. alle elektriciteitsproductie). Deze casus leverde de belangrijkste inzichten die hebben geleid tot de structurering van ZA in Hoofdstuk 2.

Hoofdstuk 5 is een casus waarin pLCA wordt toegepast op de productie van zand en grind. Procesgroep en Eerste Orde bijdragen (bijdragen van producten aan de productie van beton) werden beoordeeld. Deze ZA benaderingen werden gebruikt om te analyseren hoe conventionele productie en productie uit recycling tot verschillende milieueffecten leiden, en om de bijdragen van zand, grind en cement aan betonproductie te tonen. Deze casus leverde als belangrijkste inzicht op dat de huidige gecombineerde Directe + Indirecte benaderingen niet effectief kunnen worden toegepast op grote groepen processen. HEM, zoals geïntroduceerd in Hoofdstuk 3, helpt om dit perspectief binnen LCA te bieden.

Hoofdstuk 6 is een studie waarin negen belangrijke industriële producten uit de *Premise* database worden geanalyseerd. ZA via procesgroep ZA en HEM werd gebruikt om het effect te beoordelen van vijftien grote productgroepen die industriële sectoren vertegenwoordigen die vergelijkbare producten produceren. De ZA benaderingen werden gebruikt om de directe en gecombineerde directe + indirecte bijdragen van deze groepen aan de negen producten te beoordelen. Procesgroep ZA is essentieel in deze analyse om te laten zien waar bijdragen (of veranderingen daarin) vandaan komen. HEM maakte het mogelijk vast te stellen dat sommige sectoren een belangrijke rol spelen als ‘verbindende’ sectoren. Deze verbindende sectoren/processen hebben zelf niet noodzakelijkerwijs grote bijdragen, maar ‘verbinden’ met andere processen in het productsysteem die wel grote bijdragen hebben. Deze analyse van indirecte bijdragen van grote procesgroepen was mogelijk dankzij de aanpassing van HEM uit de input outputanalyse (IOA) naar LCA in Hoofdstuk 3.

Gezamenlijk tonen de inzichten uit alle drie de casussen aan dat het belangrijk is om duidelijke categorieën van ZA benaderingen te definiëren en nieuwe benaderingen te ontwikkelen om nieuwe perspectieven te analyseren wanneer dat relevant is, zoals HEM.

Concluderend: door ZA benaderingen te verdelen in twee perspectiefgroepen, namelijk Direct en Indirect, en duidelijk te beschrijven hoe deze benaderingen moeten worden toegepast van een bepaalde entiteit naar een andere entiteit, is ZA beter gestructureerd. Daarnaast kunnen in de toekomst andere benaderingen aan dit kader worden toegevoegd, zoals HEM. Deze structuur biedt praktijkgebruikers een gemeenschappelijke taal om ZA benaderingen te bespreken en helpt hen te bepalen welke benaderingen zij nodig hebben voor hun werk.

Het is belangrijk dat een praktijkgebruiker begrijpt hoe ZA past binnen het doel en de reikwijdte van hun LCA studie, beschrijft hoe de ZA methodologie in een studie is toegepast en ten slotte de resultaten duidelijk interpreteert en rapporteert. Hoewel ZA een uitgebreide toolbox van benaderingen is, brengen de verschillende benaderingen elk hun eigen beperkingen met zich mee, waarvan praktijkgebruikers zich bewust moeten zijn bij het toepassen van ZA. Tot slot blijkt uit deze thesis ook dat het gebruik van meerdere ZA benaderingen in studies in veel gevallen zinvol is, omdat dit meerdere perspectieven en diepere inzichten op dezelfde onderliggende resultaten kan bieden.

Wel dient opgemerkt te worden dat in deze thesis alleen ZA benaderingen uit de literatuur zijn bestudeerd. LCA is een toegepast vakgebied en er bestaan veel verschillende LCA softwarepakketten, elk met hun eigen functionaliteiten. Deze softwareopties zouden eveneens beter bestudeerd moeten worden. LCA software is de ‘laboratoriumapparatuur’ van LCA praktijkgebruikers en het vermogen om de werking van deze apparatuur te verifiëren is essentieel voor het vertrouwen in de resultaten die in dit vakgebied worden gegenereerd.

Verder richt deze thesis zich op ZA toegepast op gekarakteriseerde resultaten (bijv. na de omzetting van CO_2 en CH_4 emissies naar ‘klimaatverandering’). Hoewel de meeste studies zich momenteel richten op gekarakteriseerde resultaten, kan het toepassen van ZA op inventaris-, genormaliseerde of gewogen resultaten ook nuttige inzichten opleveren en dient dit binnen LCA niet te worden vergeten.

Chapter 1
Introduction

1.1 Life Cycle Assessment

Life cycle assessment (LCA) has become the main method to calculate the environmental performance of products and services. LCA offers a systems perspective that quantifies environmental impacts from resource extraction to end-of-life, enabling prioritization of improvements and avoiding burden-shifting.

LCA comprises four phases (ISO 14044, 2006): 1) Goal and scope definition, 2) life cycle inventory (LCI) modeling, 3) life cycle impact assessment (LCIA), and 4) interpretation.

Goal & scope definition establishes the intended application, reasons and audience, and specifies the product system, functions and functional unit, system boundary, allocation procedures, LCIA approach, data requirements, and assumptions as needed.

LCI analysis compiles, validates and calculates quantitative inputs and outputs for each included process, relates them to the functional unit, and iteratively refines system boundaries and allocation according to cut-off criteria and sensitivity analysis. Generally, for LCA studies, a large database with many interconnected processes like ecoinvent (Wernet et al., 2016) is used to represent large parts of the economy and complex supply chains, and the most important processes of what is studied are modeled in detail by the practitioner.

LCIA selects impact categories, category indicators and characterization models and calculates category indicator results (characterization), optionally with normalization, grouping and weighting.

Interpretation identifies significant issues from the LCI/LCIA, evaluates completeness, sensitivity and consistency, and then formulates conclusions, acknowledges limitations and makes recommendations aligned with the study's goal and scope for decision-making.

Conducted iteratively, LCA relies on the interpretation phase to surface key issues and guide targeted improvements across the goal and scope, inventory, and impact assessment phases. Clear interpretation is thus essential to improve LCA and translate results into actionable insights for industry and policy.

Many LCA studies today use ecoinvent (Wernet et al., 2016) or databases derived from it (e.g. Agribalyse (Colomb et al., 2015) or *Premise* (Sacchi et al., 2022)) as background processes. Ecoinvent is an LCI database with well over 20000 unit processes which are linked together in an attempt to model the global economy from a life-cycle perspective. This database is used by practitioners who model their own foreground sections of specific interest, and then link those to processes in these background databases, such as electricity production or production of metals. The use of background databases helps to save substantial time for practitioners as they can take such data from a database instead of modeling everything themselves. Moreover, it helps to standardize the field with one major source of data. One challenge of such large databases is developing an understanding of the causal relationships between the foreground processes of the practitioner and impact, where impacts may occur deep in a supply chain.

LCA became even more useful and relevant for policy when the scientific community started to explicitly assess possible impacts of new technologies in the future. While this practice has had several names, prospective LCA (pLCA) is currently most common (Arvidsson et al., 2024). The assessment of new or emerging technologies requires changes to the product systems used in these studies to represent future scenarios. While at first this was often done by altering the most important processes in the foreground, studies should also include changes in the background following the same future scenarios for better consistency, for example, changes in the electricity grid (Mendoza Beltran et al., 2018). At first, tools like Presamples (Lesage & Mutel, 2019) and Wurst (Mutel, 2017b) were used to make large scale changes to databases. By now, *Premise* (Sacchi et al., 2022) has become the most used tool to do this.

Premise allows practitioners to generate futurized versions of the ecoinvent database. It is based on scenarios reflecting high-level storylines on change in the environment and society. These storylines are based on combinations of global warming in Representative Concentration Pathways (RCPs) (Van Vuuren et al., 2011) and how well global society adapts to and mitigates climate change in Shared Socioeconomic Pathways (SSPs) (O'Neill et al., 2014). These storylines are implemented in Integrated Assessment Models (IAMs) which project quantitative results on how large-scale metrics such as Gross Domestic Product, Population and electricity production change into the future. Each IAM has its own modeling approaches to follow certain scenarios. *Premise* finally makes use of these quantitative IAM outputs and maps these outputs to changes in the ecoinvent LCI database. These databases can then be assessed at different combinations of time and scenarios.

Whether a practitioner does 'conventional' LCA or takes a more advanced approach like pLCA, it is always important to understand clearly what contributes to impacts in a study and how. Contribution Analysis (CA) is the most common tool that is used to understand contributions while assessing to what level specific processes, flows or other entities such as life cycle stages (e.g., production, use, and end-of-life) or impact scores to weighting contribute to impacts.

Furthermore, in pLCA scenario-driven changes are introduced that influence the pressures and impacts calculated for the future. These scenario-driven changes may shift contributions in non-intuitive ways, increasing the relevance of supporting the interpretation phase with a proper CA. It is hence essential that CA is better structured and understood so that impacts in LCA may be better understood and acted upon.

1.2 Understanding contributions to environmental impacts in LCA

In the interpretation phase of an LCA study, CA is frequently used to gain further insight from the LCA results or learn how to make findings actionable. CA has become essential for accurately understanding, analyzing and communicating LCA results. CA is used for 1) Finding important contributors to impacts (Guinée et al., 2002; Hauschild et al., 2018; James & Galatola, M., 2015; Laurent et al., 2020), 2) Identifying data quality problems or mistakes in modelling (Guinée et al., 2002; James & Galatola, M., 2015), and 3) Selecting parameters for sensitivity analysis (Guinée et al., 2002; Hauschild et al., 2018; Laurent et al., 2020). CA is always applied to analyze the contribution *from* some entity *to* another entity. E.g. the contributions *from* processes *to* characterized results.
Despite its wide use, there is no definition that encompasses all current uses of CA. There are different approaches that take different perspectives to contributions. The availability of different approaches and lacking definition of CA may cause confusing, unclear or even irreplicable results.

Problems related to unclear use of CA undermine the credibility of LCA studies and the entire field.

One important distinction between CA approaches is how they assess impacts. The original approaches that were introduced (Heijungs & Kleijn, 2001; Heijungs & Suh, 2002) assess Direct contributions (Srocka & Montiel, 2021) (e.g. the CO_2 emitted directly from a coal powerplant to produce electricity). This focus on Direct contributions has certainly been useful but, as Heijungs & Kleijn (2001) already noted, limited in scope. These approaches cannot indicate how contributions relate to the studied functional unit. There are newer approaches that aim to solve this limitation of these older approaches, through including Indirect contributions as well (e.g. the CH_4 released during the mining of coal for electricity production to be included as contribution for electricity production). Being able to understand the 'connecting' role of processes (Reinhard et al., 2016) is important, for example, if the electricity production from coal would be replaced with electricity from solar, this would also remove the need to produce the coal for that electricity. Understanding what contributes to impacts and through what ways is essential to be able to reduce these impacts.

As CA approaches are not well structured or defined, not all questions regarding contributions can be answered currently. One example is to analyze the Indirect contribution from a group of processes, such as an entire industry sector or region. Current approaches cannot effectively do this type of analysis. The Hypothetical Extraction Method (Hertwich et al., 2024; Miller & Lahr, 2001), from the field of Input-Output analysis which is neighboring the field of Industrial Ecology (Pauliuk et al., 2017) does provide such insights, though it is unclear if that approach could be adapted to LCA and what insights it could provide.

1.3 Contribution Analysis in prospective LCA

While it is already important in LCA to understand what contributes to impacts, pLCA adds an additional challenge: impacts for the same functional unit will generally change between scenarios and with that, have changing contributions to those impacts as well. With these changes, it becomes important to understand what contributes to these changes. This means not just understanding the total impact change, but deeply understanding how the scenario changes that were made affect impacts, as these causal relationships are often difficult to understand in the complexities of modern LCI databases.

In current pLCA practice, the state-of-the-art is to use *Premise* (Sacchi et al., 2022) as futurized background database. While this tool is highly valuable, there is a strong focus on climate change effects in *Premise* because the IAM source data is mainly focused on climate change scenarios. While climate change is undeniably an important matter, other potential environmental challenges also exist. Examples include sand scarcity, water scarcity, or decreases in biodiversity.

Prospective LCA case studies are a good way to learn more about CA since they include the additional challenge of interpreting changing scenarios. While many sectors are already included in *Premise*, the potential future environmental impacts of many more products and services must still be studied to help gain insight into possible problems and steer policy. While there is currently no set way to prioritize what materials to study first, it makes sense to study materials with one or more of these three qualifiers: 1) materials that have high impacts per unit produced, 2) materials that are produced in large quantities or 3) materials that could see major changes in how or how much they are produced.

Cobalt is one example of a material that while not produced in large quantities, is expected to see demand increases up to 10-20 times up to 2050, depending on the scenario (Deetman et al., 2018). Cobalt is generally co-produced with copper or nickel and is used in Lithium-Ion batteries. With large increases in electric mobility and use of mobile electric devices such as laptops and smartphones, demand will increase.

As this is a material with relatively low production volume and strong expected growth in demand, it is interesting to assess how the contributions to the life cycle environmental impacts of cobalt production could change in future scenarios like ore grade decline or shifts in electricity production.

Contrastingly, sand and gravel are two products with a low per-unit impact and very high production volumes. Furthermore, another issue is the growing scarcity of sand and gravel used in construction (Giljum et al., 2000; Ioannidou et al., 2017; Peduzi, 2014; Torres et al., 2017). Sand and gravel are key components of concrete and need to meet stringent quality standards to be fit for this purpose. With an expected growing demand for concrete for the coming decades (Deetman et al., 2020; Watari et al., 2023), alternative sources of sand and gravel may need to be found and it is important that these do not pose negative environmental trade-offs. As these materials have low per-unit impacts but high production volumes, the production of sand and gravel is a contrasting case to the production of cobalt to further assess CA in practice.

Both the extent of changes made to *Premise* and the limited focus on climate change raise a question on how these changes affect LCA results from these futurized LCI databases. While it is documented clearly *what changes* are made on the inventory level in *Premise*, because of the network relationships between processes, it remains unclear *what effects* these changes have throughout *Premise* databases on LCA results. Assessing the contributions from aggregated production sectors to a variety of products can provide a deeper understanding of both CA and the effects different scenarios of *Premise* have in pLCA.

1.4 Problem statement and Research question

The analysis in the sections above lead to the following problem statement. LCA is a key method to understand environmental impacts but improvements can still be made to the method. Amongst others, CA in LCA needs to be better understood. First of all, CA approaches need to be structured and where needed formalized. An overarching definition of CA that encompasses current uses and a consistent terminology in approaches needs to developed such that LCA practitioners can better communicate their results and understand the results from other practitioners. Furthermore, since current CA approaches don't offer the ability to assess the Indirect contribution of groups of processes such as industry sectors or regions, it should be studied whether an approach such as the Hypothetical Extraction Method from Input Output Analysis could provide such a role in LCA.

Presenting these CA approaches by developing a structured framework is useful but also has limitations. Applying approaches to CA in practice will provide a richer insight into what works in CA and what doesn't. It is also important to make use of pLCA in these cases since, as discussed before, pLCA provides additional interpretative challenges through changes in scenarios. For this we use the three cases suggested in section 1.3: cobalt, sand and gravel, and a broader analysis for nine commonly used industrial products included in the pLCA tool *Premise*.

In sum, this thesis makes the case for better structuring and defining CA and to extend it with an approach that can include the Indirect contribution from large groups of processes and to learn from CA in the context of pLCA through a variety of case studies.

This thesis therefore investigates the following Research Question:

How can Contribution Analysis be structured and utilized to better analyze environmental impacts in Life Cycle Assessment?

This is answered using the following sub-questions:

1. How can Contribution Analysis be structured and formalized?

2. How can indirect contributions from groups of processes be better quantified and understood in LCA?

3. What can we learn from Contribution Analysis results in practice, applied to prospective LCA of 3 cases?
    - Prospective LCA of Cobalt production
    - Prospective LCA of Sand and Gravel production
    - Prospective LCA of Nine commonly used products from *Premise*

1.5 Outline

This thesis is structured as follows:

Chapter 2 - This chapter provides an overarching definition of CA that covers current uses of the term and structures different approaches. The approaches are demonstrated using a small example case study and the differences between approaches are discussed. Finally, this chapter provides recommendations for practitioners on which approaches to use when and how to report them.

Chapter 3 - Introduction of the Hypothetical Extraction Method to LCA through introducing a four step process and provides the mathematical framework to perform it. HEM is demonstrated as an approach to CA using a small example case study and a larger example using ecoinvent.

Chapters 4-6 are case studies implementing CA in pLCA with the goal to learn from practical application.

Chapter 4 - A case study demonstrating pLCA on the production of cobalt. This case study assesses different future scenarios of cobalt production and demand and models different production variables according to those scenarios. CA is used to assess the Direct contributions to impacts of cobalt production.

Chapter 5 - A case study demonstrating pLCA on the production of sand and gravel. This case study assesses the conventional production and recycling of sand and gravel based on future scenarios. CA is used to assess the contributions to sand and gravel production as well as the contribution of sand and gravel in concrete production.

Chapter 6 - A study where nine important products from the *Premise* database are assessed. This study assesses what actually contributes to impacts of these products and how those impacts change in different scenarios. CA is used to assess the contribution from fifteen industry sectors, both directly and indirectly.

The outline of these core chapters is also shown in Figure 1.1 visually and shows how each of the methodological chapters (2-3) relate to the case study chapters (4-6).

Chapter 7 - Finally, Chapter 7 answers each sub-question based on the preceding chapters and uses this information to answer the research question. The limitations and possible future work based on this study are further discussed, and further reflections are provided.

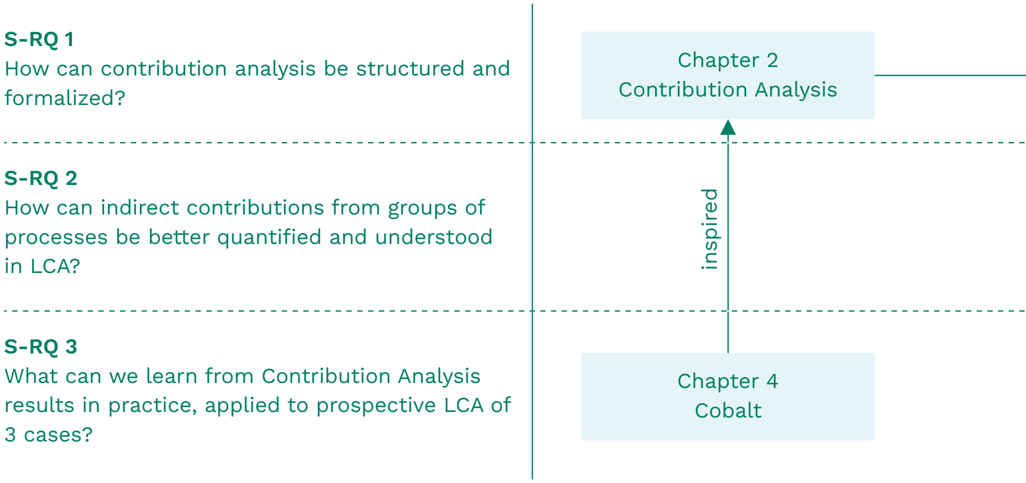
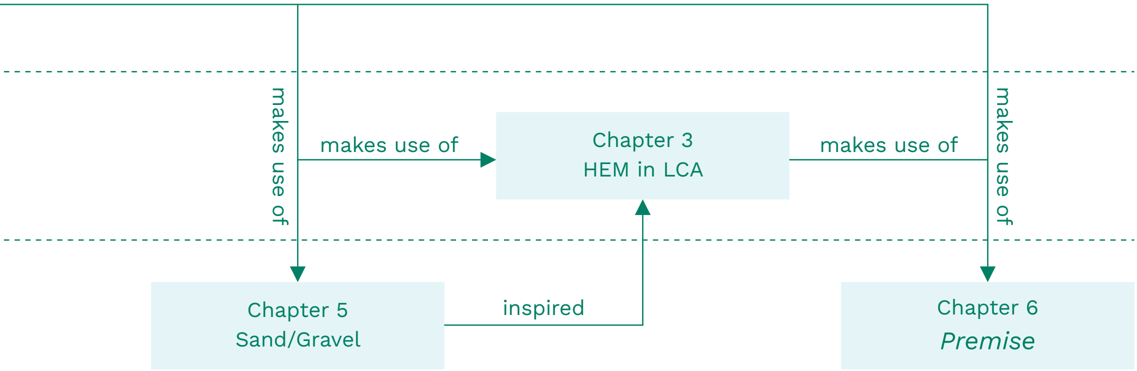


Figure 1.1 - Visual overview of connections between core chapters of this thesis and how they relate to the sub-research questions.


Chapter 3
HEM in LCA
makes use of
makes use of
makes use of
makes use of
Chapter 5
Sand/Gravel
inspired
Chapter 6
Premise

Chapter 2
Contribution Analysis in LCA: an overview of approaches and when to apply them

Authors Marc van der Meide, Reinout Heijungs, Jeroen Guinée, Mingming Hu, Bernhard Steubing

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The Supplementary Information (SI) to this chapter is available at the website of the publisher.

Abstract

Purpose: Contribution analysis (CA) is an essential method to understand and communicate Life Cycle Assessment (LCA) results. Different approaches to CA have been used to answer different questions. However, it is often unclear which approach is used in LCA studies, leaving confusion as to how contributions are actually assessed. This makes a correct interpretation or replication difficult and can even lead to ill-founded conclusions. This study aims at a clear terminology for transparent CA communication.

Method: First, we introduce eight approaches to CA used in the literature. Then, we introduce an example case study to compare each CA approach against. We then discuss the eight approaches, discussing *from* what and *to* what they contribute. We also make a distinction between the *direct* and *indirect* perspectives, where *direct* contributions are *from* Elementary Flows (EF) of processes, *indirect* contributions are *from* all EF of processes contributing to the intermediate flows (products).

Results and discussion: We identify and describe several approaches for *direct* CA: (a) Individual Elementary Flow CA, for specific individual EFs *from* single processes (Individual EF CA). (b) EF CA, for one EF across all processes, e.g. all CO_2 flows. (c) Process CA, for all EFs per process e.g. contribution to Climate Change impact *from* the process ‘electricity production from coal’. (d) Grouping can also be applied to these approaches, e.g. Process group CA for all ‘electricity production’ processes. *Direct* and *indirect* contributions can also be quantified: (e) First-Tier CA, measuring the *direct* contribution of the Functional Unit (FU) process and *indirect* contribution of each intermediate flow of the FU. (f) Life Cycle Stage CA, e.g. calculating the contributions of life cycle stages like ‘production’, ‘use’ and ‘end of life’. (g) Finally Path CA -often visualized in Sankey diagrams-, e.g. showing the ‘path’ contributions take to the FU. We compare the results, advantages and disadvantages of each approach, discuss general limitations of CA, and give recommendations on reporting CA.

Conclusion: Our study can help guide practitioners in choosing relevant CA approaches for their studies to gain better insights and more transparently communicate and report their results. This should contribute to a higher quality and more reproducible body of LCA literature and more well-founded conclusions.

2.1 Introduction

Life cycle assessment (LCA) has become the main method to calculate the environmental performance of products and services. The four phases of LCA (Goal and Scope definition, Inventory Analysis, Impact Assessment and Interpretation) are closely intertwined. In the interpretation phase of an LCA study, Contribution Analysis (CA) -also called Hotspot Analysis (James & Galatola, M., 2015) and historically called Dominance Analysis (Heijungs et al., 1992) or gravity analysis (ISO, 2006)- is frequently used to gain further insight from the LCA results or how to make this information actionable. For example, manufacturers may want to gain insight into which suppliers or internal processes they can best change to reduce the environmental impacts of their products. Consequently, CA has become essential for accurately understanding, analyzing and communicating LCA results.

CA achieves this through:
- Finding important contributors to impacts -often termed 'hotspots'- that can assist in finding product system improvements (Guinée et al., 2002; Hauschild & Huijbregts, 2015; James & Galatola, M., 2015; Laurent et al., 2020),
- Identifying data quality problems or mistakes in modelling (Guinée et al., 2002; James & Galatola, M., 2015),
- Selecting parameters for sensitivity analysis (Guinée et al., 2002; Hauschild & Huijbregts, 2015; Laurent et al., 2020).

Despite the near-universal use of CA in the LCA field, a complete and precise definition of CA is lacking. CA is always applied to analyze the contribution *from* some entity *to* another entity. E.g. the contributions *from* processes *to* characterized results. The ISO 14044 (2006) standard describes CA to determining the contribution *from* life cycle stages or groups of processes *to* the total result (2006 Annex B2.3 p. 36). But in practice CA has also often been applied to determine the contributions *from* other entities such as elementary flows (EFs), processes or characterized results. The '*to*' part is notably imprecise and could be the Life Cycle Inventory (LCI) result or any level of Life Cycle Impact Assessment (LCIA). Many other descriptions of CA exist in literature, all missing certain entities as with the ISO 14044 (2006) or not differentiating what the analysis contributes *from* or *to*. (Guinée et al., 2002; Hauschild et al., 2018; Heijungs et al., 1992; Heijungs & Kleijn, 2001; Heijungs & Suh, 2002;

Klöpffer & Grahl, 2014; Laurent et al., 2020; Noh et al., 1998; Reinhard et al., 2016, 2019).

In addition to a complete and precise definition of CA, there are different approaches that take different perspectives on finding contributions. The availability of different approaches and lacking definition of CA may cause confusing, unclear or even irreplicable results. Examples of these problems can be found randomly in the literature: CA is often not replicable as it's not reported *from* what CA is applied or because processes, process groups or life cycle stages are not defined or mixed up (Bałdowska-Witos et al., 2020; Battisti & Corrado, 2005; Duan et al., 2022; Eksi & Karaosmanoglu, 2018; Gorrée et al., 2002; Hesser et al., 2017; Leccisi & Fthenakis, 2021; Niero et al., 2015; Panepinto et al., 2015; Pradeleix et al., 2015; Roux et al., 2016; Scipioni et al., 2013; Zink et al., 2014). Many of these studies apply life cycle stage analysis with life cycle stages that are not clearly defined. Next, figures from Bałdowska-Witos et al. (2020), Battisti & Corrado (2005), Duan et al. (2022) and Leccisi & Fthenakis (2021) are challenging to interpret. More importantly, Zink et al. (2014) and Pierobon et al. (2018) don't make clear in their studies why the use of contribution analysis would be required to satisfy the goal of their LCA study. Finally, Zink et al. (2014), Pierobon et al. (2018) and Panepinto et al. (2015) share results, but never interpret this data in their studies. Such ill-defined CA applications often lead to non-replicable results, which undermines the credibility of these LCA studies. However, the average LCA practitioner is hardly to blame for this, as there is no clear overview of what approaches exist and how or when to apply them.

Some positive examples of CA in literature exist as well: Examples of well documented CA are Eksi & Karaosmanoglu (2018), who provide detailed reporting of their methodology and which processes belong to each life cycle stage, Gorrée et al. (2002), who provided substantial discussion of CA results, and Zink et al. (2014), who made good use of figures. Most studies apply CA only to impact category results, though some also consider CA to other entities like weighted results (Bałdowska-Witos et al., 2020; Duan et al., 2022).

In this study, we aim to structure, explain and provide a clear terminology for different CA approaches. We believe this will guide LCA practitioners to better understand contribution analysis and the LCA results obtained from CA, help practitioners make more conscious choices regarding CA, and better document and communicate contribution analysis results in future LCA studies. We proceed by introducing a general approach and illustrative case study used to demonstrate all approaches we discuss. We then discuss five *direct* approaches; Individual Elementary Flow Contribution Analysis, Elementary Flow Contribution Analysis, Process Contribution Analysis, Elementary Flow Group Contribution Analysis and Process Group Contribution Analysis. After this, we discuss three approaches that show both *direct* and *indirect* contributions; Tiered Contribution Analysis, Life Cycle Stage Contribution Analysis and Path Contribution Analysis. Finally, we discuss and compare the different approaches to CA.

2.2 Method

2.2.1 General approach

For this article, we use a slightly adapted definition of contribution analysis from Guinée et al (2002 p. 110) and ISO 14044 (2006): *A step of the Interpretation phase to assess the contributions from entities like individual life cycle stages, (groups of) processes, elementary flows and indicator results to the overall (or a partial) LCI or LCIA result (e.g. as a percentage).* We use the terms and definitions of ISO 14044 (2006) where possible.

From an examination of a small fraction of the body of LCA literature, and from our own experience, we have identified the following general contribution analysis approaches:

- Direct CA, including:
  - Individual EF CA,
  - EF CA,
  - Process CA,
  - EF group CA,
  - Process group CA,
- First-Tier CA,
- Life cycle stage CA,
- Path CA.

In the following chapters, each approach is described as follows:
Goal - Describes for what the approach may be useful,
Description - Identifies how each approach is performed on a high level,

Example - Example of results, we introduce a simplified LCA case study below that we use across all approaches,
Advantages and limitations - Advantages and limitations specific to the approaches.

We describe and demonstrate each of these approaches in terms of contributions to characterized results and discuss contributions to other entities like LCI and normalized results in the discussion. We focus on process-LCA (Heijungs et al., 2022) and do not discuss methods exclusive to Input-Output (IO)-LCA, such as Power Series Expansion (Suh & Heijungs, 2007) or the Path Exchange Method (Lenzen & Crawford, 2009). We demonstrate each of the approaches in the context of a simplified case study and in the Supplementary Information (SI) 1.7 a system using the ecoinvent database ecoinvent (Wernet et al., 2016) to demonstrate benefits and limitations of these approaches with systems consisting of many more processes and EFs. For each of the approaches, we provide a full step-by-step mathematical description in SI 1 and an Excel file with all calculation steps applied to the case study in SI 2. All results in this study are rounded and may not add up to totals exactly, but the full results are presented in the Excel file of SI 2.

2.2.2 Illustrative case study

In order to exemplify the different CA approaches discussed in the following, we use a simplified case study. The product system of the simplified case study is comprised of the production and use of a fridge. We use the functional unit (FU) of 'cooling 10 kilogram food for 8 years to 6° Celsius', we assume that this is the lifetime of the fridge and shorten the FU in the further text to 'cooled food'. The case consists of six simplified unit processes and two elementary flows, as shown in Figure 2.1. The flow amounts of the unit processes are quantified in Table 2.1. In the simplified case study, we characterize the climate change impact (expressed in kg $CO_{2eq.}$) adopting the Global Warming Potential for 100 years (GWP100) and assuming the GWP100 for carbon dioxide (CO_2) is 1 kg $CO_{2eq.}$/kg CO_2 emitted and for methane (CH_4) is 29.8 kg $CO_{2eq.}$/kg CH_4 emitted (IPCC, 2022). The total climate change score is 976.9 kg $CO_{2eq.}$ for 'cooling food for 8 years to 6° Celsius'.

Process name	Functional flow (Product/Service)	Intermediate flows	Elementary flows
Coal mining	Coal: 1 kg	Electricity: 0.04 kWh Steel: 0.001 kg	CO_2: 0.05 kg CH_4: 0.01 kg
Electricity production	Electricity: 1 kWh	Coal: 0.4 kg Steel: 0.001 kg	CO_2: 0.8 kg
Iron ore mining	Iron ore: 1 kg	Electricity: 0.1 kWh Steel 0.001 kg	
Steel production	Steel: 1 kg	Electricity: 0.1 kWh Coal: 0.8 kg Iron ore: 2 kg	CO_2: 1.6 kg
Fridge production	Fridge: 1 unit	Electricity: 150 kWh Steel: 40 kg	CO_2: 150kg
Use	Cooled food: 1 year	Electricity: 150 kWh Fridge: 0.125 unit	

Table 2.1 - Unit process inventory for the six simplified processes, showing functional, intermediate and elementary flows for every process. Positive intermediate flows are process inputs, positive elementary flows are process outputs.

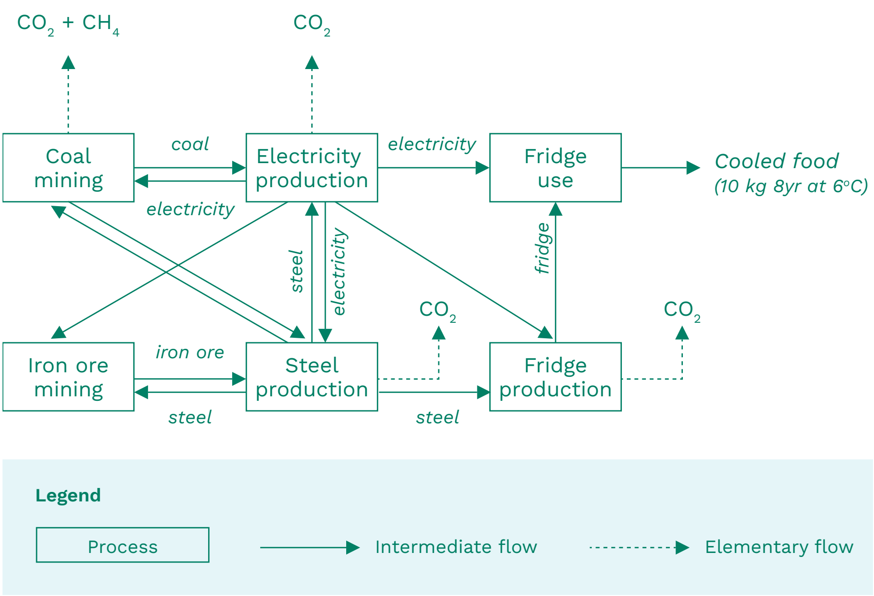


Figure 2.1 - Product system for the simplified example case, the functional unit is 'cooling 10 kg food for 8 years to 6o Celsius', shortened as 'Cooled food'. The system consists of six unit processes and two distinct elementary flows.

This simplified case study is meant for illustration of different CA approaches only and should not be used to draw any conclusions with regard to the environmental performance of fridge use or any of the other processes presented. Specifically for ‘coal mining’, which has much lower direct CO_2 emissions in reality and ‘fridge production’, which in our case has CO_2 emissions to represent some polluting process. We consider e.g. fuel inputs that would cause CO_2 emissions to these processes to be cut-off. We make these unrealistic changes to better demonstrate the different approaches to CA with a simple example, at the cost of some realism. We provide a more realistic case study for the ‘use of a fridge’ using the ecoinvent database (Wernet et al., 2016) in SI 1.7, though that example still meant to illustrate the differences between the different CA approaches, not to assess real-life ‘cooling of food’.

2.3 Direct approaches to Contribution Analysis

There are five direct approaches to contribution analysis:

- Individual Elementary Flow Contribution Analysis,
- Elementary Flow Contribution Analysis,
- Process Contribution Analysis,
- Elementary Flow group Contribution Analysis
- Process group Contribution Analysis.

Each of the direct approaches provides a different level of disaggregation of contributions, providing different insights into the contributions. The direct approaches show only *direct* contributions. *Direct* contributions are the contributions caused by the elementary flows (EFs) *from* a process where those flows occur (Srocka & Montiel, 2021), e.g. the CO_2 emitted from electricity production by burning coal in a power plant is a *direct* contribution *from* the process ‘electricity production with coal’. In contrast, *indirect* contributions are the contributions caused by the production *from* an intermediate flow (e.g., a product like ‘electricity’, from the process ‘electricity production’) from a process, this would include the contributions *from* all EFs of all processes *indirectly* needed to produce that intermediate flow in the required amount. An example of *indirectly* emitted CO_2 would be CO_2 emitted during the production of steel for the powerplant. In short; *direct* contributions are *from* processes, *indirect* contributions are *from* other processes contributing through the intermediate flows (e.g. products).

Each of the direct approaches makes use of the same disaggregated result from an LCA and was established over two decades ago (Heijungs & Kleijn, 2001; Heijungs & Suh, 2002). As the direct approaches are closely related, we discuss the advantages and limitations together at the end of this chapter.

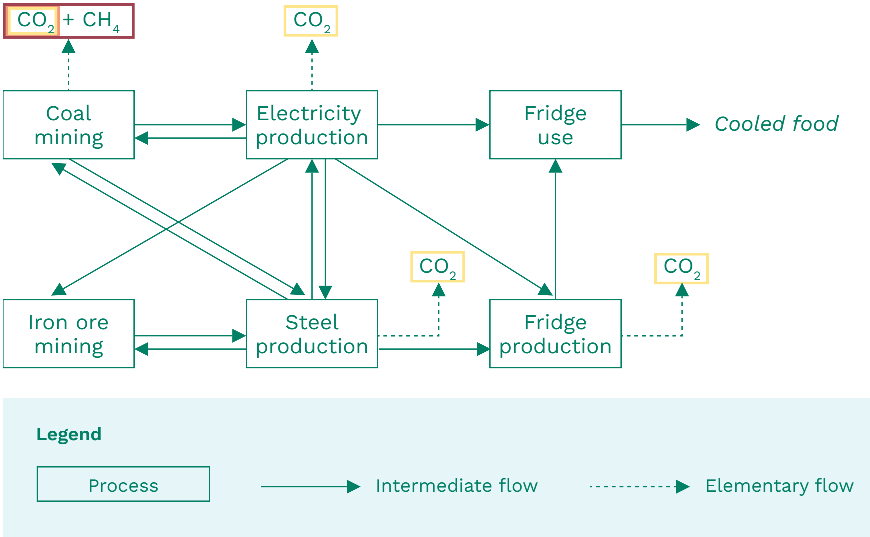
2.3.1 Individual Elementary Flow Contribution Analysis

Goal
Contribution Analysis *from* specific individual elementary flows (EF) caused by distinct processes, -individual flow contributions in short-, represents the most disaggregated approach in Contribution Analysis. There are two goals a practitioner can achieve with this approach: Either investigate specific individual flows the practitioner may be interested in, or identify which individual flows contribute most to the result. A practitioner could use this to investigate contributions *from* individual elementary flows of specific processes e.g. the climate change impact *from* CO_2 emitted by electricity production with coal. Another example could be to identify outliers in the data.

Description
This approach is based on the disaggregated results of an LCA calculation. The contributions are calculated such that the format is a matrix with EFs as rows and processes as columns. Each cell in this matrix represents an individual characterized result for the combination of the specific EF and process. We show how this could be calculated in SI 1.3.1. As this matrix contains the disaggregated contributions, we call this the contribution matrix. The contribution matrix shows all *direct* contributions, i.e. the impacts associated with the EFs coming from a process. When all numbers in the contribution matrix are summed, they are equal to the total characterized result.

Example
We show an example of the approach to the characterized results *from* individual flows with the example system in Figure 2.1 B. Subfigure B shows the individual flow contributions in orange for the individual flow contribution *from* CO_2 of ‘coal mining’. We also show the results for this approach in a stacked bar-chart in Figure 2.3 A.

A | System



B | Contribution matrix

Climate change ($kgCO_2eq.$)		Processes					
		Coal mining	Electricity production	Iron ore mining	Steel production	Fridge production	Fridge use
Elementary flows	CO_2	17.2	620.9	0	65.9	150	0
	CH_4	102.3	0	0	0	0	0

$\Sigma_{PROCESS}$

C | EF contributions

Climate change ($kgCO_2eq.$)		Processes
		$\Sigma_{PROCESS}$
Elementary flows	CO_2	854
	CH_4	102.3

Σ_{EF}

D | Process contributions

Climate change ($kgCO_2eq.$)		Processes			
		Coal mining	Electricity production	Steel production	Fridge production
Elementary flows	Σ_{EF}	119.5	620.9	65.9	150

*Figure 2.2 - **A** Overview of the system for the production of 'cooled food'. **B** Contribution matrix, showing the contributions from specific individual elementary flows (EF) originating of distinct processes to characterized results. The orange entry shows the contribution from 'CO_2' of 'Coal mining' to 'climate change'. **C** EF contributions, showing the contributions from EFs to characterized results. The yellow entry shows the contribution from 'CO_2' to 'climate change'. **D** Process contributions, showing the contributions from processes to characterized results. The red entry shows the contribution from 'Coal mining' to 'climate change'. Note that all impacts are caused from the provision of the FU and all process contributions of 0 have been removed.*

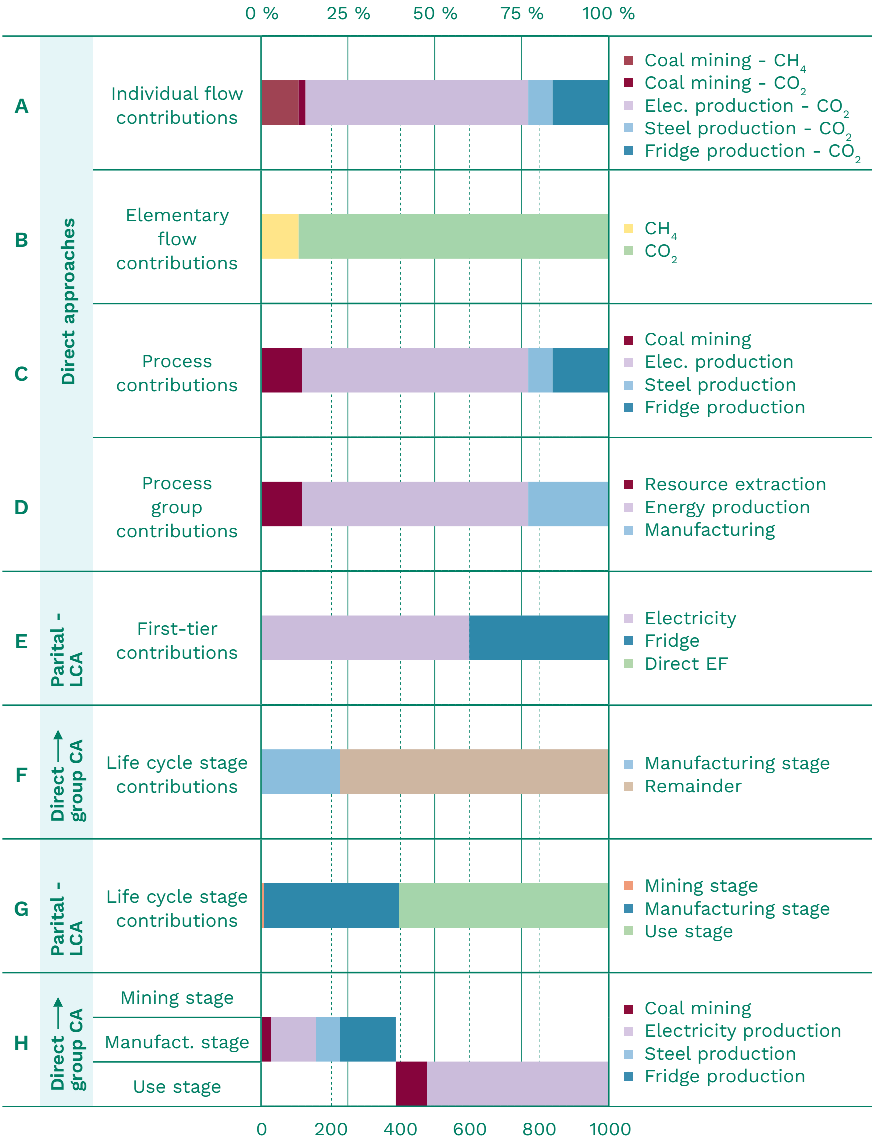


Figure 2.3 - Different contribution analysis results to characterized results of the simplified case study compared. ***A*** *Individual flow CA.* ***B*** *EF CA.* ***C:*** *Process CA.* ***D*** *Process group CA.* ***E*** *First-Tier CA.* ***F*** *Group Life Cycle Stage CA.* ***G*** *Partial-LCA Life Cycle Stage CA.* ***H*** *Process contributions to Life Cycle Stages.*

2.3.2 Elementary Flow Contribution Analysis and Process Contribution Analysis

Goal

The goal of the next two approaches is to find the contributions *from* a process or EF. A practitioner could use process CA to investigate contributions *from* specific processes e.g. the climate change impact from electricity production with coal. A practitioner may use this to identify which processes or EFs in the system have the highest *direct* contributions to climate change.

Description

These two approaches can transparently reduce the amount of generated data from individual flow contribution analysis while still providing a high level of detail.

These approaches are applied by summing one of the two axes of the contribution matrix. For EF CA, the processes (columns) are summed, one result per EF (row) is left. For Process CA, the EFs (rows) are summed, one result per process (column) is left. This is also demonstrated in SI 1.3.2.

Example

The results for these approaches are shown in Figure 2.2 C for EF and Figure 2.2 D for process contributions. The figure shows how the number of results can be effectively and transparently reduced. As an example, the process contributions *from* 'coal mining' are shown in red and EF contributions *from* CO_2 are shown in yellow. The results are also shown in Figure 2.3 B and C in context with the other approaches.

2.3.3 Elementary Flow Group and Process Group Contribution Analysis

Goal

The goal of these two approaches is to find the contributions from a group of EFs/processes. A practitioner could create groups for two reasons; either to transparently reduce the amount of datapoints, or because those EFs/processes are logically connected. A practitioner could use process group CA to assess contributions from a group of processes e.g. the climate change impact from the process group containing all processes related to electricity production. This approach is useful to find *direct* impacts of related processes (e.g. all transport processes) or EFs and to reduce the amount of data to interpret.

Description

Contribution analysis *from* process groups and EF groups are approaches that exchange levels of detail with a smaller and easier to interpret number of results. These two approaches build on the previous two approaches and reduce the number of results further, aiding in interpretation.

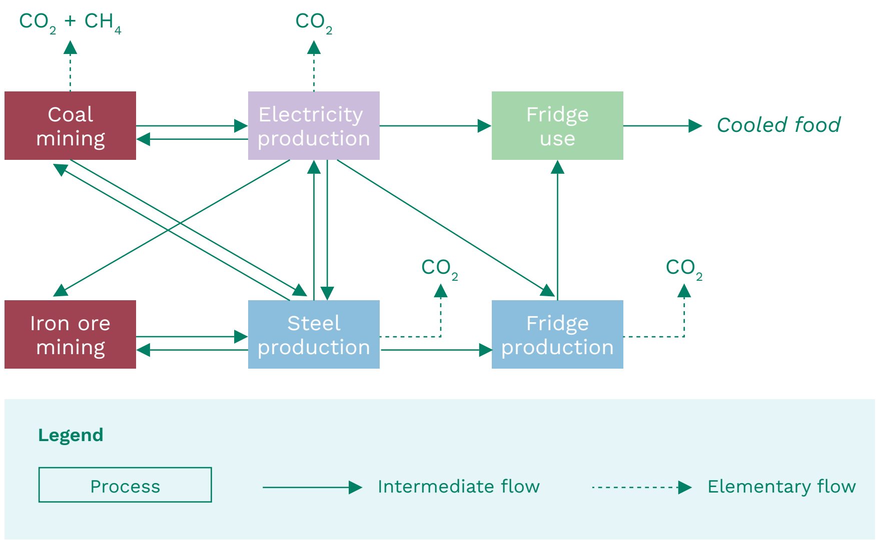
Grouping is done based on metadata. The metadata are attributes about the data, e.g. data about the EF/process. This can for example be done by grouping EFs based on EFs in different compartments, e.g. grouping all CO_2 flows from 'air', 'air, urban' etc. or grouping on an element, e.g. all flows containing carbon. For processes, this can for example be done by grouping with the same product name, location, or other relevant information such as industry sectors (e.g. ISIC sectors in ecoinvent). Such metadata could be provided by LCI database developers or be provided by the practitioner in the form of 'tags', such as 'disposal stage' or 'pesticide'. In SI 1.3.3, we demonstrate a mathematical approach transforming EF or process contributions into grouped results.

When using EF/process groups, the practitioner must be aware that the EF/process must always be in exactly one group. The entity cannot be in more than one group, or it would be double counted. Each entity must also be in one group, or its impact will not be counted. For grouping on pre-existing metadata (like product name) this would not be a problem, but attention should be paid to this when using custom tags, where all entities in a CA need to be tagged. In practice, entities that do not belong to a group could be aggregated together in a 'remainder' group to simplify this process, though a practitioner should be explicit about that choice.

Example

We show results for Process Group CA in Figure 2.4. The grouping is done based on four tagged categories, which are also color-coded for clarity. As shown, the groupings are based on tags for 'Resources extraction', 'Energy production', 'Manufacturing' and 'Use'. It is still possible for the groups to have no impact (e.g. 'Use'). The results are shown in Figure 2.3 D in context with other approaches.

A | System



B | Process contributions (tagged)

Climate change ($kgCO_2eq.$)		Processes					
		Coal mining	Electricity production	Iron ore mining	Steel production	Fridge production	Fridge use
Elementary flows	Σ_{EF}	119.5	620.9	0	65.9	150	0

C | Process group contribution

Climate change ($kgCO_2eq.$)		Processes			
		Resources extraction	Electricity pro-duction	Manufacturing	Use
Elementary flows	Σ_{EF}	119.5 (119.5 + 0)	620.9	215.9 (65.9 + 150)	0

*Figure 2.4 - **A**: Overview of the system for the production of 'cooled food' with four groups: 'Resource extraction' in red, 'Energy production' in purple, 'Manufacturing' in blue and 'Use' in green. **B**: Process contributions, marked with the groups. **C**: Process group contributions, showing the contributions from process groups to characterized results.*

2.3.4 Advantages and limitations of the direct approaches

The three levels (1: individual flow CA, 2: EF/process CA and 3: EF/process Group CA) have a few different tradeoffs between each other based on the level of disaggregation they provide. Where individual flow CA gives the highest level of resolution available, the number of results generated may quickly become too much for effective interpretation with larger systems than this simplified case study. The contribution matrix in Figure 2.2 B has 12 entries, two for each process. If two EFs and two processes were added, this would become 32, already well over double the amount. Modern databases like ecoinvent (Wernet et al., 2016) have ~5,000 EFs and ~20,000 processes. While the vast majority of these entries would be zero, the number of results would still be sizeable.

With all these approaches, due to the potential number of results, many results would likely only contribute a small fraction of the total. Sorting the contributions by magnitude and applying a cut-off to show only the most impactful contributors may help to provide insight.

A major downside of the direct approaches is that the results may in some cases be counter-intuitive, trivial or not helpful. An example of a counter-intuitive result is that, while the use process of the fridge is naively considered to be the major contributor *to* climate change, the tables in Figure 2.2 B-D show that its *direct* contribution to climate change is zero. The 'fridge problem' -where one would intuitively expect the use of the fridge to be responsible for part of the contribution- was first introduced by Heijungs & Kleijn (2001) and is caused by the fact that these direct approaches only show *direct* contributions. This problem of assigning *indirect* contributions cannot be resolved by direct approaches to contribution analysis. Similar to the 'fridge problem', an example of a trivial result would be to find that the only contributor to 'resource extraction' is a mining process, though this again comes down to the same question of *indirect* contributions, we show a triviality example in Table SI 12 in SI 1.3.1. While the mining processes *directly* contributes to resource extraction, other processes require those resources. In the following chapters we discuss different approaches that can answer questions from this *indirect* perspective.

Finally, there is a specific challenge to the grouping approaches: These approaches require more input from the practitioner by defining groups, attention needs to be paid to double-counting or dropping flows. These groups need to be clearly defined and if a 'remainder' is used, this needs to be communicated clearly. Modern LCA software can help with grouping, for example based on metadata present in modern LCA databases.

2.4 First-Tier Contribution Analysis

2.4.1 Goal

First-Tier contributions (sometimes also called product contributions, first-level, first-order or n-1 contributions) are the contributions from the (intermediate and elementary) flows required in the process delivering the FU.

The goal of First-Tier CA is to find the contributions *from* the intermediate flows (products) consumed and *direct* EFs emitted by the process providing the FU, this is an *indirect* perspective. A practitioner could use First-Tier CA to investigate the contributions *from* 'Electricity' on the fridge use. This would, in contrast to the process contributions for electricity production, include all *indirect* contributions related to the production of electricity as a product (e.g. the coal burned for electricity production and the steel produced for the power plant). Another example could be a manufacturer wishing to find the impact of components (compressor, insulation, frame, etc.) used in the fridges they produce.

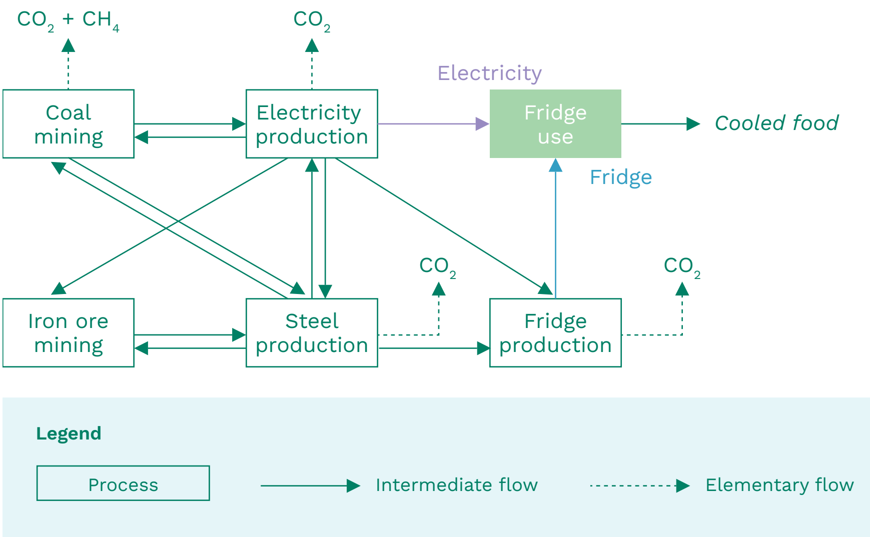
2.4.2 Description

This approach is fundamentally different from the direct approaches as these results cannot be calculated from the contribution matrix. Instead, this approach makes use of partial-LCA: Partial-LCA splits the FU into different Partial-FUs, with all parts combined still accounting for the original FU. Partial-LCA allows practitioners to assess the contributions *from* each of these Partial-LCAs.

In First-Tier CA, the FU is split into one Partial-FU for the process delivering the original FU one for each intermediate flow into that process.

First-Tier CA can only be applied to FUs where exactly one product or service is consumed. The first Partial-FU delivers the original FU minus all intermediate flows connected to the process of the FU. All Partial-FUs are scaled to the amount required for the original FU. We show this in Figure 5 A and B, in SI 1.4 we explain and demonstrate Partial-LCA for First-Tier CA in more detail.

A | System



B | One FU to Patrial-FUs

	Cooled food
Coal	0
Electricity	0
Iron ore	0
Steel	0
Fridge	0
Cooled food	8

→

Electricity	Fridge	Fridge use
0	0	0
600 (8*75)	0	-600 (8*-75)
0	0	0
0	0	0
0	1 (8*0.125)	-1 (8*0.125)
0	0	8

C | First-tier contributions

Climate change ($kgCO_2eq.$)		First-tier contributions		
		Electricity	Fridge	Fridge use
Elementary flows	Σ_{EF}	574.6	381.74	0

*Figure 2.5 - **A**: Overview of the system for the production of 'cooled food' with First tier marked: The process 'Fridge use' in green, and the intermediate flows 'Electricity' in purple and 'Fridge' in blue. **B**: Full functional unit (FU) and Partial FUs, split for the original process and each of the intermediate flows. **C**: First-Tier contributions, showing the contributions from the First-Tier (direct contribution from the process 'Fridge use' and indirect contributions from the intermediate flows 'Electricity' and 'Fridge') to characterized results.*

As an example, the contributions of 'Electricity' for the fridge use would be found by calculating the partial-LCA result for the intermediate flow of (***75 kWh/year*8 year***) 600 kWh Electricity (as derived from the Electricity input for the use process in Table 2.1)

The First-Tier results show the *direct* contribution *from* the process delivering the original FU and the *indirect* contributions *from* the intermediate flows consumed by that process.

2.4.3 Example

We show the results in Figure 2.5 C. We also show the comparative results in Figure 2.3 E. Note that the contribution from 'Electricity' in Figure 2.5 C is higher than the process contribution impact of 'Electricity production' in Figure 2.2 D, these values differ, as First-Tier contributions *from* 'Electricity' show the contribution of not only 'Electricity production' (for 600kWh), but also other *indirect* impacts from other processes required to produce that electricity. Also note that we include 'Direct EF' in Figure 2.3 E representing the 'Use' process, though the contribution is zero.

2.4.4 Advantages and limitations

There are three major advantages to this approach. First, the number of results is reduced to the number of intermediate flows of the process delivering the FU plus one for the *direct* EF contributions, which aids in interpretation. Second, the approach partially solves the problem of trivial results. For example, the contributions to 'mineral extraction' would now be shown not *from* the mining process, but as a part of the impact of the intermediate flows of the process delivering the FU, we demonstrate this in SI 1.4. Third, as full LCA calculations are used on each of the Partial-FUs, other CA approaches may be applied to the Partial-LCAs, we discuss this further in section 2.5.3.

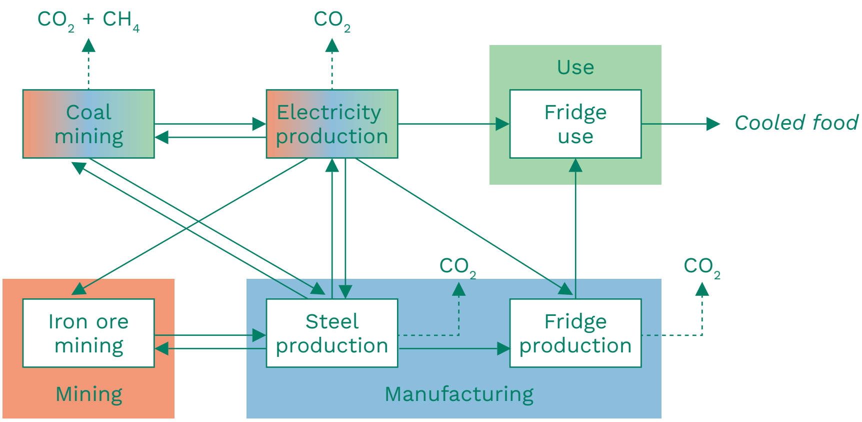
There are a few disadvantages to this approach. Despite the results being non-trivial, a substantial amount of information is removed from the results. As only the contribution from the first level is counted, this approach cannot provide deeper insight into the source of the contributions of the inputs. Finally, this approach can only be applied to FUs consisting of one product or service, though this approach could be applied sequentially to resolve this. A FU consisting of multiple products, for example a multi-functional process "basket of functions" (Majeau-Bettez et al., 2014) could be assessed sequentially for every function.

2.5 Life Cycle Stage Contribution Analysis

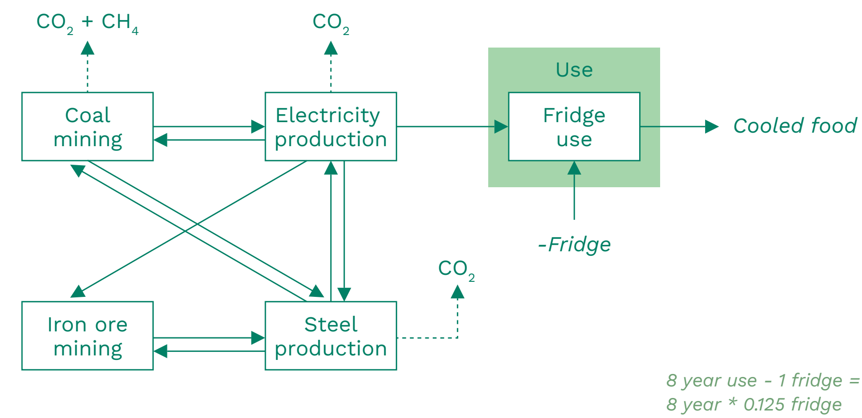
2.5.1 Goal

Contribution Analysis *from* life cycle stages shows the contributions of different life cycle stages. For this study, we define a life cycle stage as: An interdependent sequence of one or more processes connected by their intermediate flows and producing a functional flow. What processes are part of which life cycle stage should be chosen by a practitioner as useful units of enquiry for a specific question they want to answer. Life cycle stages can be connected through consuming the functional flows of other life cycle stages. Not all processes need to be assigned to a life cycle stage, as the underlying product system does not change, the un-assigned processes will contribute to the life cycle stages indirectly. Figure 2.6 A shows three examples of life cycle stages. Note that in this simplified example, 'Electricity production and 'Coal mining' are not part of a life cycle stage, but will still indirectly contribute to all of the life cycle stages. Two other examples from this system could be a stage of the two processes 'Iron ore mining' and 'Steel production' called 'Steel', or one consisting of the two processes 'Coal mining' and 'Electricity production' called 'Energy'. In general, useful life cycle stages may be 'Production', 'Use' and 'End of Life', with relevant processes chosen by the practitioner. Note that, although life cycle stages and their contributions are a cornerstone of the Product Environmental Footprint (PEF) method (European Commission, 2013; Zampori & Pant, 2019), the guidelines provide examples of life cycle stages but never explicitly define or formalize the concept.

A | System and Life Cycle stage contributions



B | Partial system and results for 'Use'



Climate change ($kgCO_2eq.$)		**Process contributions (to 'Use' stage)**			
		Coal mining	Electricity production	Steel prodution	Fridge production
Elementary flows	Σ_{EF}	85.16	488	1.4	0

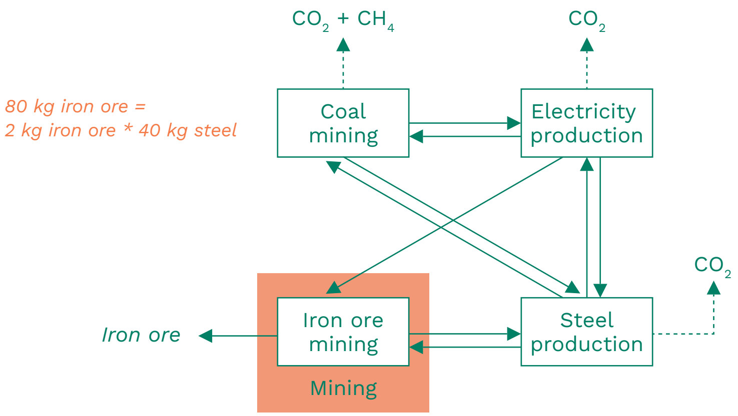
Legend

Process — Intermediate flow — Elementary flow

C | Partial-LCA life cycle stage contributions

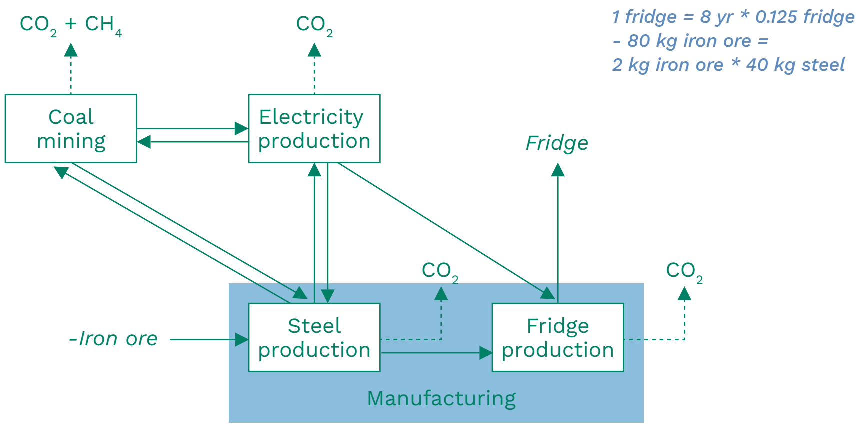
Climate change ($kgCO_2eq.$)		Life Cycle Stagecontributions		
		Mining stage	Manufac. stage	Use
Elementary flows	Σ_{EF}	574.6	381.74	0

D | Partial system and results for 'Mining'



Climate change ($kgCO_2eq.$)		Process contributions (to 'Mining' stage)			
		Coal mining	Electricity production	Steel prodution	Fridge production
Elementary flows	Σ_{EF}	1.2	6.5	0.2	0

E | Partial system and results for 'Manufacturing'



Climate change ($kgCO_2eq.$)		**Process contributions (to 'Manufacturing' stage)**			
		Coal mining	Electricity production	Steel prodution	Fridge production
Elementary flows	Σ_{EF}	33.2	126.3	64.4	150

*Figure 2.6 - **A**: Overview of the system for the production of 'cooled food' with three life cycle stages: 'Mining' in orange, 'Manufacturing' in blue and 'Use' in green. **B**: Partial system for life cycle stage 'Use' and Process contributions to 'Use stage' characterized results. **C**: Partial-LCA life cycle stage contributions, showing contributions from life cycle stages to characterized results. **D**: Partial system for life cycle stage 'Mining' and Process contributions to 'Mining stage' characterized results. **E**: Partial system for life cycle stage 'Manufacturing' and Process contributions to 'Manufacturing stage' characterized results. Also showing grouped process contributions from processes in the stage marked in blue.*

The goal of this approach is to find contributions *from* individual life cycle stages. A practitioner could use Life Cycle Stage CA to assess the contributions of various -practitioner defined- stages of production e.g. contributions *from* a 'materials production' stage. This approach can be useful to find contributions for life cycle stages along a supply chain a manufacturer has control over.

We discuss two different approaches to Life Cycle Stage CA; Process Groups and Partial-LCA. Both approaches require careful input from the practitioner to define and communicate the life cycle stages.

2.5.2 Group Life cycle stages

Description

Group Life Cycle Stage CA is based on the direct process grouping approach by tagging processes to life cycle stages and -if required-creating a 'remainder' group, as described in section 2.3.3. As this approach is a specialized use of process group CA, it carries the same advantages and disadvantages, most relevant here is that this approach can only show *direct* contributions. To use the example of Figure 6 A and the life cycle stages defined above, the upstream processes of 'electricity production' and 'coal mining' would both (indirectly) contribute to all life cycle stages and as such could not be 'tagged' into a life cycle stage and are part of a 'remainder' group.

Example

We show this result in Figure 2.3 F. As can be seen, the majority of the contribution comes from the 'remainder' group, with the direct contributions of the life cycle stages being low or zero.

Advantages and Limitations

While grouped life cycle stages may be able to reduce the number of results, this approach has the same limitations as discussed in section 2.3.4, most importantly, the approach cannot show *indirect* contributions, i.e. the 'fridge problem'.

2.5.3 Partial-LCA Life cycle stages

Description

Partial-LCA Life Cycle Stage Contribution Analysis applies Partial-LCA to calculate contributions of different life cycle stages, this allows to find both *direct* and *indirect* contributions *from* life cycle stages. Contrasting with First-Tier CA from section 2.4 though, the Partial-FUs are used to differentiate life cycle stages throughout the product system. A way of transforming life cycle stages into Partial-FUs is with 'modular LCA' as formalized by Steubing et al. (2016). The splitting of the original FU (into one FU for every Life Cycle Stage) enables the Life Cycle Stages to be calculated. In this simplified example, the life cycle stage 'Manufacturing stage' would produce 1 fridge and consume 80 kg iron ore from 'Mining stage'. More iron ore is required in the system for steel in other end-uses, but this is not considered directly in this life cycle stage, though it is considered for the total impact. We explain and demonstrate Partial-LCA life cycle stage contribution analysis in SI 1.5. As Partial-LCA is applied, the contributions *from* each life cycle stage sum to the total impact.

Example
The results of a partial-LCA life cycle stage contribution analysis show the contribution *from* each life cycle stage. We show an example of the three life cycle stages 'Mining', 'Manufacturing' and 'Use' for the simplified fridge product system in the Figure 2.6 A. We also show how the results compare to those of the other CA approaches in Figure 2.3 G. Depending on the question of the practitioner, these results may provide more insight into the life cycle stages compared to Group based results shown in Figure 2.3 F.

In the simplified example, the resulting contributions *from* each of the three life cycle stages is shown in the Figure 2.6 C. Important to note here is that the 'Use' life cycle stage is responsible for the majority of the total impact through its *indirect* contribution, while its *direct* contribution is 0. A part of the direct contribution *from* 'Coal mining' and 'Electricity production' is now associated with the each of the life cycle stages. This is another way of applying Partial-LCA to solve the 'fridge problem'.

Advantages and Limitations
The main advantage of this approach compared to the previous ones is that not only can it reduce the amount of results, it can reduce complexity in interpreting the results of an LCA -especially when large databases are used- as the contributions from only a few life cycle stages need to be considered compared to the contributions from many processes, EFs or groups, we discuss this further in SI 1.7.

As Partial-LCA is applied to calculate results, an important implication for this approach is that other CA approaches can be applied to the partial results, which allows for deeper insights into the system studied. We show this for process contributions to the life cycle stages in Figure 2.3 H and Figure 2.6 B and D-E. We also apply process grouping to differentiate between direct and indirect contributions in Figure 2.6 E. We discuss this use of other CA approaches to Partial-LCA results further in SI 1.5. Finally, life cycle stage contributions can also be grouped, we demonstrate this in SI 1.5.3.

The major downside of this approach is that it requires more modelling effort from the practitioner, who needs to define life cycle stages and the functional flows of the processes that need to be cut-off between life cycle stages, as further described in SI 1.5.

2.6 Path Contribution Analysis

2.6.1 Goal

Following from First-Tier CA, a practitioner may want to investigate the First-Tier contributions for another intermediate flow (e.g. what are the First-Tier contributors for the fridge?), expanding this first tier to paths of contributions. Results from this type of approach are often shown in a Sankey diagram (Sankey, 1898).

The goal of Path CA is to find how contributions *from* intermediate flows throughout the product system lead to the final LCA score. A practitioner could use Path CA to investigate through what intermediate flows (e.g. products) the production of electricity *indirectly* contributes to the final impact. Another example could be to find which components and sub-components of a fridge may be responsible for what *indirect* contributions.

2.6.2 Description

This approach shows the contributions *from* intermediate flows between processes. Path CA makes use of the networked structure of product systems which can be traversed and considers the contribution at any intermediate flow the product system, scaled to the FU. As the contributions are not *to* the FU but instead *to* any intermediate flow in the system, the contributions do not add up to the total LCA result. For this reason, this approach should not be considered contribution analysis in the strict sense, though this fact does not diminish its widespread use and practical usefulness to assess contributions, which is why we still discuss this approach.

While Sankey diagrams have been used abundantly in reporting contribution results in LCA, to our knowledge this approach was only formalized for inventory results recently by Srocka & Montiel (2021), who call this 'Upstream contributions'. However, we do not agree with this naming as contributions could also be counted from 'downstream' processes, e.g. with waste treatment. The approach by Srocka & Montiel (2021) calculates the Path contributions for all intermediate flows in the system at once, we demonstrate the approach in SI 1.6, also for characterized results. The Path contributions can also be calculated for (a part of) the product system iteratively, which can be more efficient for large systems.

2.6.3 Example

We show a Sankey diagram of the simplified case study in Figure 2.7. The figure shows the Path contributions through the system. Caution must be paid in interpretation of the figure: While the Path contributions (lines connecting the boxes) are shown as a percentage of the total impact, they should not be summed, as explained earlier.

2.6.4 Advantages and Limitations

Path CA has two advantages. First, it can show contributions throughout the product system. This can help identify key processes and intermediate flows that affect results highly. Such processes could have a low (or no) *direct* contribution themselves, but instead have a 'connector' role (Reinhard et al., 2019), 'accumulating' contributions through their intermediate flows. Secondly, Path CA can also answer questions regarding the responsibility for *indirect* contributions. For example, in Figure 2.7, we show that 'Electricity' does not only have the biggest contribution *to* 'use' but also *to* 'fridge production', where the *indirect* contribution from 'Electricity' is higher than the *direct* contribution of the process itself.

There are also some strong limitations to this approach: Firstly, graphical representation is complex, due to the fact that the LCA results do not add up to the total impact (double counting, as explained in SI 1.6.1), these results should not be shown in traditional graphs like bar charts. The results can be shown through a Sankey diagram or a tree structure. However, these can make it harder to compare alternatives to each other. Another limitation is that the approach is limited to a

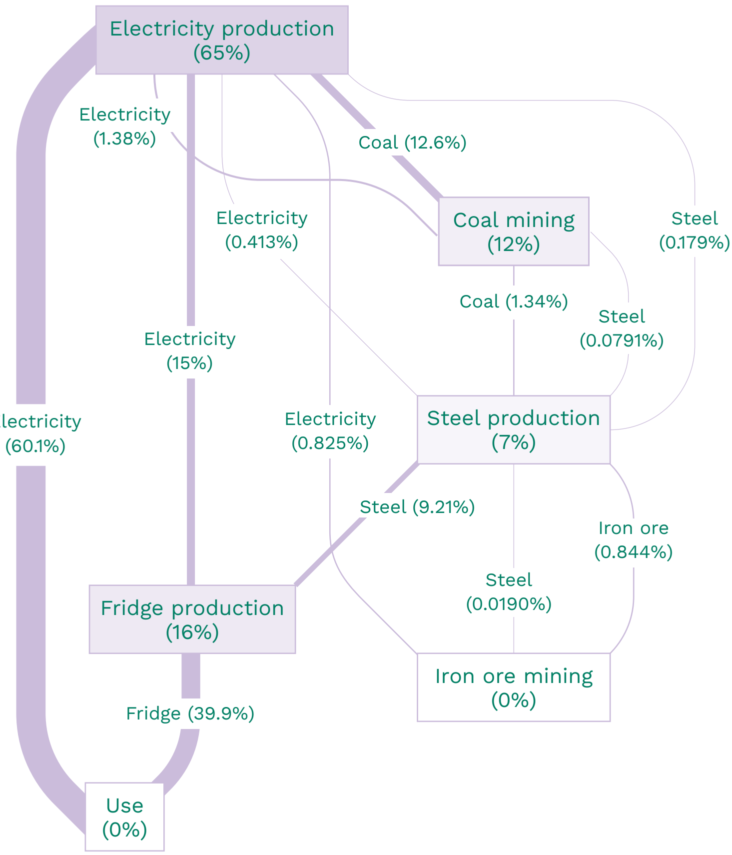


Figure 2.7 - Sankey figure of the Path contributions for the production of 'cooled food'. Each box represents a process, each line an intermediate flow between processes. The percentages for processes are the relative direct contributions. The percentages for the intermediate flows are the relative indirect Path contributions at these intermediate flows.

FU of one product, like First-Tier contributions. Additionally, Srocka & Montiel (2021) identify an additional limitation to their approach: Open loops -i.e. loops including the FU- cannot be computed. The iterative approach has the advantage that a cut-off can be applied, thus limiting the number of results.

2.6.5 Similar approaches to Path Contribution Analysis

Two similar approaches to Path CA are from Reinhard et al. (2019), who demonstrate a similar concept with the 'connector perspective', though they applied this to every product in the product system at once, instead of to a singular FU, limiting use in normal practice. The other is Contribution Trees in Srocka & Montiel (2021, Section 7.4.3), where contributions are shown in a tree instead of a network. We discuss the difference between Path contributions and contribution trees in SI 1.6.2.

Other similar approaches to Path CA are Structural Path Analysis (Suh & Heijungs, 2007; Waugh, 1950), Path Exchange method (Lenzen & Crawford, 2009) and Output contributions (Suh, 2004). However, these approaches are mainly limited to IO-LCA and can be challenging or impossible to apply to process-LCA (Heijungs et al., 2022; Suh & Heijungs, 2007). We refer to Heijungs & Suh (2002), Lenzen & Crawford (2009), Suh & Heijungs (2007) and Suh (2004) for further discussion of these approaches.

2.7 Discussion

2.7.1 Contribution Analysis to other entities

So far, we only discussed Contribution Analysis to characterized results (or partial characterized results), as this is most commonly shown in literature. CA can, and has been, applied to other entities as well. In Table 2.2 we give an overview to which entities each CA approach we discussed is compatible with.

To / From	Life Cycle Inventory (EF)	Characterized result	Normalized result	Weighted result
Individual flow	SI 1.3.1	Sec. 2.3.1 / Fig. 2.2B		
EF	SI 1.3.2	Sec. 2.3.2 / Fig. 2.2C		
Process		Sec. 2.3.2 / Fig. 2.2D		
EF group		SI 1.3.3		
Process group		Sec. 2.3.3 / Fig. 2.4B		
First-Tier	SI 1.4	Sec. 2.4 / Fig. 2.5C		
Life Cycle stage		Sec. 2.5 / Fig. 2.6		
Path	SI 1.6	Sec. 2.6 / Fig. 2.7		

Partial-LCA group		SI 1.5.3			
Characterized result					
Normalized result					

Table 2.2 - Overview of the CA approaches: from approach (rows) to entity (columns). Grey cells show that an approach can be applied to that entity. Where relevant, we refer to the section and figure where the approach to that entity is discussed in the cell.

For the life cycle inventory, CA cannot be applied *from* processes or process groups, as the EFs in those processes cannot be combined without characterizing them (combining ‘kg CO_2’ and ‘m^2 of land use’ is not possible without characterizing the EFs).

As Partial-LCA results have the same format as ‘regular’ LCA results -just for each partial FU-, each of the approaches could also be applied to partial-LCA, keeping in mind the limitations of those approaches. As an example; it could be useful to apply process CA *to* the Partial-LCA life cycle ‘Manufacturing’ (as shown in Figure 2.3 H). Conversely, Partial-LCA results can also be grouped, e.g. First-Tier contributions grouped into ‘materials’, ‘energy’ and ‘transport’.

For normalization and weighting, the same approaches can be used as *to* characterized results. Though the contributions *from* characterized results *to* normalization and *to* weighting could also be applied. Finally, *from* normalized results *to* weighted results could be used.

2.7.2 Comparison of CA approaches and their domain of application

As demonstrated in Figure 2.3 and Figure 2.7, each approach to CA provides different results and insights by assessing the same system from different perspectives. While the direct approaches use the same information, First-Tier, Partial LCA Life Cycle Stage analysis and Path Contributions require additional calculations to provide results.

The approaches we demonstrated above vary in the resolution of results they can give. In Table 2.3 we provide an overview of key aspects to each of the approaches. Because LCA results may provide a large amount of information, having high resolution is not always advantageous. The individual flow, process and EF CA approaches are best applied when looking for contributions from specific entities, with cut-offs applied to reduce the number of results, or when working with small systems. The grouping, First-Tier, life cycle stages and Path approaches are primarily useful with larger systems, where they can be effectively used to reduce the amount of information, we show this with an example using the ecoinvent database (Wernet et al., 2016) in SI 1.7. While Partial-LCA Life Cycle Stage CA requires more input from the practitioner compared to the other approaches due to the definition of life cycle stages for their system, we see this approach as a particularly useful approach to provide actionable results. We also note that with larger systems, most, if not all approaches would benefit from additional input, mostly in the

		Example research question	Examples (to characterized results)
Direct approaches	Individual Flows	Which individual EFs from which processes contribute how much?	- Top contributions from individual EF caused by a process
	Elementary Flow (EF)	Which EFs contribute how much?	- Top contributions from EFs
	Process	Which processes contribute how much?	- Top contributions from processes
	EF Group	Which EF Groups contribute how much?	- Contribution from all carbon-containing flows
	Process Group	Which Process Groups contribute how much?	- Total contribution from electricity inputs - Contribution from specific ISIC sector
Direct +	First-Tier	Which intermediate flows and EFs contribute how much?	- Contributions from inputs-to and production-of a fridge
	Life Cycle Stage	Which life cycle stage contributes how much?	- Life Cycle contributions from each stage
	Path	Which intermediate flows form paths of major contributions?	- Intermediate flows that contribute to final result

Table 2.3 - Comparison of key aspects of CA approaches to characterized results. The columns show key aspects: example research questions, examples, resolution of results (how detailed are the results?), perspective (can the approach show direct, indirect or both perspectives?) and finally potential challenges for interpretation and additional inputs needed from a practitioner.

form of cut-offs or groupings to reduce the amount of results. Each of the approaches can be useful and the practitioner should choose which are most relevant to the questions they want to answer.

Another main difference is whether the approach shows only *direct* results or also *indirect* results. A notable example is the difference between Figure 2.3 C and E. If we consider ‘electricity production’ (a process) and ‘electricity’ (an intermediate flow) , these may at first sight be considered the same, but the former shows the *direct* contribution of the process, while the latter show the *indirect* contribution of the product. This means the impacts will be different. On the one hand the contribution of ‘electricity’ is increased as it includes contributions from other processes (e.g. ‘coal mining’), on the other hand, the contribution

Resolution	**Interpretation challenges and additional inputs**
Highest	- Amount of contributions, can be reduced by sorting and cut-off. - Direct contributions only: the ‘fridge problem’.
High	
Depends on group size	- Requires definition of groups (could automated through metadata). Any ‘remainder’ groups must be made clear. - Amount of contributions, can be reduced by sorting and cut-off. - Direct contributions only: the ‘fridge problem’.
Low	- First tier inputs do not give insight into deeper sour-ces of contributions than the first tier.
Depends on life cycle stage amount	- Requires definition of life cycle stages and how they connect.
Depends on cut-off	- Does not necessarily show the entire system or full impacts. Loops and FUs consisting of multiple pro-cesses may form interpretation challenges.

is decreased as not all electricity is consumed by 'use', some is also used by other processes (e.g. 'fridge production'). The net effect of both is a higher impact compared to 'electricity production' in this simplified example, but this will depend on the case.

Partial-LCA Life Cycle Stage CA is a required method by the PEF method (European Commission, 2013; Zampori & Pant, 2019). In the PEF, 'Raw material acquisition', 'Manufacturing', 'Distribution', 'Use' and 'End of life' are required as life cycle stages for which contributions must be reported. Building further on this, EN 15804+A2 (2019) introduces even more sub-modules. These could be calculated as individual life cycle stages, after which the life cycle stage results could be grouped into the full modules, as we demonstrate in SI 1.5.3. Another use of grouping of life cycle stages is the application of the Scopes (1: direct, 2: indirect from electricity, 3: all other) from the GHG protocol (2004) and ISO 14064 (2018), as we discuss in SI 1.5.3.

Finally, we mention some other notable approaches of CA we have not discussed in more detail: The identification of processes in the ecoinvent database (Wernet et al., 2016) that contribute highly to many different impact categories through differentiating between *direct* contribution and *indirect* contribution perspectives (Reinhard et al., 2019), who name this causer and connector perspective respectively). Identifying the importance of capital goods in the ecoinvent database (Frischknecht et al., 2007). The analysis of abiotic resources in the ecoinvent database (Rørbech et al., 2014). These approaches can also be useful to practitioners in specific cases, though their use is not common in literature.

2.7.3 Limitations to Contribution Analysis

While one of the most important limitations to CA was summarized as the 'fridge problem' (trivial or counter-intuitive results) introduced by Heijungs & Kleijn (2001), we have shown that this is only a limitation of CA approaches that show *direct* results. This limitation can be resolved by using approaches that show *indirect* results as well.

There are still three major limitations to all discussed approaches to CA that should be taken into account when using any approach: the use of negative numbers, missing data and the verifiability of results.

Firstly, the occurrence of negative numbers in LCA results (Heijungs & Kleijn, 2001). Note that here we discuss numbers below 0, this does not imply anything about the desirability of that result. Negative numbers can occur in various cases: Negative elementary flows (e.g. CO_2 uptake in forestry), negative characterization factors (e.g. atmospheric SO2 as a decreasing global warming effect), or negative intermediate flows due to substituted processes (avoided production). Negative numbers void the use of pie-charts and can make it more difficult to interpret results effectively, especially with relative representations. We discuss some examples and approaches to present negative numbers in SI 1.8.

Secondly, Heijungs & Kleijn (2001) also point toward the limitation of missing data; contribution analysis can only show contributions of what is modeled. While this limitation may seem obvious, this limitation is especially relevant in two cases: 1) when using CA as input for sensitivity analysis or 2) when using CA in early project phases when there are still data gaps or detailed data may not be available.

While Heijungs & Kleijn (2001) only discussed the direct approaches to contribution analysis, these limitations are still important for all approaches we have discussed here.

Finally, when performing LCA, it is important to be able to verify that results are correct and the calculations are performed correctly. We suggest practitioners -especially academics-, make use of software that allows users to inspect the algorithms such that they can be verified to provide correct results.

2.7.4 Reporting Contribution Analysis

In reporting CA, we recommend reporting the following points to ensure the CA is better replicable and useful for the study it is applied in:

- What approach is used and to what entity it is applied,
- Additional information relevant to the approach:
  - Cut-offs if any,
  - What EFs/processes are in groups and if a remainder is used,
  - Processes in Life Cycle Stages and the functional flow of those stages,
  - The specific software or tool -and version- used, as implementations may vary with different tools,

- How the chosen approach helps answer their research question,
- Results should be available in tabular form (either in main text or appendices),
    - Results can optionally be reported in a graph, e.g. a stacked bar chart like Figure 2.3.

Some examples are:
- 'We use EF Group Contribution Analysis to LCI results to investigate carbon containing EFs in Excel (provided in SI x), all other EF are grouped as 'rest'.'
- 'This study applies Process Contribution Analysis to find major contributing processes to 'resource extraction' with a cut-off of 5% contribution, the resulting processes are used in sensitivity analysis in software x version y.'
- 'First-Tier Contribution Analysis is used to find the 'climate change' impact *from* components in a fridge with python (code provided in SI x) to inform supplier choices.'

As demonstrated in the examples above, describing a CA approach doesn't require much space in a report or manuscript, but providing this description can considerably improve clarity and replicability for readers about what the practitioner has done.

Finally, CA is sometimes applied in combination with sensitivity/uncertainty analysis. When this is the case, contributions of individual entities may change through different calculations, which may be relevant to report as well. We note here that this would not be possible in the stacked bar chart we use in Figure 2.3, as uncertainty ranges could not be combined as such, though each contributing entity may be shown as an individual bar with an uncertainty marker. This is discussed in more detail in Heijungs (2024).

2.8 Conclusion

With this study, we set out to structure, explain and provide a clear terminology for different CA approaches. We introduced the *from*-*to* relationship, classified different approaches based on the *from* and discuss *to* what they can be applied. Furthermore, we also make a distinction between the *direct* and *indirect* perspectives on contributions and how these perspectives help answer different questions. Through discussing each approach with its goal, workings, advantages and disadvantages as well as comparing the results of each approach to the same simplified case study, we have shown the different insights each approach can provide and in what cases which approach may be most useful. Additionally, we formalized the use of Partial-LCA for First-Tier CA and Life Cycle Stage CA, and expanded on the use of Path CA for LCIA results.

As we have shown with this overview, each of the approaches has its place in the toolbox of the LCA practitioner and can be used to provide different insights into LCA results. Which approach is best applicable is best judged on the question that needs to be answered. Applying multiple approaches is recommended to gain deeper insight and complementary perspectives on results. This study can help those new to LCA, as well as experienced practitioners and LCA software developers to gain deeper insight into these approaches, especially by referring to SI 1 and SI 2 where each approach is presented in more detail and calculations are presented.

Through applying the right CA approach for the question and case at hand, we hope practitioners can gain better insights and more transparently communicate and report their results. This should contribute to a higher quality and more reproducible body of LCA literature and more well-founded conclusions.

Acknowledgements

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Chapter 3
Hypothetical Extraction Method in Life Cycle Assessment: Method and Uses

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The Supplementary Information (SI) to this chapter is available at the preprint server.

Abstract

Hypothetical Extraction Method (HEM) is an approach in Input Output Analysis (IOA) used to assess the effects of *'target'* economic sectors have on other sectors. If we interpret HEM in a Life Cycle Assessment (LCA) context, HEM could be described as 'assessing the contribution of processes (or groups of processes) to the impact of other processes', making this another potential Contribution Analysis (CA) approach. In this study, we introduce HEM in LCA and demonstrate how HEM may provide different insights compared to the already existing CA approaches in two example case-studies. We do this by showing how HEM may be applied in LCA in four steps: 1) defining a scenario for extraction, 2) extracting *target* processes, 3) calculating results for the *original* and *'remaining'* system and 4) calculating results for the *target* processes. We then demonstrate HEM in LCA using two different example case-studies and compare HEM against other CA approaches. We also demonstrate process contributions to the *target* and *remaining* sections, allowing deeper insight into results. With this study we have shown how and when HEM can be a useful approach for CA in cases where current CA approaches may be lacking, providing an additional CA approach to the LCA practitioner in understanding impacts from their systems.

3.1 Introduction

Hypothetical Extraction Method (HEM) is a method in Input Output Analysis (IOA) used to assess the effects economic sectors have on other sectors (Hertwich et al., 2024). To do this, a counterfactual scenario is created where the *'target'* sector (Dente et al., 2018) is extracted from the IOA model and results are re-calculated. The difference between the *original* result and the HEM scenario is considered to be caused by the extracted *target* sector.

HEM can be used for many different use-cases such as assessing the contribution of sectors to carbon footprints of products and consumption baskets (Hertwich, 2021; Rasul & Hertwich, 2023), assessing the 'importance' of an economic sector to other sectors in terms of consumption (Miller & Lahr, 2001) or assessing the effect of disruptive events (Dietzenbacher et al., 2019; Haddad et al., 2021). For an extensive overview of examples we refer to Miller & Lahr (2001) and Hertwich et al. (2024).

Even though IOA and Life Cycle Assessment (LCA) have similar mathematical structures, HEM is not used in LCA, though their similar structures could make this possible.

If we loosely interpret the goal of HEM 'assessing the impact of sectors on other sectors' to an LCA context, we find something like 'assessing the impact from processes (or groups of processes) to other processes'. This could be interpreted as similar to Contribution Analysis (CA) (what is the contribution of x to the total?) (Guinée et al., 2002; Heijungs & Kleijn, 2001). Through the extraction, this would assess not only the contribution of a process' direct contribution (Srocka & Montiel, 2021) but also all consumption of that process, meaning it would include indirect contributions as well (Reinhard et al., 2016; van der Meide et al., 2025). Other CA approaches that assess both direct and indirect contributions are First-Tier CA (van der Meide et al., 2025), assessing contributions of products feeding into the Functional Unit (FU). Life Cycle Stage CA (van der Meide et al., 2025), dividing the system into relevant sections of the supply chain such as 'production' and 'use'. And Path/Sankey CA (Srocka & Montiel, 2021), showing the 'path' contributions take to the FU. While these approaches each have their own unique strengths, they cannot be used to assess large groups of processes, for example industry sectors or regions effectively.

CA approaches could also be applied to systematically assess system-wide changes, applying it at another level than CA. Some examples are: Finding 'causer' and 'connector' processes in LCI databases (Reinhard et al., 2016), where these processes either have direct (Srocka & Montiel, 2021) or indirect (van der Meide et al., 2025) contributions, respectively. Two other examples are the identification of important capital goods in an LCI database (Frischknecht et al., 2007) and an analysis of abiotic resources in an LCI database (Rørbech et al., 2014).

While there are already various approaches to assessing indirect contributions in LCA, approaches to assess the indirect contribution from large groups of processes, such as sectors or regions do not currently exist. The objective of this study is to introduce HEM in LCA as a new approach to CA and demonstrate how HEM may provide different insights compared to the already existing CA approaches. We formalize the method in LCA and demonstrate with a simplified case study how it may be used and how results may be interpreted. Next, we compare it against other approaches with the simplified case study. After this, we also demonstrate HEM using a much larger example using the ecoinvent LCI database (Wernet et al., 2016) to simulate a more realistic case study. Finally, we discuss how HEM in LCA may help LCA practitioners to find new insights and discuss the nuances between different CA approaches.

3.2 Method

3.2.1 Notation

We demonstrate the approach in vectorized format. We use *italic lower case* for scalar values, ***bold lower case*** for vectors and ***BOLD UPPER CASE*** for matrices. Column vectors are written as $\boldsymbol{v}$, while row vectors are written as $\boldsymbol{v}^T$. All results presented are rounded, we refer to the excel file SI 2 for unrounded results.

3.2.2 Mathematical structure of LCA

We shortly introduce the mathematical structure of LCA based on Heijungs & Suh (2002) and the SI of van der Meide et al. (2025). LCA is generally done as IO-LCA or as process-LCA (Heijungs et al., 2022). In this study the focus is on process-LCA where applying IOA methods has traditionally been challenging or impossible (Heijungs et al., 2022; Suh & Heijungs, 2007), we also shortly discuss their differences in SI 1.1. We refer to Heijungs & Suh (2002) for an extensive introduction to the mathematical background of LCA and van der Meide et al. (2025) for a more extensive treatment of CA in LCA.

We start with the known information; $\boldsymbol{A}$, $\boldsymbol{B}$, $\boldsymbol{f}$ and $\boldsymbol{q}^T$. Here, $\boldsymbol{A}$ is the technology matrix, $\boldsymbol{B}$ is the Elementary Flow (EF) matrix, $\boldsymbol{f}$ is the functional unit (FU) vector and $\boldsymbol{q}^T$ is the characterization vector.

The technology matrix $\boldsymbol{A}$ has processes as columns, with inputs (consumption) to that process as negative values and the produced product as a positive value for output. Each row in $\boldsymbol{A}$ shows how much of the product/service the given process produces is consumed in other processes. The EF matrix $\boldsymbol{B}$ shows which interventions each process causes as an EF in the environment as columns. It has the same amount of columns as $\boldsymbol{A}$.

First, a scaling vector $\boldsymbol{s}$ is calculated, this represents how many times each process needs to produce its product to fulfil the FU expressed by $\boldsymbol{f}$:

$$\boldsymbol{f} = \boldsymbol{A}\,\boldsymbol{s} \;\rightarrow\; \boldsymbol{s} = \boldsymbol{A}^{-1}\,\boldsymbol{f} \tag{1}$$

Next, $\boldsymbol{B}$ and $\boldsymbol{s}$ can be multiplied to calculate the inventory results vector $\boldsymbol{g}$, which shows all EFs emitted or consumed to fulfill the FU $\boldsymbol{f}$:

$$\boldsymbol{g} = \boldsymbol{B}\,\boldsymbol{s} \tag{2}$$

Finally, the inventory results vector is characterized to a characterized result h by multiplying by the characterization vector $\boldsymbol{q}$:

$$h = \boldsymbol{q}^T\,\boldsymbol{g} \tag{3}$$

Or:

$$h = \boldsymbol{q}^T\,\boldsymbol{B}\,\boldsymbol{A}^{-1}\,\boldsymbol{f} \tag{4}$$

As the results from eq. (2) and (3) only show one characterized result for every FU and every impact category, these don't show any insights into what processes or EFs contribute to the total result. These results can be disaggregated to show which process causes each EF for the given FU, turning the inventory into a contribution matrix $\boldsymbol{g} \rightarrow \boldsymbol{G}$ (Srocka & Montiel, 2021).

To calculate the contribution matrix, the $\boldsymbol{s}$ and $\boldsymbol{q}$ vector are diagonalized. Diagonalizing means putting the values of the respective vector on the diagonal of a square $\mathbf{0}$ matrix of the same size.

This leads to adjustments of eq. (2) and (3) below:

$$\boldsymbol{G} = \boldsymbol{B}\, diag(\boldsymbol{s}) \tag{5}$$
$$\boldsymbol{H} = diag(\boldsymbol{q})\ \boldsymbol{G} \tag{6}$$

Through the above adjustment, $\boldsymbol{G}$ and $\boldsymbol{H}$ become matrices with a value ($\boldsymbol{g}$ for inventory or h for characterized results) for each process as a column and each EF as a row.

3.2.3. Example case

We demonstrate HEM in LCA based on a simple case study example of four processes; coal mining, electricity production, iron ore mining and steel production. We show the system in Figure 3.1 and define the inventory of these processes in Table 3.1. We use this simplified example system to demonstrate the principles of HEM in LCA, show example results and compare similar approaches to HEM using this example system. We will focus primarily on the production of '1kg steel' as FU, it will be make clear in instances where this is not the case. As an impact category, we use climate change (GWP 100) from the IPCC (2022), characterizing CO_2 emissions as 1 $kgCO_{2eq.}$/kg and CH_4 emissions as 29.8 $kgCO_{2eq.}$/kg.

We strongly emphasize that this example is exclusively for the demonstration of HEM and is not meant to represent reality nor to assess the actual impact of processes within this system.

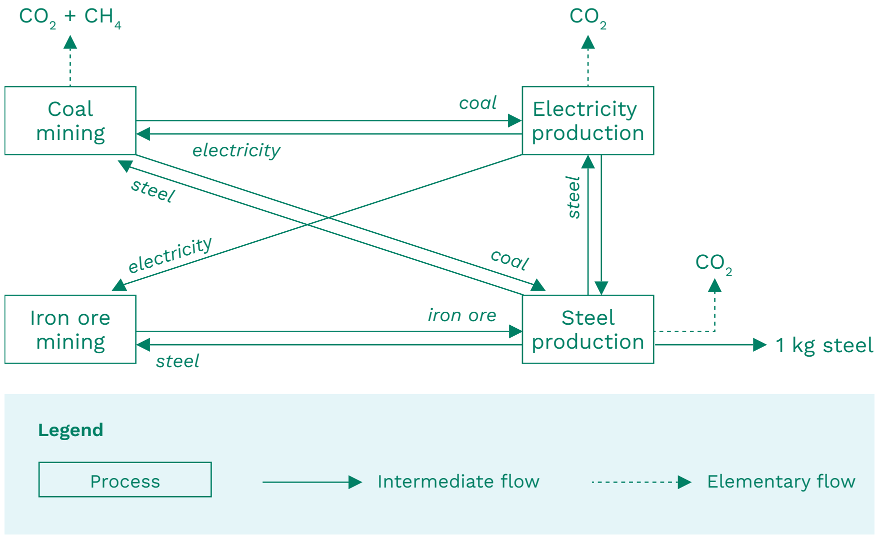


Figure 3.1 - Product system for the example case study.

Process name	Functional flow (Product/Service)	Intermediate flows	Elementary flows
Coal mining	Coal: 1 kg	Electricity: 0.04 kWh Steel: 0.001 kg	CO_2: 0.05 kg CH_4: 0.01 kg
Electricity production	Electricity: 1 kWh	Coal: 0.4 kg Steel: 0.001 kg	CO_2: 0.8 kg
Iron ore mining	Iron ore: 1 kg	Electricity: 0.1 kWh Steel 0.001 kg	
Steel production	Steel: 1 kg	Coal: 0.8 kg Iron ore: 2 kg	CO_2: 1.6 kg

Table 3.1 - Inventory table for the example case study, showing functional flow, intermediate flows and EF per process.

Based on Table 3.1 above, we get the following technology matrix $\boldsymbol{A}$, EF matrix $\boldsymbol{B}$ and characterization vector $\boldsymbol{q}^T$ from the description above:

$$\boldsymbol{A} = \begin{bmatrix} 1 & -0.4 & 0 & -0.8 \\ -0.04 & 1 & -0.1 & 0 \\ 0 & 0 & 1 & -2 \\ -0.001 & -0.001 & -0.001 & 1 \end{bmatrix} \quad \boldsymbol{B} = \begin{bmatrix} 0.01 & 0 & 0 & 0 \\ 0.05 & 0.8 & 0 & 1.6 \end{bmatrix} \quad \boldsymbol{q}^T = \begin{bmatrix} 29.8 \\ 1 \end{bmatrix}$$

Where the rows/columns from the top/left in technology matrix $\boldsymbol{A}$ are ‘Coal mining’, ‘Electricity Production’, ‘Iron ore mining’ and ‘Steel production’. For the EF matrix $\boldsymbol{B}$ and characterization vector $\boldsymbol{q}^T$, we first list CH_4 and then CO_2.

3.2.4. Applying HEM to LCA

In general the steps of applying HEM in IOA is that a counterfactual (hypothetical) scenario is created where one or more target sectors are removed (extracted) and results are re-calculated without for the *‘remaining’* sectors. The difference between the *original* result and the *remaining* result is the effect from the extracted *target* sector.

The goal of HEM in IOA is to assess the effect of a sector on other sectors in a final result can be translated to the context of LCA. Here, the goal becomes ‘assessing the contribution a process (or group of processes) has on the final result from the FU’. We develop HEM in LCA further with this goal in mind. As the mathematical structure differs, our approach is slightly different as well.

To apply HEM to LCA, we need to take 4 steps:

1. Define an HEM scenario
2. Extract the processes
3. Calculate the results for the *original* and *remaining* system
4. Calculate the results for the *target* processes

In the further text, in all cases that could apply to one or multiple processes, we will refer to this as ‘processes’ in plural for brevity. In specific instances where only one or the other is meant, it will be made clear.

We emphasize that the 'H' in HEM stands for Hypothetical, meaning that we do not truly assume that the *target* processes would suddenly 'not exist', the extraction is rather a tool to assess the contribution of the *target* and/or *remaining* processes to the total result.

All information to replicate this approach conceptually or in small product-systems can be found in this article and its SI, the code make use of this approach or to replicate it using Brightway2 (Mutel, 2017a) on real-world systems is provided in van der Meide (2025a).

HEM scenario definition

First, the practitioner must choose *target* processes to extract. The *target* processes can be any set of processes of interest for the question the practitioner is trying to answer. This grouping can be based on the process metadata (information describing the process, like name, product, location or an industry sector (e.g. as given in ecoinvent metadata (Wernet et al., 2016)). The processes should have some relationship to each other that makes them relevant to extract together. For example, a practitioner could choose all ecoinvent processes with the Central Product Classification (CPC) (UN, 2015) Division '14: Metal ores' and they could assess the contribution of products classified as such to the final result. Another example could be, if the practitioner would choose all processes with the location 'NL' in an LCI database, the practitioner could assess the impact processes in the Netherlands have on the final result, mirroring the regional example Miller and Lahr (2001) give.

Extracting processes

After defining an HEM scenario, we calculate the scaling vector $\boldsymbol{s}$ (following eq. (1)) for the *original* system and the *remaining* system. As Miller and Lahr (2001) discuss, there are several options to extract sectors. In process-LCA, the list of options is more limited because we use a different mathematical model. The mathematical format of process-based LCA (Heijungs et al., 2022) makes it impossible to calculate results for any FU if the reference flow of any process is '0' (not producing anything), this reduces the amount of options we can use compared to Miller and Lahr (2001). We discuss this further in SI 1.2. Taking these limitations into account, the following four options in Table 3.2 are possible approaches to HEM in LCA with corresponding case numbers from Miller and Lahr (2001) for comparison.

Case	Description
1	Extracting the processes from the technology matrix, decreasing its size (deleting both the rows and columns).
2a	Extracting both *consumers* (row values) and *consumption* (column values) of the target processes, resulting in processes that are both un-used and 'empty' (replacing all process flow values except reference flow with 0).
3a	Extracting all *consumers* (row values) of the *target* processes in the technology matrix, resulting in processes that are un-used (replacing all process flows *from* this process with 0).
3b	Extracting all *consumption* (column values) of the *target* processes in the technology matrix, resulting in 'empty' processes (replacing all process flows to this process with 0).

Tabel 3.2 - Options to extract processes for HEM in LCA. The numbering of the cases is the same as in Miller and Lahr (2001)

While the first option (case 1) seems most intuitive, this first option could be potentially challenging as it changes the size of matrices, making it harder to keep consistent links between the *original* system and the HEM scenario for comparison later.

The second option (2a) may seem like a good option as it 'isolates' the processes and maintains the matrix sizes. Though making the extracted processes have 'no consumption' is not ideal as the *target* processes would always have '0' impact due to not consuming anything.

The third option (3a), would (similar to case 2a) also 'isolate' the processes. However, if one or more of the extracted processes in question is part of the FU, this would now still show what that process would consume from the *remaining* system (or from other extracted process), thus being a better representation for all processes that could be in the FU.

The last option (3b) would still 'isolate' the *target* processes, and remove their associated impacts to the system, this makes the results equivalent to option 2a in LCA. However, as explained with case 3a, this form of isolation would not be representative in case processes in the FU are part of the extracted processes.

We continue with option 3a as this allows for most interpretability of the system, and as we show later, can still differentiate between direct and indirect impacts from the extracted *target* processes by combining HEM with process CA. We demonstrate all four options further in SI 1.2 and show that all four cases give the same result in LCA if the FU does not contain the extracted process.

While in IOA the interest often lies in the technology matrix, in LCA, the interaction of the processes with the environment is very important to consider as well. This means that with HEM in LCA we also extract the EF matrix $\boldsymbol{B}$.

We show the extraction of 'electricity production' from our example system below. This gives us the *remaining* system $\boldsymbol{A}^*$ and $\boldsymbol{B}^*$, marked with a '*' to show these are changed. We also mark the changed items in yellow. Note here that we mirror the superscript notation for *remaining* and *target* systems (*, o) of Hertwich et al. (2024) for consistency:

Matrix - *Original* system

$$\boldsymbol{A} = \begin{bmatrix} 1 & -0.4 & 0 & -0.8 \\ -0.04 & 1 & -0.1 & 0 \\ 0 & 0 & 1 & -2 \\ -0.001 & -0.001 & -0.001 & 1 \end{bmatrix}$$

$$\boldsymbol{B} = \begin{bmatrix} 0.01 & 0 & 0 & 0 \\ 0.05 & 0.8 & 0 & 1.6 \end{bmatrix}$$

Matrix - *Remaining* system case 3a

$$\boldsymbol{A} = \begin{bmatrix} 1 & -0.4 & 0 & -0.8 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & -2 \\ -0.001 & -0.001 & -0.001 & 1 \end{bmatrix}$$

$$\boldsymbol{B} = \begin{bmatrix} 0.01 & 0 & 0 & 0 \\ 0.05 & 0 & 0 & 1.6 \end{bmatrix}$$

Results for the Original and Remaining system

With the extraction complete, the remaining scaling vector $\boldsymbol{s}^*$ can be calculated (following eq. (1) again) from the $\boldsymbol{A}^*$ technology matrix. Where $\boldsymbol{s}^*$ is a *partial* scaling vector of the FU for the *remaining* system. A partial scaling vector represents a partial fulfilment of the *original* FU, where all partial scaling vectors together fulfil the full FU (van der Meide et al., 2025).

We can calculate the inventory for both the *original* ($\boldsymbol{g}$) and *remaining* system ($\boldsymbol{g^*}$) with eq. (2). We can logically take this a step further to now calculate characterized results with eq. (3) for the *original* ($\boldsymbol{h}$) and *remaining* ($\boldsymbol{h^*}$) systems.

Results for the Target processes

So far, we have calculated results for the *remaining* processes (the hypothetical extraction), we take this a step further to find results for the *target* processes as well, which is the goal of HEM. As we discussed above, the scaling vector $\boldsymbol{s^*}$ is a partial scaling vector, making $\boldsymbol{g^*}$ the partial inventory. As our FU did not change, the difference between the partial inventory and the *original* inventory will caused by the extraction of the *target* processes. We can calculate the *target* inventory by subtracting the partial inventory $\boldsymbol{g^*}$ from the *original* inventory $\boldsymbol{g}$:

$$\boldsymbol{g^o} = \boldsymbol{g} - \boldsymbol{g^*} \tag{7}$$

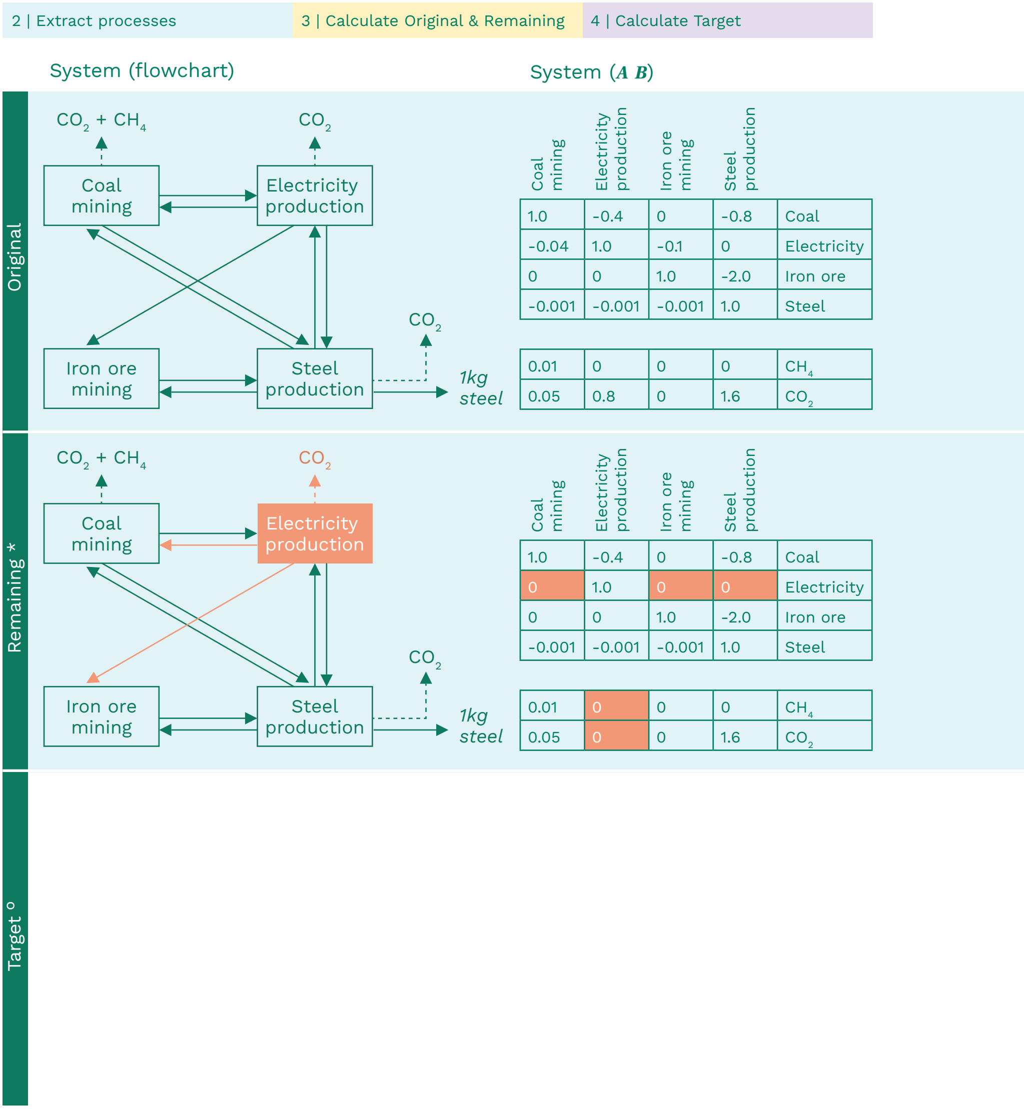
Note that eq. (7) can also be applied to a diagonalized instance of $\boldsymbol{g}$, as $\boldsymbol{G}$, this is shown in the example later. We can then calculate the characterized results $\boldsymbol{h^o}$ for the *target* as well by again using eq. (3).

In the context of HEM in LCA, the inventory and characterized results of the *target* system should be interpreted as the EFs or impact caused by the products or services provided by the *target* processes. This would include both the direct and indirect EFs or impacts. In other words, all the EFs that are caused to produce all intermediate flows of the *target* throughout the entire system (in the example, the CH_4 emitted to mine the coal to produce the electricity). The inventory and characterized results of the *remaining* system are from everything else. We show how this may be interpreted in the results section.

Following from eq. (7), if we sum the partial *target* and *remaining* inventory vectors, we still have the original inventory vector ($\boldsymbol{g} = \boldsymbol{g^*} + \boldsymbol{g^o}$). While this may seem trivial, it is important to note, as this does guarantee that this approach is not double (or under) counting. By splitting the inventory into two partial inventories, we can assess the contribution of both the extracted processes and the *remaining* system to the full result.

Alternatively, applying eq. (5) to $\boldsymbol{s}$ and $\boldsymbol{s^*}$ and then applying eq. (7) allows us to assess the contribution matrices of both the *target* processes and *remaining* system, as well as their characterized versions by applying eq. (6). These last steps allow us to assess contributions to the partial target processes and *remaining* system.

Finally, a careful reader may have noticed we do not apply eq. (7) to the scaling vector $\boldsymbol{s}$ but to the inventory $\boldsymbol{g}$. We do this as we also change



Original:

Coal mining	Electricity production	Iron ore mining	Steel production	
1.0	-0.4	0	-0.8	Coal
-0.04	1.0	-0.1	0	Electricity
0	0	1.0	-2.0	Iron ore
-0.001	-0.001	-0.001	1.0	Steel
0.01	0	0	0	CH_4
0.05	0.8	0	1.6	CO_2

Remaining *:

Coal mining	Electricity production	Iron ore mining	Steel production	
1.0	-0.4	0	-0.8	Coal
0	1.0	0	0	Electricity
0	0	1.0	-2.0	Iron ore
-0.001	-0.001	-0.001	1.0	Steel
0.01	0	0	0	CH_4
0.05	0	0	1.6	CO_2

Figure 3.2 - Graphical overview of calculation steps for HEM. First, processes are extracted (blue), next, the original and remaining system are calculated (yellow) and finally, the target is calculated (pink).

the EF matrix $\boldsymbol{B}$, which would affect the inventory independent of the scaling vector. This detail is discussed further in SI 1.4. We provide a visual overview of the last three steps in Figure 3.2.

Scaling vector ($\boldsymbol{S}$) | Inventory matrix ($\boldsymbol{G}$) | Characterization matrix ($\boldsymbol{H}$)

$\boldsymbol{s} = \boldsymbol{A}^{-1}\boldsymbol{f}$

0.9	Coal mining
0.24	Electricity production
2.0063	Iron ore mining
1.0031	Steel production

$\boldsymbol{G} = \boldsymbol{B}\,diag\,(\boldsymbol{s})$

Coal mining	Electricity production	Iron ore mining	Steel production	
0.009	0	0	0	CH_4
0.045	0.189	0	1.605	CO_2

$\boldsymbol{H} = diag\,(\boldsymbol{q}^T) * \boldsymbol{G}$

Coal mining	Electricity production	Iron ore mining	Steel production	
0.267	0	0	0	CO_2eq
0.045	0.189	0	1.605	CO_2eq

$\Sigma \boldsymbol{H} = 2.106$ kg CO_2eq

$\boldsymbol{s}^* = \boldsymbol{A}^{*-1}\boldsymbol{f}$

0.8	Coal mining
0	Electricity production
2.0056	Iron ore mining
1.0028	Steel production

$\boldsymbol{G}^* = \boldsymbol{B}^*\,diag\,(\boldsymbol{s}^*)$

Coal mining	Electricity production	Iron ore mining	Steel production	
0.008	0	0	0	CH_4
0.04	0	0	1.604	CO_2

$\boldsymbol{H}^* = diag\,(\boldsymbol{q}^T) * \boldsymbol{G}^*$

Coal mining	Electricity production	Iron ore mining	Steel production	
0.239	0	0	0	CO_2eq
0.04	0	0	1.604	CO_2eq

$\Sigma \boldsymbol{H}^* = 1.883$ kg CO_2eq (89.4%)

$\boldsymbol{G}^{\circ} = \boldsymbol{G} - \boldsymbol{G}^*$

Coal mining	Electricity production	Iron ore mining	Steel production	
0.001	0	0	0	CH_4
0.005	0.189	0	0.001	CO_2

$\boldsymbol{H}^{\circ} = diag\,(\boldsymbol{q}^T) * \boldsymbol{G}^{\circ}$

Coal mining	Electricity production	Iron ore mining	Steel production	
0.028	0	0	0	CO_2eq
0.005	0.189	0	0.001	CO_2eq

$\Sigma \boldsymbol{H}^{\circ} = 0.223$ kg CO_2eq (10.6%)

3.3 Results

3.3.1 Interpreting HEM results

For our example case, we extract the *target* process 'electricity production' as shown in the method and calculate the results for a FU of '1kg steel'.

We calculate the following scaling vectors from equation (1). Note that values are rounded:

$$\boldsymbol{S}^T = \begin{bmatrix} 0.9 & 0.24 & 2.\,.. & 1.\,.. \end{bmatrix} \qquad \boldsymbol{S}^{*\,T} = \begin{bmatrix} 0.8 & 0 & 2.\,.. & 1.\,.. \end{bmatrix}$$

Based on these scaling vectors, we calculate the following LCI from eqs. (5) and (7) and characterized contribution matrices with eq. (6):

$$\boldsymbol{G} = \begin{bmatrix} 0.009 & 0 & 0 & 0 \\ 0.045 & 0.189 & 0 & 1.605 \end{bmatrix} \qquad \boldsymbol{H} = \begin{bmatrix} 0.267 & 0 & 0 & 0 \\ 0.045 & 0.189 & 0 & 1.605 \end{bmatrix}$$

$$\boldsymbol{G}^{*} = \begin{bmatrix} 0.008 & 0 & 0 & 0 \\ 0.04 & 0.189 & 0 & 1.604 \end{bmatrix} \qquad \boldsymbol{H}^{*} = \begin{bmatrix} 0.239 & 0 & 0 & 0 \\ 0.04 & 0 & 0 & 1.604 \end{bmatrix}$$

$$\boldsymbol{G}^{o} = \begin{bmatrix} 0.001 & 0 & 0 & 0 \\ 0.005 & 0.189 & 0 & 0.001 \end{bmatrix} \qquad \boldsymbol{H}^{o} = \begin{bmatrix} 0.028 & 0 & 0 & 0 \\ 0.005 & 0.189 & 0 & 0.001 \end{bmatrix}$$

Note again that as $\boldsymbol{G}^*$, $\boldsymbol{G}^o$ and $\boldsymbol{H}^*$, $\boldsymbol{H}^o$ are partial results, they sum to the total result $\boldsymbol{G}$ and $\boldsymbol{H}$ respectively. The results above are rounded, the full results are available in SI 2.1.

As $\boldsymbol{G}^o$ represents the partial inventory of the *target* processes, it does not just represent the direct, but also indirect elementary flows of processes in the system. This is because we 'extracted' not only the production of electricity, but also all production (coal, steel, iron ore for the steel etc.) needed for the production of that electricity, thus also including indirect impacts.

In HEM, the *target* processes never contribute to the *remaining* impact, but the *remaining* processes can contribute to the *target* impact. We show the results for the *target* and *remaining* system and the direct contributions to both in Figure 3.3 A. Here, we can see that the HEM *target* 'electricity' is contributing 10.58% of the impact to climate change to steel. In the first row of Table 3.3 we see this contribution is made up of both 8.98% direct contribution for 'electricity production', as well from indirect contributions from 'coal mining' and 'steel production' needed to produce that electricity. For the *remaining* system, the contributions are from 'coal mining' and 'steel production' without any contribution from 'electricity production'.

	Electricity production/ Electricity	Coal mining	Steel production	Connector	Total
HEM Target	8.98%	1.57%	0.03%		10.58%
Electricity life cycle stage	8.96%	1.56%	0.01%		10.52%
Path (electricity)	8.84%	1.71%	0.02%		10.58%
Causer/Connector	8.98%		1.74%	10.72%	

Tabel 3.3 - Direct and Indirect contribution results of 'electricity' or 'electricity production' for 'steel production'. Percentages have been rounded to 2 digits to show differences, complete results are available in SI 2.1.

Example case: Comparison of HEM to other Contribution Analysis approaches

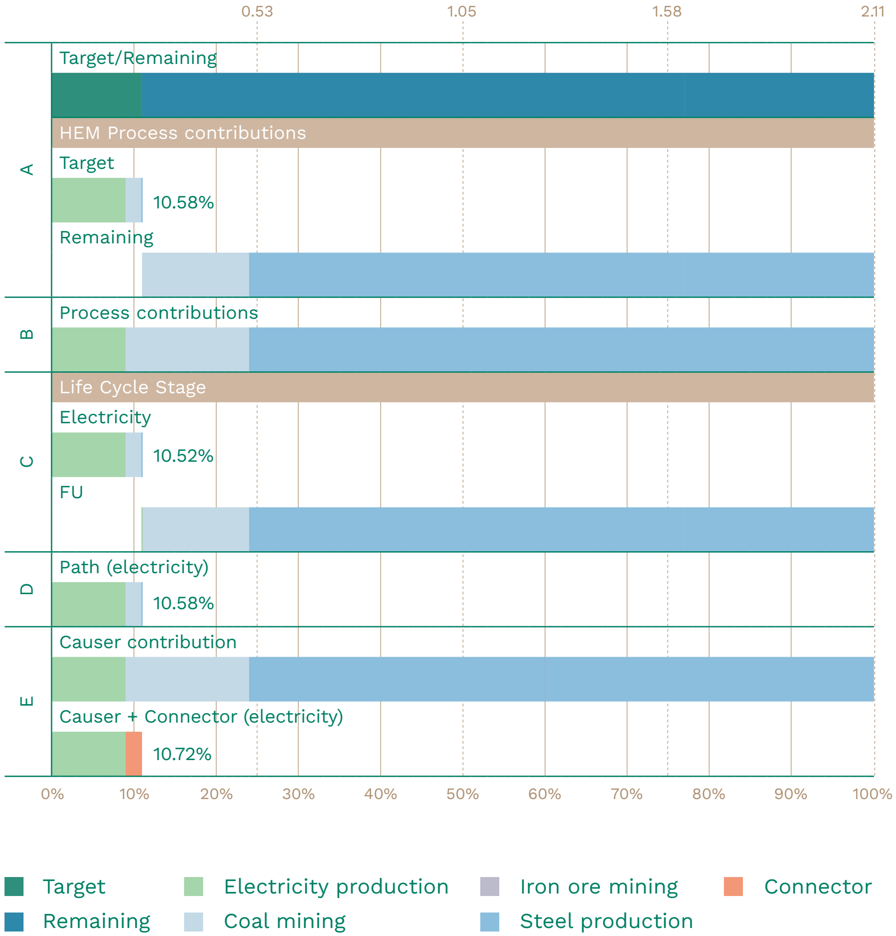


Figure 3.3 - Contribution Analysis results for different approaches for the production of 1kg steel and the extraction/contribution of 'electricity'. Top numbers are the climate change impact in kgCO_2eq., the bottom numbers are in percentage contribution. ***A*** *Contribution of both the target processes and remaining system. Also showing the process contributions to the target and remaining system.* ***B*** *Process contributions.* ***C*** *Process contributions to Life Cycle Stages.* ***D*** *Path contributions at 'electricity production'.* ***E*** *Causer and Connector contributions for 'electricity production'. Note that causer contributions are the same as process contributions.*

Extracting the Functional Unit
It could happen in an analysis that the practitioner wants to extract the processes that provide the FU. With case 3a we use for the extraction, this is possible. We demonstrate this with the example system by now taking '1kWh of Electricity' as a FU.

Intuitively one may assume that the contribution would just be 100%, as the extracted process is causing 100% of its direct and indirect contribution. However, the results show a different picture when using case 3a (though we do find the assumed 100% contribution when using the other extraction cases). Through the extraction of the direct impacts (in $\boldsymbol{B}^*$) and consumption of electricity by the other processes (in $\boldsymbol{A}^*$), we have created a situation where our *remaining* system contribution would show the impact of everything *needed* for the production of electricity, except for the electricity itself. The *target* would now show the direct contribution of 'Electricity production' and the indirect contribution of all electricity that would be consumed in the system to produce that electricity. Extracting the FU is the only instance where case 3a is different from cases 2a and 3b in terms of results. We discuss this further and show results for this in SI 1.3 and show results for all cases where the FU is extracted in SI 2.3.

3.3.2 Comparison with other approaches

For our comparison with other approaches, we extract 'electricity production' and use '1kg Steel' as FU. Full results are presented in SI 2.1.

Process contributions
When comparing HEM results against direct process contributions (Figure 3.3 B), we see that applying HEM to 'electricity production' not only accounts for the direct, but also indirect impacts of electricity production.

Life Cycle Stage Contribution Analysis
For the Life Cycle Stage contributions (van der Meide et al., 2025), we assume a life cycle stage consisting of the process 'electricity production' only. We show the process contributions to the life cycle stage and remainder of the system in Figure 3.3 C. We note the total impact is still the same (no double counting) but that the contribution of the life cycle stage is lower. The exact differences *within* the life cycle stage

are shown in Table 3.3. The difference with HEM is because the partial-FU of the life cycle stage only considers the direct use of electricity for the production of the FU. Other 'indirect' use, e.g. the electricity needed to produce coal to produce electricity is excluded. This is an important conceptual difference between HEM and Life Cycle Stage contributions, where HEM completely 'isolates' the processes through 'extraction' and Life Cycle Stage contributions instead consider direct use for the FU only.

Path Contribution Analysis
For Path contributions (Srocka & Montiel, 2021), the impact of 'Electricity' (Figure 3.3 D) is the same compared to HEM. In this case, we see that a lower contribution is attributed to 'Electricity production', while a higher contribution is attributed to 'Coal mining' in Table 3.3. Through the extraction of processes, HEM effectively breaks infinite loops between processes (e.g. coal is needed to produce electricity and electricity is needed to produce coal), where Path contributions does not, which leads to different attributions of contribution. As shown in Table 3.3, the contribution from 'Electricity production' is lower than the direct process contribution of the same process, we discuss this in more detail in SI 1.6.

As long as a singular process is extracted, the total result will be the same, however, when multiple processes are extracted, results may differ, as these could (indirectly) affect each other, this would lead to double counting in Path contributions. We discuss this in some more detail in SI 1.6.

Causer and Connector Contribution Analysis
Causer and Connector contributions (Reinhard et al., 2016) are more useful for systematic analysis of databases than 'regular' CA, but here we use this approach to assess the contributions of electricity production. We find two major differences compared to HEM: Firstly, we find higher contributions compared to HEM (Figure 3.3 E). Secondly we find only the aggregated contribution for 'connector' (indirect contributions), without any possible disaggregation of the processes that are in this group, which may not be ideal in CA.

While the direct contributions are the same (given that the FU amount is the same as the amount of product produced by that process), the indirect contributions are higher. Reinhard et al. (2016) point to double counting of their method for connector contributions, while they did not consider this a major issue for their specific use case, double counting should be avoided in CA.

3.3.3 Applying HEM using ecoinvent

Having demonstrated this approach to a small example, we now demonstrate HEM with a simple (but much larger) example using ecoinvent v3.11 (Wernet et al., 2016). The code for this example is available at (M. van der Meide, 2025a). We show the contribution of mining processes to the production of copper. As a Functional unit, we use 1 kg of 'copper cathode' from 'Market for copper, cathode, GLO'. We extract processes based on metadata, we use the CPC classification '14: Metal ores' (and processes with underlying classifications). All processes with this classification are extracted. To assess climate change impact, we use the GWP 100 method from the IPCC (2022).

Applying HEM to this example, we find the results in Figure 3.4 A. Here, we see that the *target* 'mining' contributes about 39% of the impact. To gain further insight, we then assess the process group contributions to both the *target* and *remaining* groups, grouping the processes by the reference product names. This shows us that both the *target* and *remaining* sectors are heavily affected by contributions from 'electricity', though the production of this electricity may happen in entirely different locations for the *target* and *remaining* systems.

We now compare HEM to grouped process contributions. The process group contributions only show the direct contributions. In Figure 3.4 B we have two groups; the processes in the *target* and *remaining* groups. Here, we find that the *target* 'mining' has almost no direct contribution. In Figure 3.4 C we also compare against the three main process groups and a remainder, grouped based on reference product. Here we find no mining processes. This shows us that while considering direct contributions may show *sources* of contributions, indirect contributions can show how these contributions connect to the FU (Reinhard et al., 2016).

From these results, a producer of copper may conclude that while they may be able to switch to more sustainable sources of electricity for their production processes, a large part of the electricity related impacts come from mining.

Ecoinvent: Comparison of HEM to other Contribution Analysis approaches

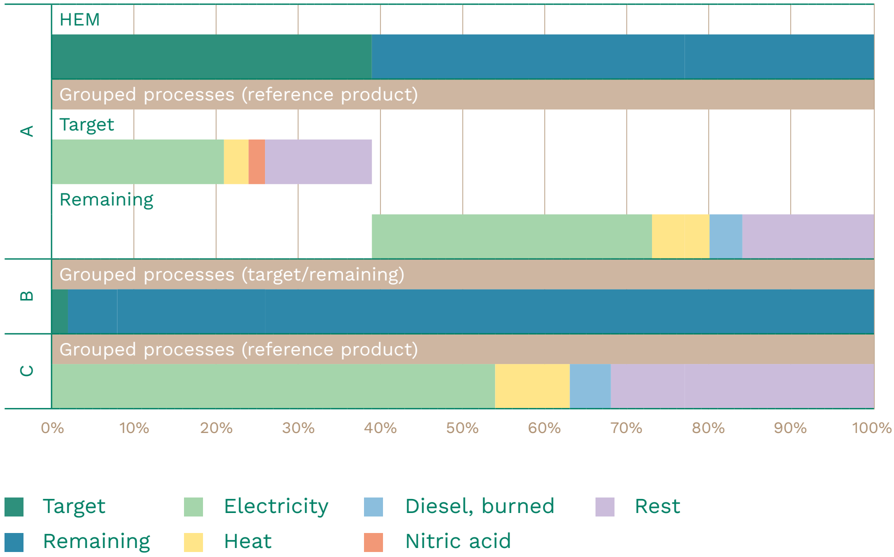


Figure 3.4 - Contribution Analysis results for different approaches for the production of 1kg 'copper, cathode' and the extraction/contribution of 'Metal, ores' in ecoinvent. The bottom numbers are in percentage contribution. ***A*** *Contribution of both the target processes and remaining system. Also showing the grouped process contributions to the target and remaining system. Grouped by reference product name, showing highest three contributing process groups and 'rest'.* ***B*** *Grouped process contributions, grouped by 'target' and 'remaining'.* ***C*** *Grouped process contributions, grouped by reference product name, showing highest three contributing process groups and 'rest'.*

Comparing approaches that show indirect contributions becomes more challenging in larger examples. Path Contributions can be calculated and are shown in SI 1.7. While calculating these results is easy, interpretation becomes complex as there are many production routes from 'ore' to the final product for the production of copper, some consisting of multiple processes in a chain. Combining these into a single 'minging' group is difficult due to interdependencies of these processes. For Life Cycle Stage contributions, we run into the same issue, where a life cycle stage would need to be defined for each production route, making this not only time consuming but also error-prone to ensure the life cycle stages don't overlap in this complex supply chain.

3.4 Discussion

Above, we have shown how HEM may be applied in LCA through: 1) defining a scenario, 2) extracting processes, 3) calculating results for the *original* and *remaining* system and 4) calculating results for the *target* processes. We have discussed interpretation of HEM results and have compared HEM against other CA approaches. That said, we want to emphasize that this should be considered as an additional approach for CA that may be useful in specific cases, not a replacement of existing ones.

The main advantage of HEM in LCA is that it allows practitioners to assess contributions of processes anywhere in the system, independent of their 'network' relationship between each other in the supply chain but also independent of their relationship to the FU. We have shown that this may be a useful approach when making use of large LCI databases and many processes may need to be assessed with our example using the ecoinvent LCI database (Wernet et al., 2016). Further uses could be to identify highly contributing sectors or countries, or this could be identifying suppliers or materials, that are important to a manufacturer.

3.4.1 Other applications for HEM

Another use-case of HEM may mirror that of Reinhard et al. (2016) where HEM can be used to systematically assess contributions from processes (or groups of processes) to other processes in an LCI database. These results could be used to prioritize database improvements while not double-counting impacts.

Furthermore, HEM could also be applied partially in two ways: 1) Reducing the 'extracted' amounts instead of completely removing them, making HEM this very similar to Sensitivity Analysis (Heijungs & Kleijn, 2001) (e.g. extracting half of the use of electricity). 2) Targeting the extraction of single uses of a product instead of all uses (e.g. the extraction of electricity use in coal mining), making the extraction more targeted. Both partial approaches may be useful, though the use-cases for this may be limited and it would be very important to carefully document what is extracted.

3.4.2 Comparison against other CA approaches

Life Cycle Stage CA bears a lot of similarity to HEM and both approaches avoid double counting, though the main difference is that HEM considers the use of all of the reference product from the *target* processes, where Life Cycle Stage CA only considers the direct use from the FU. Similarly, Path contributions are also close in results, though Path CA under-counts the contribution compared to process CA, implying that the contributions would be lower than they actually are.

As we have shown, both Life Cycle Stage CA and Path CA quickly become challenging to apply and interpret once many processes are involved. This use-case is where HEM becomes particularly useful; large systems and many *target* processes, especially if the direct 'supply chain' link between the FU and the *target* processes may be unclear.

Another comparison we made was with 'causer' and 'connector' contributions (Reinhard et al., 2016), here we find that we can calculate the same kind of results, but without double counting. Furthermore, HEM can apply this method to groups of processes, making it more useful for larger systems, where the contribution of a single process is likely to be low. Another advantage to HEM is that we are able to apply process contributions to the *remaining* system and *target* processes, allowing additional insight into results that was previously not possible.

One approach to HEM in LCA that we have not yet discussed but is technically similar is how Volkart et al. (2018) extract processes from their system to avoid double counting in a coupling of LCA with Partial Equilibrium models. While their stated goal is entirely different (avoiding double counting), they effectively use a similar approach (extracting processes similar to case 3a). Another difference is that we also explore the use of process contributions within the *remaining* system and *target* processes to gain more insight into results.

3.4.3 Limitations of HEM

CA is generally applied to answer one of two kinds of questions: 'What entities contribute to the total?' and 'What is the contribution of this entity to the total?'. The former is more an explorative question, while the latter is more an investigative question. While some approaches may be applied to answer both questions (Direct CA, First Tier CA, and Path CA), HEM and Life Cycle Stage CA are most useful for the last type of question, where the practitioner wants to gain deeper insight into a specific part of their model. This will limit the amount of use-cases HEM is relevant in LCA.

Furthermore, a main limitation is that there are currently no standard software tools to apply HEM in LCA for practitioners. That said, we do share the code we used to apply HEM in our ecoinvent example in van der Meide (2025a). This could be modified into a more generic software package in the future.

Next, one limitation that applies both to HEM and all other CA approaches; the usefulness of the approach will entirely depend on the quality of the data used and whether that is sufficient for the question at hand.

One more limitation comes when HEM in LCA is compared to HEM in IOA, in the latter, it is often used to analyze trade relationships, through extracting regions (Miller & Lahr, 2001). This use-case would be harder in process-LCA as such data is not well represented in LCI databases such as ecoinvent (Wernet et al., 2016). That said, especially since version 3.10, ecoinvent has included more trade information in every version, so it remains to be seen how much of a problem this will remain into the future.

Finally, changes to the technology matrix are made, this brings two possible questions. The first is on stability of results, when looking closely at each of the cases to implement HEM in LCA, it turns out each already has commonly used analogs in LCA and they pose no risk to calculations, as discussed further in SI 1.5. The second is on the computational load of re-calculating the scaling vector, one additional solution to the scaling vector needs to be found for each HEM calculation, which common LCA software such as Brightway2 (Mutel, 2017a) can do in well under a second, meaning doing that calculation twice should not be an issue. Lastly, more exotic approaches to LCA such as dynamic LCA have not been considered in this study, the interplay of such approaches to LCA and contribution analysis should be studied in more detail.

3.5 Conclusion

In this study we introduced HEM from IOA as a useful CA approach in LCA and have shown how HEM may provide different insights into LCA results compared to existing CA approaches. Through our demonstration of HEM in a simplified example and a larger example using ecoinvent (Wernet et al., 2016), we have shown how HEM can be used and what insights it can provide in LCA. By comparing against several established CA approaches we have shown how and when results are different and how this can help practitioners to gain insight into results.

As we have shown, this approach can help practitioners gain deeper understanding of impacts within their systems. The methodological connections between IOA and LCA should keep being investigated by both sides to keep improving both methods.

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Chapter 4

Effects of the energy transition on environmental impacts of cobalt supply: A prospective Life Cycle Assessment study on future supply of cobalt

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The Supplementary Information (SI) to this chapter is available at the website of the publisher.

Abstract

Cobalt is considered a key metal in the energy transition, and demand is expected to increase substantially by 2050. This demand is for an important part because of cobalt use in (electric vehicle) batteries. This study investigated the environmental impacts of the production of cobalt and how these could change in the future. We modeled possible future developments in the cobalt supply chain using four variables. v1) Ore grade, v2) Primary market shares, v3) Secondary market shares, v4) Energy transition. These variables are driven by two metal demand scenarios which we derived from scenarios from the Shared Socioeconomic Pathways, a 'Business as Usual' (BAU) and a 'Sustainable Development' (SD) scenario. We estimated future environmental impacts of cobalt supply by 2050 under these two scenarios using prospective Life Cycle Assessment. We found that the environmental impacts of cobalt production could likely increase and are strongly dependent on the recycling market share and the overall energy transition. The results showed that under the BAU scenario, climate change impacts per unit of cobalt production could increase by 9% by 2050 compared to 2010, while they decreased by 28% under the SD scenario. This comes at a trade-off to other impacts like human toxicity, which could strongly increase in the SD scenario (112% increase) compared to the BAU scenario (71% increase). Furthermore, we found that the energy transition could offset most of the increase of climate change impacts induced by a near doubling in cobalt demand in 2050 between the two scenarios.

4.1 Introduction

Although it is commonly acknowledged that the energy transition will substantially increase the demand for cobalt (Deetman et al., 2018; Harald Ulrik Sverdrup et al., 2017), it is so far unknown how such a rise of demand will affect the environmental performance of cobalt supply. Cobalt is a key metal for the energy transition as it is for electric vehicles, wind turbines and other power generation technologies (Cobalt Institute, 2015). Electric vehicles require batteries and magnets, wind power requires magnets and other power generation technologies require superalloys and magnets. The highest demand for cobalt is in electric vehicle batteries, which have seen strong growth in demand over recent decades (Cobalt Institute, 2015).

Deetman et al. (2018) expect a demand increase for cobalt of 10 to 20 times by 2050 compared to 2010 due to the energy transition. Other researchers also expect a substantial increase in cobalt demand in the coming decades although there is no consensus on magnitude (Junne et al., 2020; Harald Ulrik Sverdrup et al., 2017; Tisserant & Pauliuk, 2016; Xu et al., 2020).

Different geological sources of cobalt are used for supplying different cobalt-based materials or chemicals to different end-uses. Cobalt is primarily co-mined with two major metals: copper and nickel. Roughly 60% of cobalt, although exact numbers vary by year, is co-mined with copper, specifically from sediment-hosted copper deposits processed via hydrometallurgy, which is mostly used for battery production (British Geological Survey, 2019; United States Geological Survey, 2017c). 35-40% of cobalt is co-produced from processing of nickel laterite and nickel sulfide ores, with a growing share being from nickel laterite-based production (British Geological Survey, 2019; United States Geological Survey, 2017c). Nickel laterite ores are mostly mined in open pit mines, whereas nickel sulfide ores are often mined underground. The remaining share comes from minor sources, including pure cobalt and cobalt from platinum group metals production.

Given the increasing importance of cobalt, some studies assessed environmental impacts of products which contain cobalt, such as electric vehicles (Xu et al., 2020). A detailed Life Cycle Assessment (LCA) of cobalt production based on industry data was conducted by the

Cobalt Institute (2016), though much of the study remains confidential. The study did however consider cobalt as a co-product of other metals production and, therefore, the multifunctionality of the metal mining and production processes. Farjana et al. (2019) took a more theoretical approach. Their LCA study is based on data from the ecoinvent database (Wernet et al., 2016) and Nuss and Eckelman (2014). They assessed cobalt production as presented in ecoinvent, disregarding the multifunctional nature of cobalt production. While these studies provide some insight into current impacts, the potential environmental impact of future cobalt production is currently unknown.

The environmental impacts of metal production can be influenced by different factors, such as ore grades, market shares between different production technologies, technological efficiency improvements and the source of the energy supplied to production. The ore grade, i.e., the ratio of contained metal to total ore mass, influences the amount of ore that needs to be processed to produce one unit of metal. Ore grade is a well-known factor influencing environmental impacts of copper and nickel production (Calvo et al., 2016; Chapman & Roberts, 1983; Harpprecht et al., 2021; Norgate & Rankin, 2000; Northey et al., 2014; van der Voet et al., 2018). Market shares can be divided into production from virgin resources, known as primary production, and recycling, known as secondary production. The environmental performance of cobalt production (both primary and secondary) strongly depends on the production route, applied methods and technologies s (Harpprecht et al., 2021; Li et al., 2017; Norgate et al., 2007; van der Voet et al., 2018; Yang et al., 2014). Secondary production adds to these differences through large differences in production methods like pyrometallurgical and hydrometallurgical production (Harpprecht et al., 2021; van der Voet et al., 2018). While technological improvements were considered by Harprecht et al. (2021), the influence on environmental impacts was minor. A more external factor to production is the electricity supply. As revealed by previous studies, the electricity supply could considerably reduce GHG emissions of copper and nickel production (Harpprecht et al., 2021; Norgate & Rankin, 2000, 2002; Norgate et al., 2007) as well as of cobalt production (Cobalt Institute, 2016; Farjana et al., 2019). Harpprecht et al. (2021) also considered technological improvements to production, but this was found to have only a minor influence on environmental performance. Each of these variables could be affected by changes in demand, in part due to the energy transition. In addition, these variables depend on each other. These variables should thus be considered in conjunction, taking a systematic approach considering interdependencies. So far, this has not been studied for cobalt production.

Previous studies modeled most of these variables or scenarios for such variables, either for cobalt itself or for metals related to cobalt production. While scenarios for ore grade decline of copper and nickel have been addressed by Harpprecht et al (2021) and Northey et al. (2014), none currently exists for cobalt ore grades. Future market share projections for different cobalt production routes have also not been explored yet, although future demand has been estimated, e.g. by Deetman et al. (2018). Additionally, estimates for cobalt use by category and recycling rates exist (Harper et al., 2012; Sun et al., 2019). Finally, for future developments of electricity supply, LCI background datasets are available for future scenarios of electricity production (Mendoza Beltran et al., 2018).

An approach to consider scenarios for interlinked systems in LCA is the use of background scenarios. Background scenarios can be incorporated into a background database to create a future version of supply systems. This keeps interlinkages between systems and thus allows for environmental assessments of future, interdependent systems. Mendoza Beltran et al. (2018) developed a method to generate LCI databases that represent future scenarios for global electricity production from the Integrated Assessment Model (IAM) of IMAGE (Stehfest et al., 2014). These scenarios are based on the Shared Socioeconomic Pathways (SSPs) scenarios (O'Neill et al., 2014). From these future scenarios, they mapped production efficiencies, emissions, as well as market shares of electricity production technologies onto the ecoinvent database. Harpprecht et al. (2021) have built further on the approach of Mendoza Beltran et al. (2018) and developed background scenarios for metals production (copper, nickel zinc and lead).

The use of future backgrounds is ideally suited for prospective LCA, which was previously defined as an "...approach [that] studies future technological systems and their environmental implications" (Cucurachi et al., 2018). The further development of future background databases is considered an important development in making more accurate and reliable predictions of future environmental impacts in LCA (van der Giesen et al., 2020).

In this study, we aim to gain insight into the potential future environmental impacts of cobalt production. We develop background scenarios for key variables in the cobalt supply chain using metal demand as the driver, while adhering to the overall storylines of the SSP scenarios. We use the LCA results to identify production hotspots and conduct a sensitivity analysis for important variables. Furthermore, we calculate the potential total impact of cobalt production by considering cobalt demand increases. Finally, we compare our results to previous studies for cobalt production. The results are intended to be used as background scenarios of cobalt production in future prospective LCA studies.

4.2 Methods

This study presents a prospective LCA that models four key variables for cobalt production between 2010 and 2050 in five-year time steps:

1. 'Ore grade', leading to changes in energy and resource requirements
2. 'Primary production', market shares of primary production routes
3. 'Secondary production', market share of secondary production i.e. recycling
4. 'Energy transition', changes in the electricity supply

The modeling has been done in alignment with two SSP scenarios (O'Neill et al., 2014) which drive the changes in the above variables:

1. SSP2 'business as usual' is a scenario which is considered a likely pathway in terms of difficulty in mitigating and adapting to climate change.
2. SSP2-450 'sustainable development' assumes a successful reduction in emissions to limit global warming to 2oC by the end of the century.

The modeled variables were used as changes in the background LCA model for the supply of cobalt, which is described below.

4.2.1 Background LCA model of cobalt production

As shown in Figure 4.1, we represent the supply chain of cobalt through the three principal primary production routes and two methods of recycling. We based our model on the ecoinvent v3.6 cut-off database

(Wernet et al., 2016). The three primary production routes were based on existing processes in ecoinvent: hydrometallurgical production of copper, production of nickel sulphide and production of ferronickel from nickel laterite, which are also shown in SI-1. For the production of nickel from nickel laterite, we developed an additional process 'Cobalt production from nickel laterite' to represent the refining of cobalt. Secondary production of cobalt is based on the original ecoinvent processes.

The market for cobalt was modeled by adding the three primary production routes to the existing 'market for cobalt' process. The two original sources of cobalt to the market were maintained, their market shares were fixed at 1.5% independent of other variables and other variables were not considered for these flows.

Cobalt is produced from the three production routes along with copper or nickel products. As these production systems produce multiple products, assigning impacts to any individual products requires the use of allocation to resolve the multi-functional nature of the production systems. A revenue-based allocation was conducted based on the ten-year (2006-2015) global average price and production data of the metals from the United States Geological Survey (2014, 2017a, 2017b, 2018). This led to an allocation factor of 19.1% for cobalt from copper and 4% for cobalt from nickel. Our allocation approach is explained in more detail in the SI-1, we also calculate and discuss mass-based allocation in our sensitivity analysis below.

As functional unit, we used 1 kg of cobalt metal. Four different origins were compared: each of the three primary production routes, and finally, the 'market for cobalt' considering market shares of the three main routes and recycling.

4.2.2 Scenarios

We modeled the future changes in cobalt production based on implementations of the policy scenarios 'business as usual' and 'sustainable development'. We used these scenarios as a representation of two policy directions.

As the production of cobalt is strongly related to the production of copper and nickel, we applied the primary copper and nickel demand from the Yale Major Metals (YMM) scenarios by Elshkaki et al. (2018). From the YMM scenarios, we matched the 'Market World' to our 'business as usual' scenario and the 'Equitability World' to our 'sustainable development' scenario. Demand for cobalt in various products was previously modeled in the IMAGE IAM (Stehfest et al., 2014) implementation of the SSP scenarios by Deetman et al. (2018). We used these estimates as the demand for cobalt. Finally, we used electricity production scenarios from Mendoza Beltran et al. (2018) based on the IMAGE implementation of the SSPs.

4.2.3 Variable 1: Ore grade

We used mined ore grade as a proxy for change in ore grade (Figure 4.2a). Considering the dependence of cobalt production on copper and nickel production, we used their respective future developments of ore grade as a proxy for future cobalt ore quality. A decline in ore quality means a higher energy and materials requirement to produce the same amount of metal.

Based on cumulative future demand of copper and nickel from Elshkaki et al. (2018), we modeled ore grade change through a regression model. Basing the model on cumulative demand allow us to distinguish between different metal demand scenarios. With the demand in each year, we derived the ore grade in each year for each demand scenario. Next, we used the results from the ore grade regression model as inputs for another regression model based on data from Calvo et al. (2016). This model estimates electricity and diesel requirements for mining based on ore grade, for open pit mining for copper and nickel laterite, and underground for nickel sulfide mining.

Energy requirements during the refining step of cobalt production do not seem to depend strongly on changes in ore grade (Harald Ulrik Sverdrup et al., 2017). This relationship diminishes as once a mineral concentrate is produced or the metal has been chemically extracted, the original ore has no direct bearing on downstream processing anymore. We thus assumed refining energy requirement to remain at 3.77 kWh/kg as an average of various sources (Åkre, 2008; Elsherief, 2003; Mulaudzi & Kotze, 2013; United States Geological Survey, 2011).

Finally, we linked the energy and ore grade models to exchanges in the

LCA unit processes. We did this by identifying each exchange as part of a category, like 'mining', or 'refining'. For the production of tailings during mining, tailings were linked to ore grade, e.g., a decline in ore grade from 1% to 0.95%, and therefore a relative decline of 5%, means a relative increase in tailings of 1/0.95 (i.e. 5.26% or from 100 kg to 105.26 kg). For the exchange of diesel use, diesel was linked directly to the modeled diesel requirement. For the exchange of electricity, it was linked directly to the modeled electricity requirement. Additionally, the static amount of electricity (3.77kWh/kg) required was also included on top to represent refining.

Next, other exchanges were linked. For this we mapped each exchange to two major production phases, 'mining/processing' or 'refining'. Each exchange mapped to 'mining/processing' was linked relatively to a change in electricity requirement, e.g., a relative increase in electricity requirement of 5% (from 1kWh/kg to 1.05 kWh/kg) means a relative increase in 'conveyor belt' of 5%, which would be used for transport at the mine and processing site. The recovery rate of cobalt was assumed at a fixed percentage for each source of cobalt. The implementation of this variable is explained in more detail in SI-1

4.2.4 Variables 2 and 3: Primary and secondary production

Each separate production route for producing cobalt has differences due to the use of different materials and technologies. The model is shown in Figure 4.2b. This leads to differences in their environmental performances. Variable 2 describes future market shares of different primary production routes, while variable 3 describes the secondary market shares.

Variables 2 and 3 are closely linked as cobalt consumption has a lagged effect on the amount of recycled cobalt available, as such, we modeled them together, while their effects could be assessed separately with our model. Tisserant and Pauliuk (2016) suggest that to better understand future environmental impacts of cobalt production, demand in end use categories should be modeled in combination with a database like ecoinvent. We used the future demand estimates for cobalt from Deetman et al. (2018). Although not all cobalt demand is covered in these categories, this is the only source with this level of detail. This demand is separated in different categories of material use, for which absolute quantities and market shares differ between the categories in the two scenarios.

Next, we required product lifetime and recycling rates to estimate potential quantities of recycled cobalt. We translated these use categories of Deetman et al. (2018) to categories from Sun et al. (2019), which provide estimates for such recycling data, this process is described in SI-1. Then, the cobalt demand in the new categories was used to derive the market shares of the different primary production routes (variable 2). The demand per category was further used together with lifetimes and recycling rates in a simple stock model. The stock model was used to find the production of secondary cobalt (variable 3) and is further described in SI-1. To combine variable 2 and 3, we subtract the supply of cobalt from secondary sources, as well as the supply of cobalt from the two unmodified ecoinvent processes (cobalt production, and cobalt from zinc) from the total demand to determine the market shares of primary production routes.

The resulting market shares for each of the production routes were linked to the LCA unit process of 'market for cobalt'.

4.2.5 Variable 4: Energy transition

The final variable 'energy transition' was included based on the study of Mendoza Beltran et al. (2018), which combined future scenarios from the IMAGE model (Stehfest et al., 2014) with the ecoinvent database to yield future scenario LCI databases. These future scenario LCI databases differ from the ecoinvent database in a number of aspects, including electricity production efficiency and related emissions, regional representation of electricity markets and the market shares of electricity producers. We used the SSP2 (RCP6) and SSP2-450 (RCP2.6) scenarios. The superstructure approach (Steubing & Koning, 2021) was used to practically calculate LCA results for the range of scenario LCI databases resulting from the work of Mendoza et al. (2018). Since the scenario databases based on Mendoza et al. were calculated in ten-year time steps and the resolution in our model was five-year time steps, we linearly interpolated LCI data from Mendoza et al. to obtain a five-year time step resolution. The output data from these scenarios is based on ten-year time steps, which we linearly interpolated to five-year time steps.

4.2.6 Combining variables and technical implementation

Nine different combinations of the variables described above are considered for both scenarios and analyze different kinds of interactions and effects:

1 Ore grade: Variable 1 only
2 Primary market shares: Variable 2 only
3 Market shares of primary and secondary production: Variables 2-3
4 All but the energy transition: Variables 1-3
5 The energy transition: Variable 4 only
6 - 9 Each of 1-4 including Variable 4

We modeled each variable in both scenarios using python. For the implementation of the unit processes and subsequent LCA we used the Brightway 2 (Mutel, 2017a) and wurst (Mutel, 2017b) software packages. The changes from each scenario were made through the super-structure approach (Steubing & Koning, 2021). All further analysis of the results was done in python. Each ecoinvent process used was altered following the scenario-variable-combination, starting in 2010. The full technical implementation is explained in the SI-1.

4.2.7 Sensitivity analysis

We performed a sensitivity analysis in which three modeling assumptions were altered individually. Additionally, we applied a mass-based allocation approach. All sensitivity approaches are described in more detail in SI-1.

First, we swapped our static energy requirement assumption for processing in variable 1 to one modeled with regression based on data from Sverdrup et al. (2017). Secondly, we used a different set of assumptions for cobalt-containing product categories, lifetimes and recycling rates to achieve a different set of market shares for primary and secondary production as a change for variable 2 and 3, based on data from Harper et al. (2012). Finally, we consider impacts from recycling processes differently. Instead of the 0% allocation to waste treatment co-products in the ecoinvent cutoff model (Wernet et al., 2016), we assumed a 'worst-case' 100% allocation. We made this assumption because of the high recycling rates of cobalt and to gain a better insight of the worst-case scenario of recycling impacts. For our sensitivity analysis on allocation, we applied mass based allocation based on the same ten-year production average described for the revenue-based allocation.

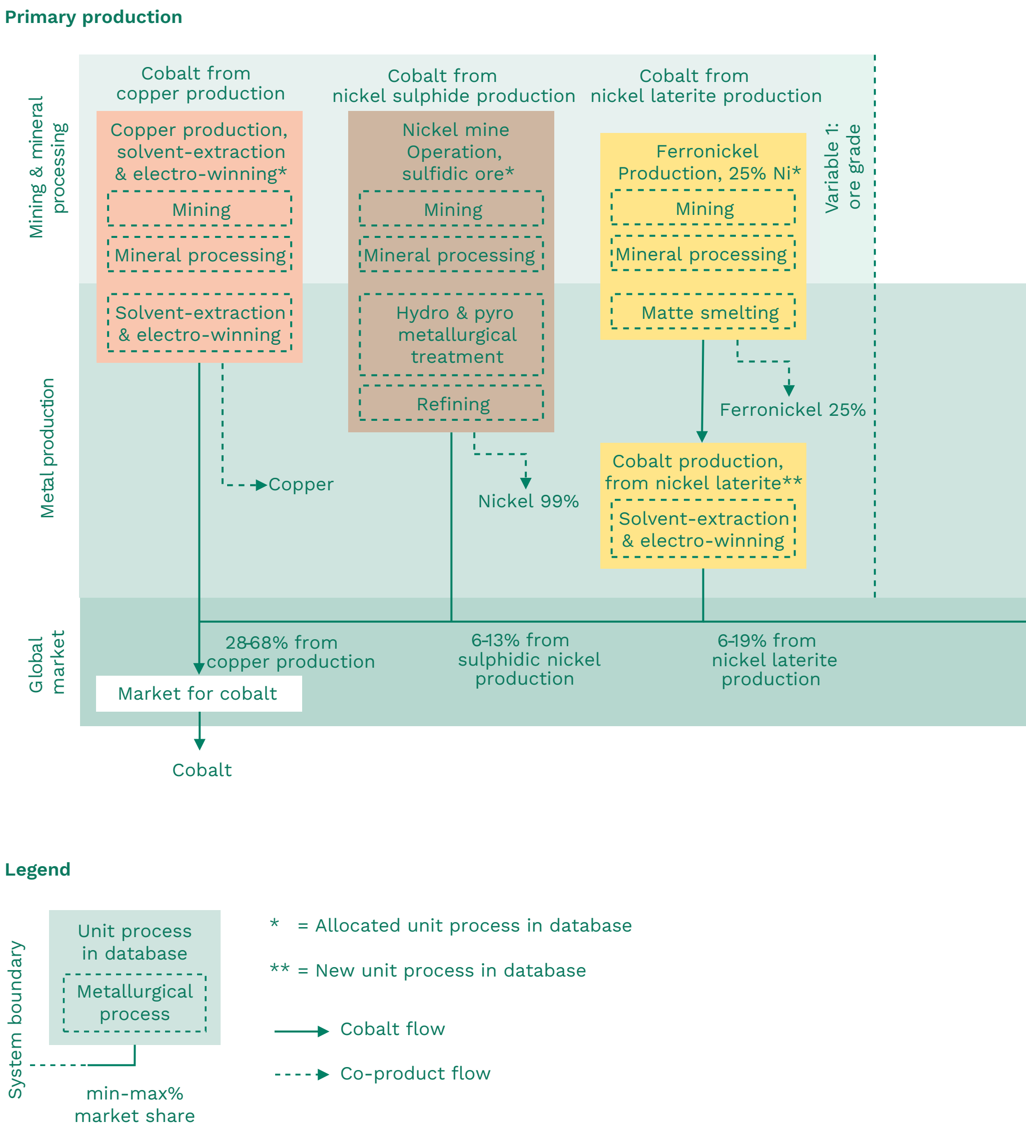
4.2.8 Impact assessment

We used six impact assessment methods:
1. Climate change (CC)
2. Fossil cumulative energy demand (CED)
3. Particulate matter formation (PMF)
4. Metal depletion (MDP)
5. Human toxicity (HTP)
6. Photochemical oxidant formation (POFP)

For CC, the IPCC 2013 (100a) method was used (IPCC, 2014), as with Mendoza Beltran et al., (2018) we considered biogenic carbon through altering the CC Characterization factors. For the other methods, the ReCiPe 2016 mid-point level methods were chosen (Huijbregts, 2016).

4.2.9 Total cobalt impacts

As a final step, we assessed the total impact of cobalt production. For this, we used the impact of cobalt from the 'market for cobalt' process per kg and multiplied it by the demand in each scenario in each year. We use this as an indication of the total environmental impact cobalt production could have up to 2050.


Primary production
Mining & mineral processing
Metal production
Global market
Cobalt from copper production
Cobalt from nickel sulphide production
Cobalt from nickel laterite production
Copper production, solvent-extraction & electro-winning*
Mining
Mineral processing
Solvent-extraction & electro-winning
Nickel mine Operation, sulfidic ore*
Mining
Mineral processing
Hydro & pyro metallurgical treatment
Refining
Ferronickel Production, 25% Ni*
Mining
Mineral processing
Matte smelting
Variable 1: ore grade
Ferronickel 25%
Copper
Nickel 99%
Cobalt production, from nickel laterite**
Solvent-extraction & electro-winning
28-68% from copper production
6-13% from sulphidic nickel production
6-19% from nickel laterite production
Market for cobalt
Cobalt
Legend
System boundary
Unit process in database
Metallurgical process
min-max% market share
* = Allocated unit process in database
** = New unit process in database
Cobalt flow
Co-product flow

Secondary production

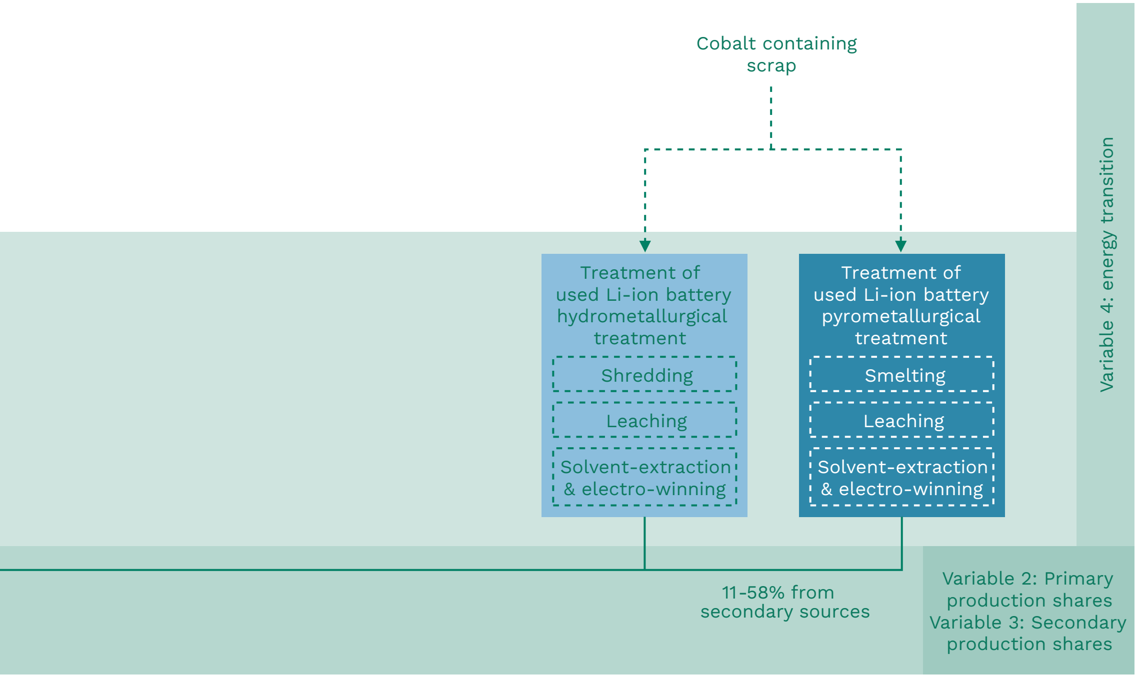
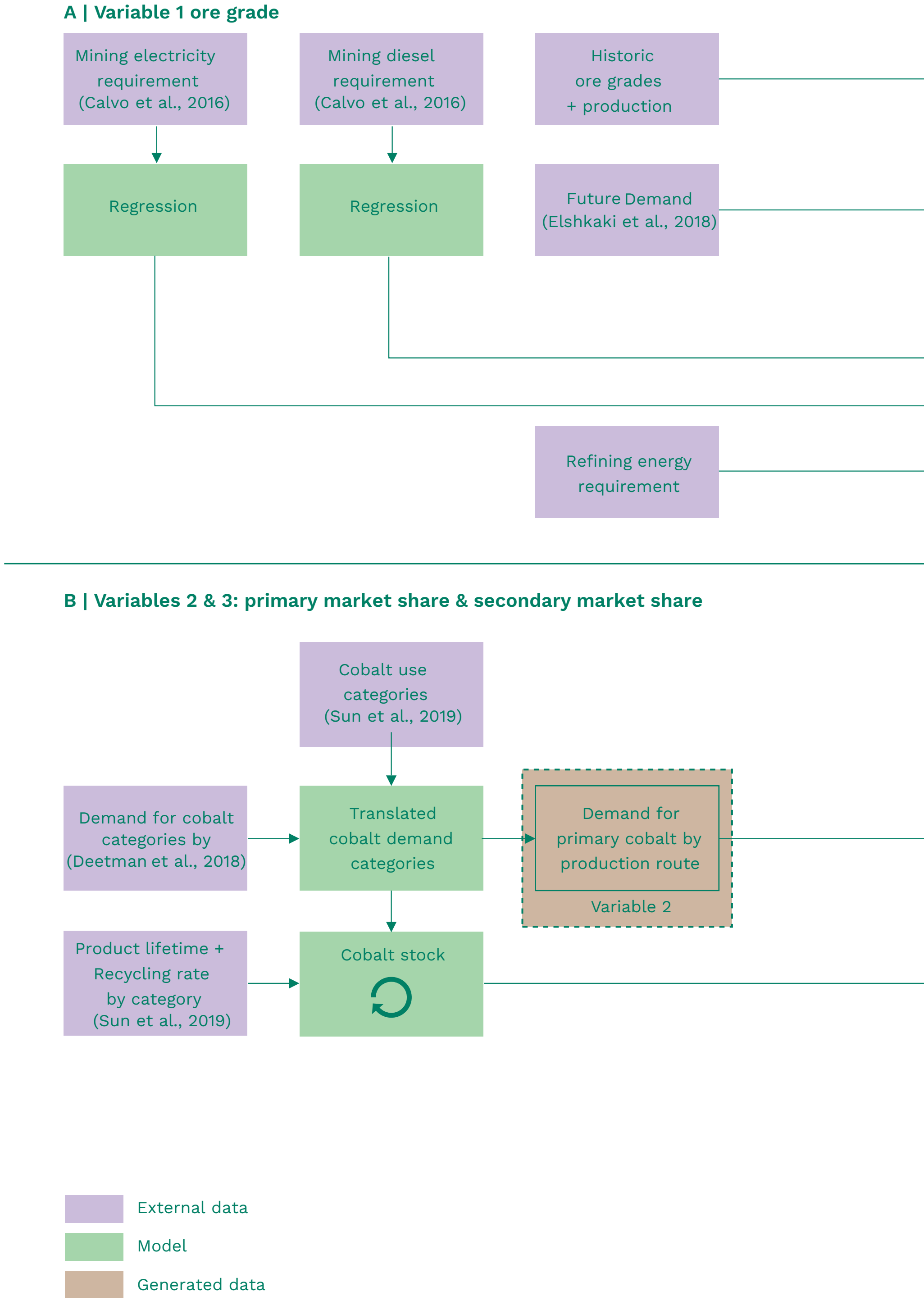
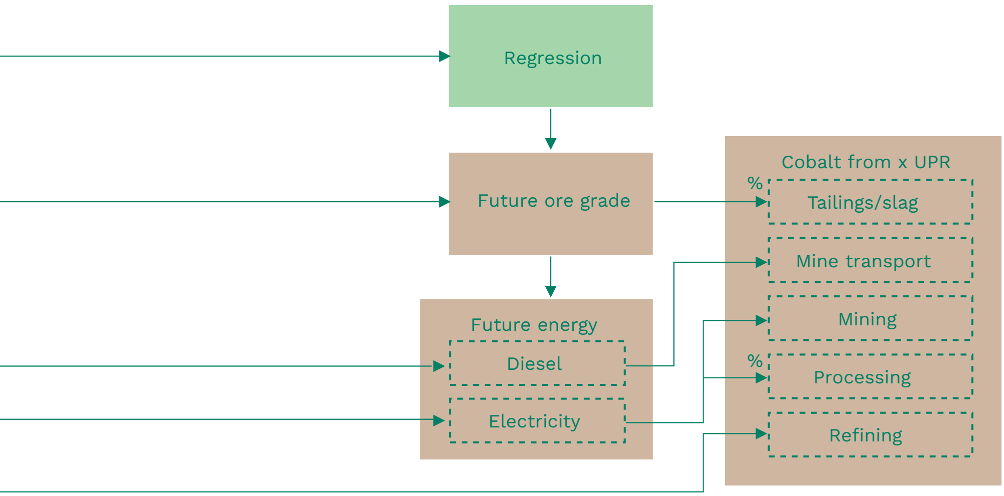


Figure 4.1 - Overview of the modeled LCI supply routes based on ecoinvent. Each of the three main primary supply routes and two secondary supply routes and their link to the 'Market for Cobalt' process are shown. The market shares refer to the modeled minimum and maximum market shares. All processes affected by a variable are shown within dotted lines.


A | Variable 1 ore grade
Mining electricity requirement (Calvo et al., 2016)
Mining diesel requirement (Calvo et al., 2016)
Historic ore grades + production
Regression
Regression
Future Demand (Elshkaki et al., 2018)
Refining energy requirement
B | Variables 2 & 3: primary market share & secondary market share
Cobalt use categories (Sun et al., 2019)
Demand for cobalt categories by (Deetman et al., 2018)
Translated cobalt demand categories
Demand for primary cobalt by production route
Variable 2
Product lifetime + Recycling rate by category (Sun et al., 2019)
Cobalt stock
External data
Model
Generated data



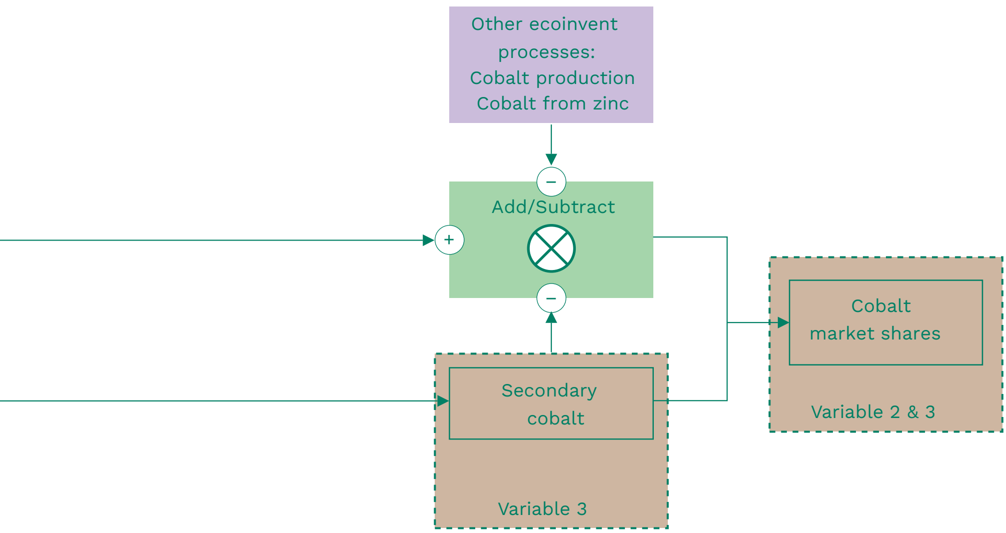


Figure 4.2 - Overview of variables 1-3. ***A*** *Variable 1. Based on historic ore grade and future demand, we modeled future ore grade, which we combined with mining electricity and diesel requirement to model future energy requirement. Which we used this to alter each exchange in a cobalt production process.* ***B*** *Variable 2 and 3. We converted demand for cobalt to different demand categories to both model primary demand routes (variable 2) and model cobalt stock with additional product lifetime and recycling rates data (variable 3). By combining primary and secondary cobalt supply, we finally modeled the combined market shares.*

4.3 Results

4.3.1 Variable models

Increases in demand for both copper and nickel lead to a decline in variable 1 (ore grade). More detailed results are of the variable changes are presented in SI-1. The change in ore grade is shown in Figure 4.3a-b. This decline is larger in 'sustainable development' scenario, caused by the higher demand for copper and nickel to enable the energy transition. For copper, the modeled ore grade declines from 0.55% to 0.35% and 0.33% in 2050 in the 'business as usual' scenario and 'sustainable development' scenario, respectively. For nickel the modeled ore grade declines from 0.8% to 0.49% and 0.45% in 2050 in the 'business as usual' scenario and 'sustainable development' scenario respectively.
The decline in modeled ore grade drives energy requirement up between 40% and 66% toward 2050, depending on the scenario, co-mined metal and mining method. Energy requirements are shown in Figure 4.3c-d. One exception to this is the diesel requirement for nickel sulfide, which is only modeled to increase between 19% and 23%. This is likely due to less diesel being used in underground mine transport.

The market shares for variable 2 and 3 (primary and secondary market shares) fluctuate over time, the total magnitude of demand increases substantially in both scenarios. The market shares are shown in Figure 4.3e-h. In both scenarios, around 2012-2015, there is a substantial increase in demand for electric vehicles (Deetman et al., 2018), which translates to an increase in demand for cobalt from copper. By 2020-2025 cobalt from recycled electric vehicle batteries becomes available for recycling, causing an increased share of secondary cobalt.

4.3.2 Life cycle impact assessment

The effects of each impact category and scenario-variable combination in 2050 relative to 2010 are shown in Figure 4.4. More detailed results are of the LCA results are presented in SI-1. Each variable modeled influences the long-term environmental impacts of cobalt production in different ways:

- Variable 1 (ore grade) increases the environmental impacts in 2050

for each production route and impact category. This illustrates the extent to which an increase in environmental impacts from just ore grade decline could be expected.
- Variable 2 (primary market shares) shows a minor decrease in PMF while having increases in the other five impact categories in 2050 in both scenarios.
- Variable 2 and 3 (primary and secondary market shares) show a slightly larger decrease in particulate matter for the 'business as usual' scenario and lower increases in the other five impact categories in 2050 compared to when only the primary market share is modelled. For the 'sustainable development' scenario, impacts in all six categories increase.
- Variable 1, 2 and 3 together show the strongest increases in impacts in the 'business as usual' scenario in 2050 for all but PMF, which is moderated slightly by the effects of the primary and secondary market. In the 'sustainable development' scenario, each impact category is substantially increased.
- Variable 4 (energy transition) leads to strong impact reductions for five impact categories, only MDP remains unchanged, as it is not affected by changing energy supply. The effects in the 'sustainable development' scenario are notably more positive for CC and fossil CED.

Variable 4, when paired with the other variable combinations becomes a balancing force in reducing the increasing impact effects of the other three variables. This balancing results in decreasing impact results in the 'business as usual' scenario for all but fossil CED. For the 'sustainable development' scenario, CC, fossil CED, and PMF decrease, while the other impact categories increase slightly.

4.3.3 Contribution analysis

In all scenario-variable combinations, electricity is the main driver for CC impacts. This remains the case, even in the best-case scenario, 'sustainable development' with only variable 4. This is shown in Figure 4.5. Fossil CED is caused for 35-40% by natural gas. In all scenario-variable combinations for PMF, cobalt and blasting (a mining activity) account for over 60% of impacts together. MDP impacts are split between concentrates and cobalt, accounting for >98% together in all cases. For HTP, tailings are responsible for >90% of impacts in all cases. Finally, POFP by blasting is responsible for >50% of impacts.

4.3.4. Cobalt production impacts over time

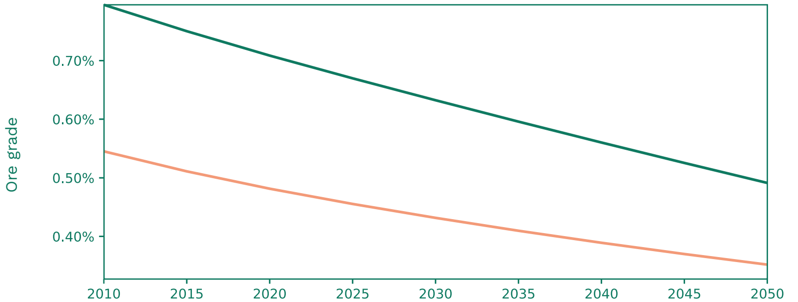
When considering the impacts from 2010 to 2050, other effects become visible, this is shown in Figure 4.6 for the ‘business as usual’ scenario. The impact-reducing effect of the secondary market share is most visible between 2010-2030, all impacts rapidly increase and decrease again, caused by the lack of secondary cobalt, as was also shown in Figure 4.3e-h. For variable 1, all impacts steadily increase over time.

For total impacts of cobalt production, we found that for CC and CED, the impacts depend heavily on the inclusion of Variable 4. As displayed in Figure 4.7, the substantial difference in cobalt demand between the two scenarios is not reflected in the environmental impact when considering the energy transition as growth in environmental impacts is decoupled from growth in demand. This decoupling would however come with a trade-off with the other impact categories studied, as also displayed in the figure. These other impact categories (PMF, MDP, HTP and POFP) have substantially higher impacts in the ‘Sustainable Development’ scenario. This could in large part be explained by the higher demand. It is also visible that the effects of the energy transition are substantially less pronounced in these impact categories.

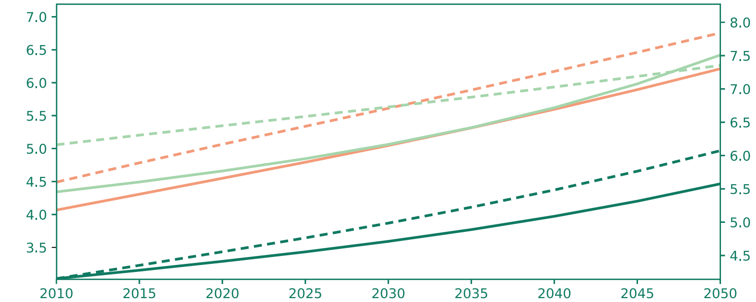
4.3.5 Sensitivity analysis

The adjustment of static processing of energy requirements for variable 1 to dynamic processing yields only very minor differences in total results. More detailed results are of the sensitivity analyses are presented in SI-1. These results are also presented in SI-1 The change in market shares in variables 2 and 3 yields decreased impacts in all six categories. This is primarily due to the estimation of a lower rate of cobalt recycling by Harper et al. (2012). When considering the 100% allocation to cobalt scenario for impacts of recycling on cobalt production, all impacts increase in the market for cobalt. With between 6.8% and 12.6% for CC, depending on the year. When combining the changed market shares and recycling impacts, final results are decreased in all six categories compared to the base line results. With between 2.7% and 29.8% for CC, depending on the year.

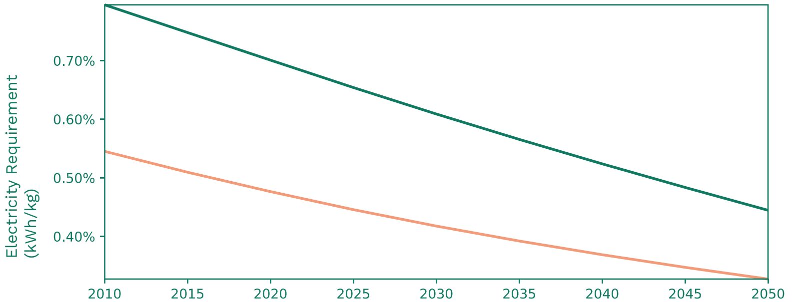
A | Modeled ore grade in the BAU scenario



B | Modeled ore grade in the SD scenario



C | Modeled Electricity and Diesel requirement in the BAU scenario



D | Modeled Electricity and Diesel requirement in the SD scenario

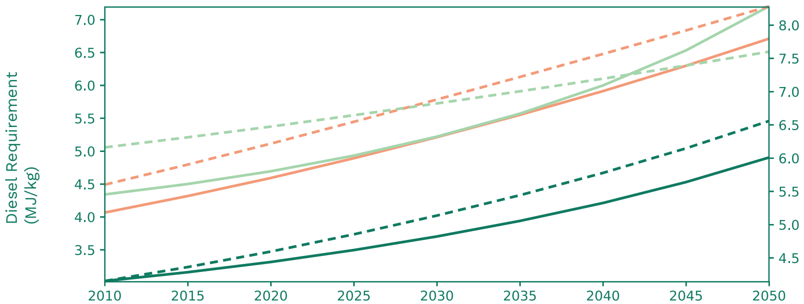


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*Figure 4.3 - **A-B** V1 ore grade in the 'Business as Usual' (BAU) scenario (A) and 'Sustainable development' (SD) scenario (B). **C-D** Electricity and diesel requirement for each source of metal for the BAU (C) and SD (D) scenarios. **E-H** Market shares of primary and secondary sources of cobalt for the BAU (E and G) and SD (F and H) scenarios. Note that the y axis in A-D does not start at 0. The data for this figure is available on a repository (van der Meide et al., 2021).*

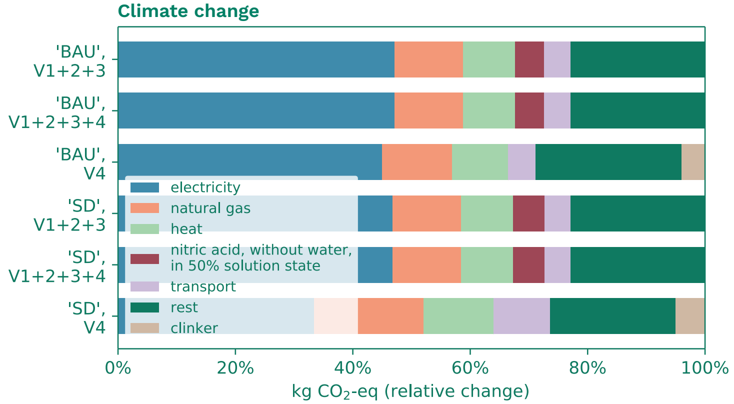
	Scenario	Variable	Climate change	Fossil cumulative energy demand	Particulate matter formation	Metal depletion	Human toxicity	Photochemical oxidant formation
Market for cobalt	BAU	V1	16%	14%	19%	7%	30%	32%
		V2	2%	2%	-4%	11%	32%	18%
		V2+3	1%	1%	-6%	10%	29%	16%
		V1+2+3	20%	18%	18%	19%	70%	58%
		V4	-10%	-17%	-3%	0%	1%	-4%
		V1+4	5%	-4%	16%	7%	31%	28%
		V2+4	-8%	-16%	-7%	11%	33%	13%
		V2+3+4	-9%	-17%	-8%	10%	30%	11%
		V1+2+3+4	9%	-1%	15%	19%	71%	54%
	SD	V1	19%	17%	23%	8%	35%	40%
		V2	2%	2%	-5%	13%	37%	20%
		V2+3	12%	10%	7%	21%	56%	36%
		V1+2+3	40%	36%	43%	34%	114%	101%
		V4	-53%	-50%	-15%	0%	-1%	-8%
		V1+4	-40%	-38%	7%	8%	33%	31%
		V2+4	-52%	-49%	-20%	13%	35%	12%
		V2+3+4	-47%	-44%	-8%	21%	55%	28%
		V1+2+3+4	-28%	-27%	24%	34%	112%	91%

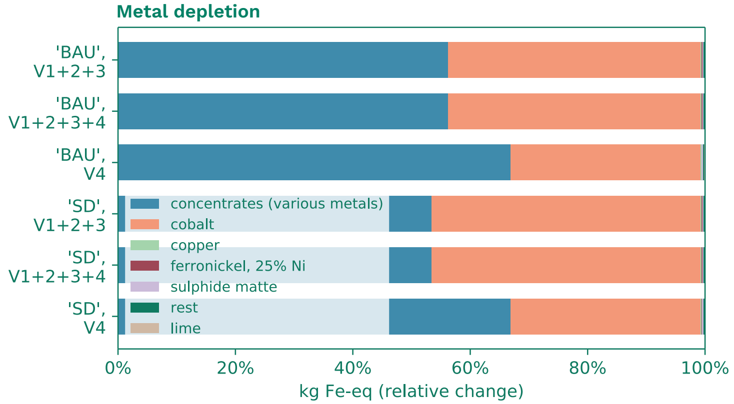
	Scenario	Variable	Climate change	Fossil cumulative energy demand	Particulate matter formation	Metal depletion	Human toxicity	Photochemical oxidant formation
Cobalt from copper	BAU	V1	40%	39%	48%	21%	36%	51%
		V4	-8%	-13%	-4%	0%	0%	-2%
		V1+4	30%	21%	43%	21%	36%	49%
	SD	V1	50%	48%	59%	25%	41%	63%
		V4	-46%	-42%	-14%	0%	-1%	-3%
		V1+4	-13%	-10%	40%	25%	40%	58%
Cobalt from nickel sulphide	BAU	V1	6%	7%	6%	5%	26%	9%
		V4	-5%	-10%	0%	0%	1%	-1%
		V1+4	1%	-4%	6%	5%	27%	8%
	SD	V1	8%	9%	8%	7%	30%	12%
		V4	-26%	-32%	-1%	0%	-6%	-2%
		V1+4	-20%	-26%	6%	7%	23%	10%
Cobalt from nickel laterite	BAU	V1	15%	13%	17%	28%	19%	17%
		V4	-8%	-11%	-11%	1%	5%	-15%
		V1+4	8%	1%	5%	29%	25%	1%
	SD	V1	20%	17%	22%	36%	25%	21%
		V4	-46%	-37%	-42%	1%	-28%	-27%
		V1+4	-29%	-22%	-23%	37%	-4%	-7%

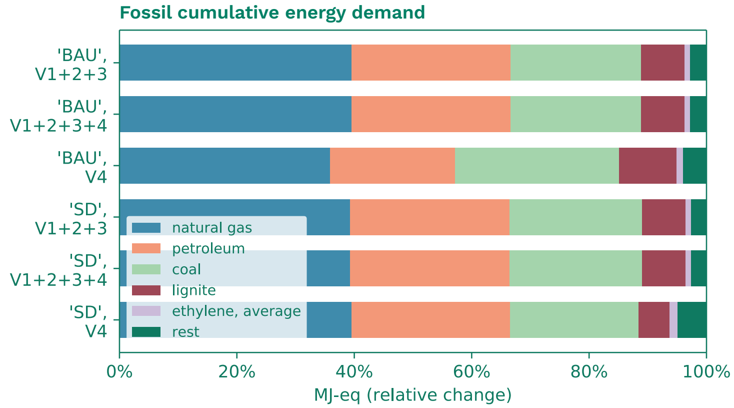
V1: Ore grade, V2: Primary market shares
V3: Secondary market shares, V4: Electricity supply
BAU: Business as Usual, SD: Sustainable Development

Figure 4.4 - Overview of relative impact changes of relevant variables in 2050 compared to 2010 in the 'Business as Usual' and 'Sustainable Development' scenarios for each production route and the market for cobalt for the production of 1kg of cobalt. The data for this figure is available on a repository (van der Meide et al., 2021).

Cobalt from ‘market for cobalt’
Relative process contributions in some scenario and variable combinations







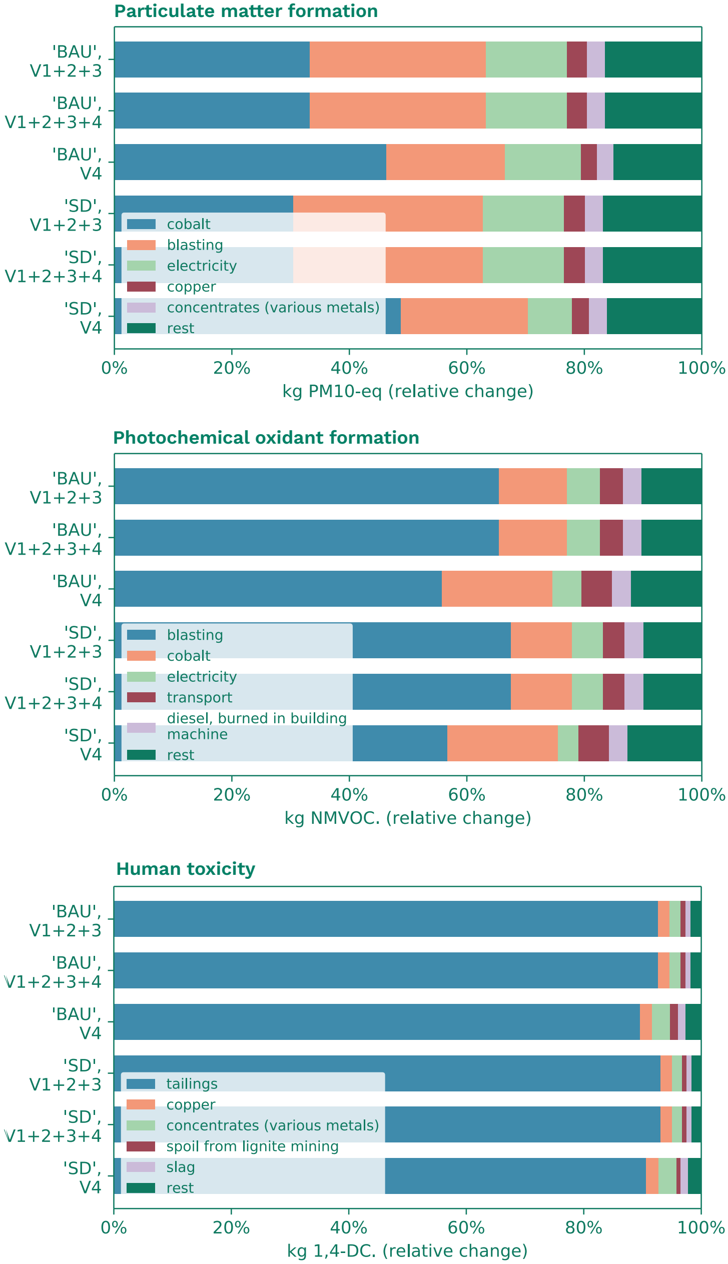
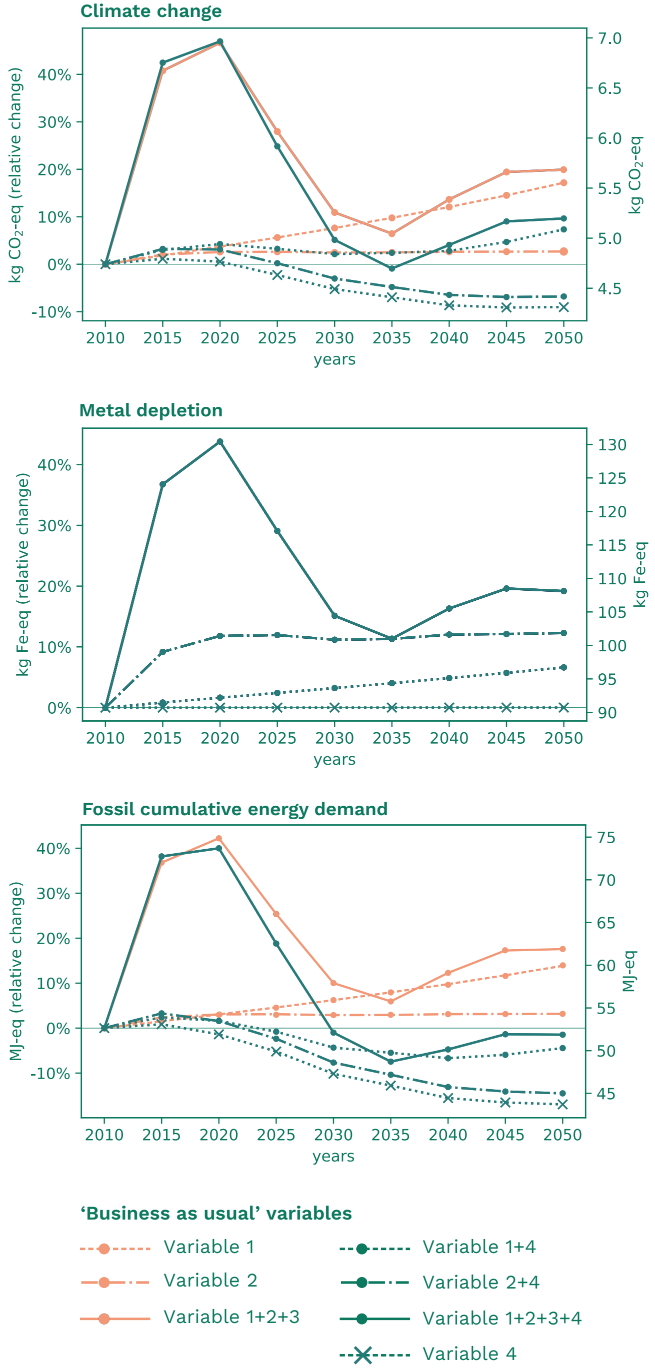


Figure 4.5 - Relative process contributions for the production of 1kg of cobalt for the Business as Usual (BAU) and Sustainable Development (SD) scenarios with variable combinations V1+2+3, V1+2+3+4 and V4. The data for this figure is available on a repository (van der Meide et al., 2021).

Impacts of cobalt from the process 'market for cobalt'
For each impact assessment method and scenario



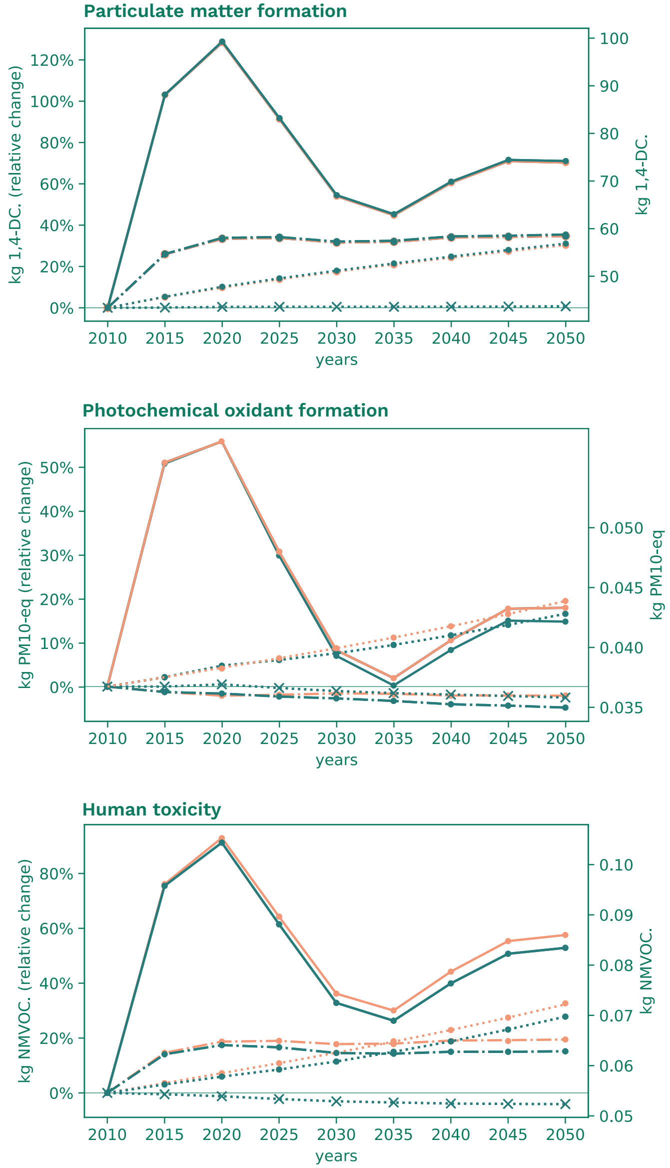
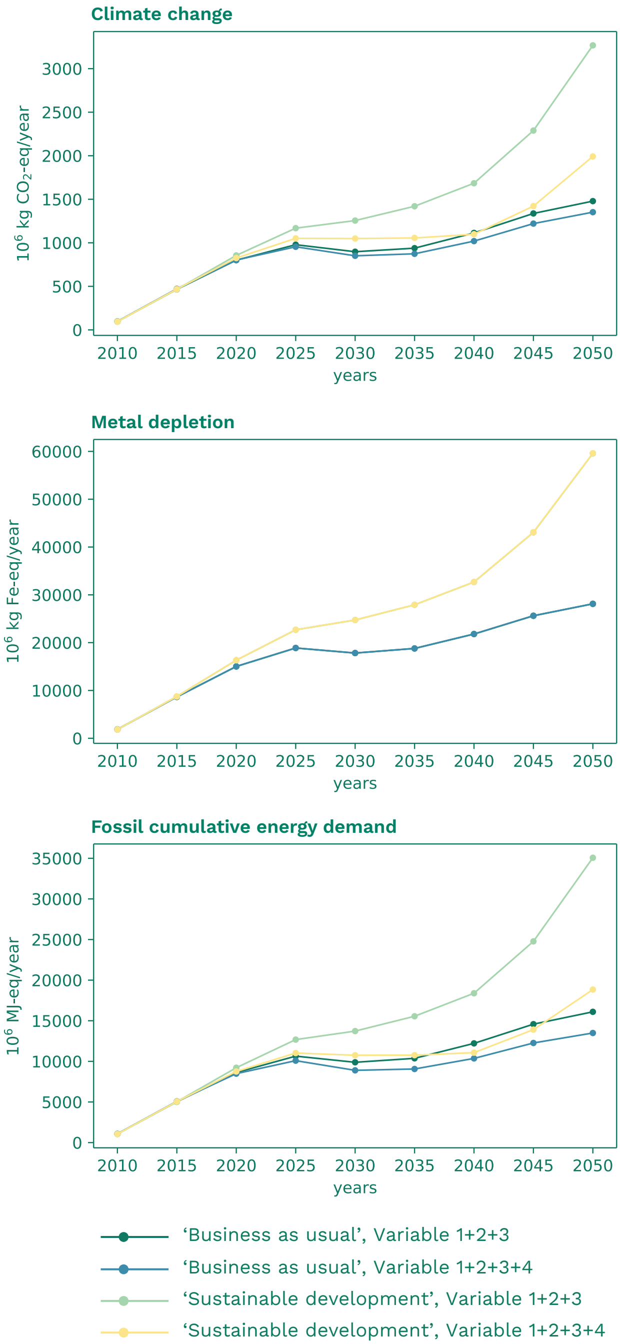


Figure 4.6 - Relative (left axis) and absolute (right axis) change in impacts for the production of 1 kg of cobalt in the 'Business as Usual' scenario for V1 ore grade, V2 primary market, V1+2+3 all variables, V1+4, V2+4, V1+2+3+4 and V4 energy transition for the market for cobalt. The turquoise lines are combined with Variable 4, energy transition, blue without. The data for this figure is available on a repository (van der Meide et al., 2021).

Impacts of cobalt from the process 'market for cobalt'
For each impact assessment method and scenario



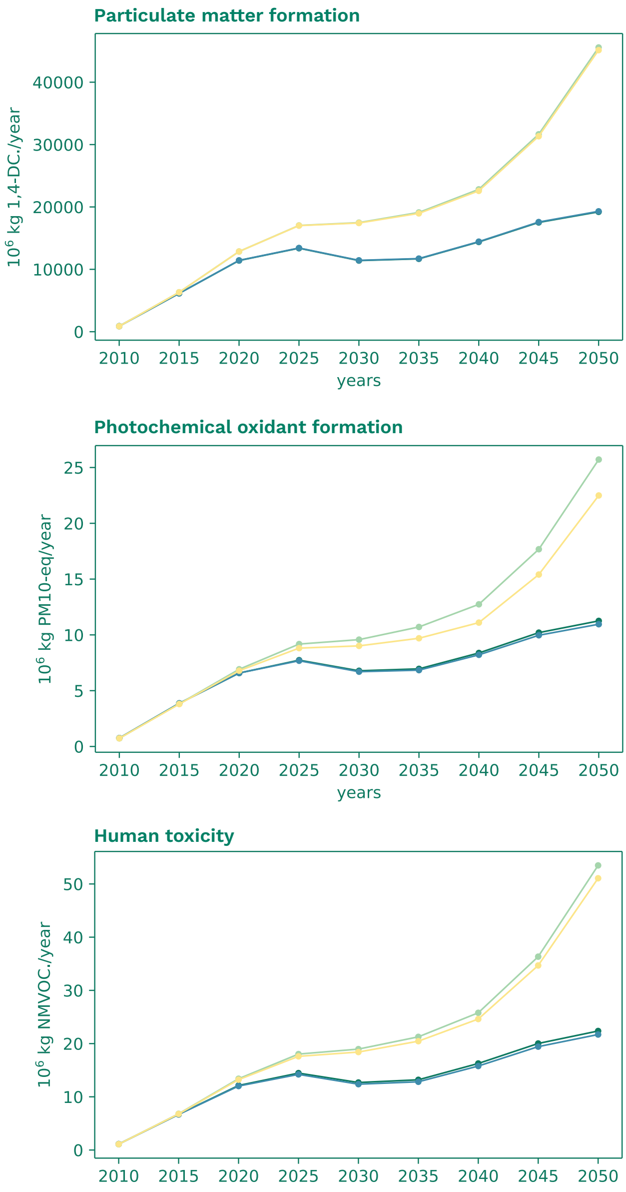


Figure 4.7 - Development of total impacts in the 'Business as Usual' (blue lines) and 'Sustainable Development' (green lines) scenarios for Variable 1+2+3 (all variables without energy transition) and Variable 1+2+3+4 (all variables). The data for this figure is available on a repository (van der Meide et al., 2021).

4.4 Discussion

The aim of this study was to determine how the environmental impacts of cobalt production could change up to 2050 and to provide a method for integrating the results into other prospective LCA studies. To achieve this goal, we modeled the impact of four factors that affect the supply of cobalt from different production routes in two scenarios between 2010-2050. The scenario results of this study could be used as background data in further studies that consider the future environmental impacts of cobalt-containing products by following the superstructure approach (Steubing & Koning, 2021). We enable the use of the superstructure approach by providing the data files in a repository (van der Meide et al., 2021).

4.4.1 Ore grade and market shares

Our model for ore grade and energy requirement allowed us to estimate future impacts of cobalt supply for two scenarios, 'Business as usual' (BAU) and 'Sustainable Development' (SD), using metal demand as a driver. We found that the higher demand for metals in the SD scenario could cause a faster ore grade decline and a higher increase in energy requirements for the production of cobalt compared to BAU.

Despite the usefulness of the models we developed, one major limitation should be considered with these results: ore quality is a complex issue that is not well modeled for most metals, including copper, nickel and cobalt. The true quality of a cobalt resource extends far beyond simple measurements such as ore grade, and should also consider the specific mineralogy, morphology and accessibility of these deposits. These factors are all highly variable between individual cobalt bearing mineral deposits and this translates into significant variability in the potential recovery, economics and environmental impacts of cobalt extraction (Dehaine et al., 2021; Mudd et al., 2013). Importantly, any evaluation of the quality of a mineral resource is dependent upon the (implicitly or explicitly) assumed economic context, and so our perception of the availability and quality of cobalt resources may change drastically if future economic conditions change. A complicating factor is the various definitions of ore grades, which are sometimes confused or aggregated with each other in LCA studies (Northey et al., 2018).

There is also considerable complexity and limited data available to understand how mined grades of by-products, such as cobalt, may evolve into the future. Long-term declines in the average grade of remaining copper and nickel resources could reasonably be expected, if market conditions and technology assumptions used to define mineral resources are static and when assuming preferential extraction of high-grade mineralization and progression along the cumulative grade-tonnage relationships for copper and nickel resources. As cobalt is a co-product of copper and nickel production, we assumed that declining ore grades of copper and nickel could be used as a proxy for changes in cobalt ore grades. Considering the inherent complexity and uncertainties underlying this assumption, the ore grades we modeled in this study should not be considered predictions, but rather loose proxies for the potential for change in resource quality.

To model the market shares for the cobalt supply, we developed a stock model and found that there could occur a period in which secondary cobalt supply is heavily outpaced by high demand for cobalt in a 'circularity gap'. Despite that cobalt has traditionally been a metal with good recycling efficiencies (Nansai et al., 2014), even with high recycling rates, sudden increases in demand will result in primary demand as secondary supplies will lag behind the demand. We also observed this result in our sensitivity analysis when using market shares and recycling estimates from Harper et al. (2012).

A limitation of our stock model is that it considers only the global supply of cobalt, which reduces applicability and ignores changes in transport requirements for cobalt from different sources. Additionally, the stock model does not assume changes in cobalt content in a product or changes in their recycling rates.

4.4.2 LCIA results in context of other cobalt production studies

Our results show that the environmental impacts of cobalt production could increase and that the magnitude of this increase is strongly influenced by the electricity supply. It should also be noted that even though impacts per unit of cobalt could be much lower in the SD scenario, the total demand would be nearly twice as high as in the BAU scenario, resulting in a total emissions growth.

Two notable previous LCA studies on the supply of cobalt have been conducted: the Cobalt Institute (2016) and Farjana et al. (2019), shown in Table 4.1. The Cobalt Institute states in their study that variability of results might be higher than with other LCA studies on metals due to the co-production nature of cobalt and the wide range of production processes and sources. As a comparison, the reported CC and CED results per mass of production for cobalt production have often exceeded the results for bulk and base metal reported by others, such as Norgate et al. (2007) and van der Voet et al. (2018).

To validate the results of our study, we compared the impacts of copper production from our process “cobalt from copper production” with impacts of copper production of other studies. This additional comparison is discussed in the SI-2. These comparisons suggest that the outcomes of this study are in line with those of other LCA studies, such as (Li et al., 2017; Memary et al., 2012; Norgate & Rankin, 2000; Yang et al., 2014).

One factor that affected our results is the use of the ecoinvent cut-off model (Wernet et al., 2016). Our stock model suggests that substantial amounts of cobalt are recycled, while the ecoinvent cut-off model allocates 0% of impacts to recycled materials. To counteract this optimistic assumption, we performed a sensitivity analysis which assumes a 100% allocation of the recycling impacts to cobalt production. This resulted in a minor increase of impacts of 12.6% in 2010 for CC. Another factor that could explain the lower impacts in our results could be that our models use the updated electricity generation data from Mendoza Beltran et al. (2018).

Study		**Database**	**CC ($kgCO_2eq$/ kg cobalt)**	**CED (MJ/ kg cobalt)**
Our study, BAU, Market for Cobalt, All variables	2010	Superstructure based on Ecoinvent 3.6 cut-off	4.3	53
	2025		5.3	63
	2050		4.7	52
Cobalt Institute (2016)		Gabi	38	653
Farjana et al. (2019)		Ecoinvent	12	141
Ecoinvent 3.6 cut-off (2016)		Ecoinvent 3.6 cut-off	9.5	127

Table 4.1 - Comparison of results with previous LCA studies on the environmental impacts of cobalt production.

4.4.3 Limitations

Two factors that were considered static are a limitation in our study. First, estimates for cobalt recovery rate were used from Crundwell et al. (2011), which is the ratio between total cobalt content of the ore versus the extracted amount of cobalt metal. These estimates could be outdated. Besides, Tisserant and Pauliuk (2016) stated that through economic mechanisms, the recovery rate of cobalt could change over time. This would depend on the supply-demand ratio, as a higher demand for cobalt would likely increase the recovery rate of cobalt and changes to process optimization could additionally decrease the recovery rates of the host metal. Such changes could alter the environmental impacts of both cobalt and the host metal production, as the process outputs could change with only minor changes to the process inputs, causing a shift in impact per unit of cobalt produced.

The second factor is that our allocation factors were derived in a simplified way. We used global ten-year average price and production values of copper, nickel and cobalt. For both copper and nickel production, only a minority of mines produce cobalt (Tisserant & Pauliuk, 2016), so we only considered production volumes of countries producing cobalt where also copper or nickel is produced. The Cobalt Institute (2016) realized a more complex allocation procedure based on physical processes, intermediate product pricing (for example for cobalt hydroxide), or cobalt and other metal pricing, which was not applied in this study due to the lack of data. However, we did apply mass based allocation as sensitivity analysis and found that this reduces impacts substantially due to the higher weightings of copper and nickel production routes.

4.4.4 Further research

Managing the environmental impacts of the energy transition will require improved understanding of material supply chains and the relationships between material and energy supply. By identifying important variables and modeling those in line with policy scenarios from IAMs, other materials could also be studied to expand the availability of prospective LCA background data for other studies. Studying materials that could have significantly changing impacts, materials that are of great importance to society or are used as commodities for many applications might prove most effective to expand the reach of this type of study. Ensuring a high degree of compatibility with background databases like ecoinvent and other future background studies like ours would also likely improve the reach and adoption of this type of study.

For our study, we identify three points:

1. Regionalizing production: We used global datasets, using regionalized data could make results more specific, this could be especially useful in combination with the electricity dataset from Mendoza Beltran et al. (2018).
2. Modeling recovery rates: For a material that is co-produced such as cobalt, the demand for it and the main metal could have major effects on the recovery rate of the co-produced material (Tisserant & Pauliuk, 2016). Modeling recovery rates of each co-product could alter both impacts and partitioning with allocation, both can have major effects on sustainability impacts.
3. Establishing models for the evolution of cobalt (and other by-product) ore grades: As there are conceptual and data difficulties in translating host metal grade scenarios (which are already highly uncertain) into grade scenarios for companion/by-product grades, particularly for some deposit types or mineralogies where host and by-product grades may not be strongly correlated.

Methods for inferring companion metal grades developed by Werner et al. (2017) could potentially be adapted to support this form of modelling.

4.4.5 Conclusion

This study demonstrates that multiple competing pressures may alter the environmental impacts of cobalt production over time. As part of this, we identified potential synergies between increased secondary production of cobalt, adoption of renewable energy in the electricity sector and the consequent reductions in the long-term environmental impacts of the mineral and metal production. Importantly, the study demonstrates that it may be possible to decouple growth in annual cobalt production and the associated depletion of high-quality mineral resources from rises in the total annual climate change impacts of cobalt production. Despite this, under both the sustainable development and business-as-usual scenarios the total demand growth results in an increase of impacts of cobalt production across all impact categories. This study demonstrates the benefits of taking a systems and life cycle approach to model and better understand interrelationships between different sectors so that the factors influencing long-term changes in environmental impacts and greenhouse gas emissions can be more clearly articulated and addressed. This should also be extended to consider the use of cobalt as a contributor to reductions in greenhouse gas emissions in other sectors of the economy, especially the energy and transport sectors through its use in battery technologies. Finally, the developed database from our study could be used as a background database in other LCA studies where the use of cobalt in the future would be relevant for the studied functional unit.

Our results indicate two major opportunities to reduce the environmental impacts of cobalt production: Firstly, improving recycling rates and efficiency could help reduce impacts of cobalt production. As a secondary effect from this, reduced primary supply could reduce rates of decline in the availability of high-grade ores and subsequently reduce potential increases in the impacts of extraction. As a second opportunity, the energy transition could help reduce the impacts of cobalt production, despite higher cobalt demand. A range of policy and technical solutions should be developed to drive improvements over time, such as increasing recycling rates of cobalt-containing products, improving recovery of cobalt in primary production processes and rapidly adopting renewable energy use in cobalt and electricity production more broadly.

Acknowledgements

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Chapter 5
Recovering sand and gravel from End-of-Life concrete: The global potential

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The Supplementary Information (SI) to this chapter is available at the preprint server.

Abstract

Concrete is a key material in our modern society and will remain an important material in the coming decades globally. Two main components of concrete, sand and gravel -together aggregates- could become scarce which may pose a significant problem the production of concrete. One option to mitigate scarcity is to recycle concrete. Two complementary technologies that have been in development for this are making this feasible; 'Advanced Dry Recovery' and 'Heating Air classification System'. Together they produce recycled sand and gravel. In this study we assess the recyclability of End of Life concrete up to 2050 in 26 regions for the production of new aggregates with a dynamic material flow analysis model and assess environmental impacts with Prospective Life Cycle Assessment. We find that recycling could reduce demand for conventional sand by 16% and gravel by 34% globally by 2050 without large increases in impacts, though impacts differ substantially per region.

5.1 Introduction

Concrete is a key material in our modern society and will remain an important material in the coming decades globally. It is an engineered material mainly made from sand, gravel, water, and cement. Production of concrete has quadrupled between 1990 and 2020 (Watari et al., 2023). Additionally, demand for concrete is expected to keep rising in most world regions up to 2050, either for new construction, maintenance and replacement of demolished buildings (Deetman et al., 2020; Harald U. Sverdrup et al., 2017). Two ingredients of concrete -sand and gravel (together aggregates)- made up 79% of all non-water resources extracted from nature in 2010 (Krausmann et al., 2017). The winning of aggregates causes land use change and hence may have biodiversity impacts. While the winning of aggregates is not carbon-intensive, the production of concrete is highly energy intensive and was responsible for 3.3 GT $CO_{2eq.}$ emissions in 2020 (Müller et al., 2024). Their large scale consumption makes it important to investigate how environmental challenges related to the use of aggregates could be limited (van der Meide et al., 2022).

Although sand and gravel seem to be abundantly available, the scarcity issue of conventionally produced aggregates has gained more scientific attention recently -though concern for sand scarcity is hardly new, see e.g. Giljum et al (2000)-. Torres et al. (2017) have shown that illegal sand mining is causing local problems in the global south. Peduzi (2014) highlights effects on biodiversity, land loss and erosion, water supply and potential damage to infrastructure. This poses a special concern to future concrete manufacturing, which demands not only a high quantity but also a high quality of aggregates, namely, construction grade sand and construction grade gravel. While construction sand is mostly discussed in the scarcity context, construction gravel can also be considered scarce, depending on the region and supply (Ioannidou et al., 2017), though the locality of scarceness is important for all aggregates. We can expect these problems to exacerbate significantly due to the growth in demand (Watari et al., 2023).

Several options have been proposed to mitigate the scarcity challenge for conventional aggregates, such as recycling secondary aggregates from end of life (EoL) concrete (Tukker et al., 2023; Zhang et al., 2022) and increasing efficiency in material use (Cao & Masanet, 2022). Zhong et al. (2022) show that to combat sand scarcity substitution is the single most effective strategy. The substantial flows of future EoL concrete projected by Deetman et al. (2020) indicate a potential worth to investigate for sand and gravel substitution by recycling secondary aggregates from the rising future EoL concrete flows.

While recycling concrete into construction grade aggregates has been an engineering and economic challenge (Ren et al., 2021; Zhang et al., 2019), two complementary technologies that have been in development in Europe over the past decade are making this feasible. They are 'Advanced Dry Recovery' (ADR) (Lotfi et al., 2017) and 'Heating Air classification System' (HAS) (Gebremariam et al., 2020). ADR works by separating concrete pieces into different sizes through a mechanical system. The output streams are recycled gravel and an intermediate. HAS works by separating the intermediate stream into two smaller streams through a thermal system. The output streams are recycled sand and a fine dust that can be used as a cement filler. The technologies could be deployed in tandem to recycle EoL concrete and reduce demand for conventional aggregates.

For ADR and HAS, some work has already been done to assess their environmental impacts with Life Cycle Assessment (LCA). Zhang et al. (2023) studied the environmental performance of the technologies, including a prospective study where the energy supply to the technologies was adjusted to future energy mixes with *Premise* (Sacchi et al., 2022). While this study provided deeper insight into material and fossil fuel footprints for EoL treatment, the potential of ADR and HAS as a technology to produce recycled sand and gravel and related environmental impacts has not been assessed.

Before the potential of recycling of EoL concrete and its environmental impacts can be assessed, we first need to better understand the relationship between availability of EoL concrete and demand for concrete. Additionally, it is not clear whether recycling concrete with ADR/HAS technologies may pose any trade-offs with environmental impacts or how these recycled aggregates compare against conventional aggregates in terms of their environmental impacts. In this study, we aim to address both of these gaps. We develop a dynamic material flow analysis model (MFA) for global aggregates and concrete to understand to what extent EoL concrete can provide secondary aggregates for future concrete production in 26 regions of the world from 2025 to 2050. We then model the potential for and environmental benefits of recycling concrete with ADR and HAS up to 2050. We do so by integrating these technologies into a prospective version of the ecoinvent Life Cycle Inventory (LCI) database (Wernet et al., 2016). We do this by linking the recycling processes to the sand and gravel markets, letting all processes in the database that consume aggregates make use of the recycled aggregates as well. We calculate potential environmental impacts using *Premise* to assess possible trade-offs from recycling. Our method is further elaborated in section 5.2. Section 5.3 provides results and finally Section 5.4 gives the discussion and conclusions.

5.2 Methods

We start by developing a dynamic MFA model to assess the global potential of concrete recycling to reduce the demand for conventional aggregates. Based on existing building material stock and flow data from Deetman et al. (2020) we build a 'recycling material flow analysis model' to show how much conventional aggregates could potentially be substituted by recycled aggregates in 26 global regions from 2025 to up to 2050.

Next, we describe the Life Cycle Assessment (LCA) goal and scope and the ADR/HAS inventories and how we integrate them with *Premise*. We do this by linking the recycling processes to the sand and gravel markets, letting all processes in the database that consume aggregates make use of the recycled aggregates as well. After this, we assess the environmental impacts of the recycling technologies compared to conventional production and assess what processes and products contribute to their impacts.

Finally, we combine both the stock model data and the calculated environmental impacts to assess any potential trade-offs at scale.

Our calculation of LCA results is done in Activity Browser 2.11.2 (Steubing et al., 2019) and the results analysis done is with Excel (available as Supplementary Information (SI) 1). The python scripts for our stock model and integration with ecoinvent data are provided as SI in van der Meide (2025).

5.2.1 Recycling material flow analysis model

To assess the availability of EoL concrete to recycle we make use of the outputs of Deetman et al. (2020), who calculate in-and-outflow of concrete in the building stock for a given year and region between 1970 and 2050. This is modeled with the IMAGE Integrated Assessment Model (IAM) (Stehfest et al., 2014) for the SSP2 scenario (O'Neill et al., 2014), which projects likely policy changes based on current and future policy plans. In this study, we only consider the recycling of concrete and use of aggregates again in concrete as data for other aggregate uses (e.g. road-fill) is lacking.

We use the stock model outflow from Deetman et al. (2020) as available material for recycling and use the inflow as demand for new concrete, we show this in Figure 5.1. We then split the EoL concrete outflow from the building stock into production shares that ADR/HAS can produce. Based on the amount of gravel/sand that can be produced from the outflow and the demand in a given year and region, we calculate a balance. The balance for sand/gravel is zero, positive or negative for every timestep and region. If the balance is zero, the demand can be satisfied exactly by the outflow of the concrete stock. If the balance is positive (more material is available than is demanded), the remainder is considered to be stored and available for future time steps in the same region. If the balance is negative (more material is demanded than is available), the remainder can be supplied from the storage, any remainder after that (e.g. when the storage is empty) must be produced as conventional concrete. Based on the balance, the market share between conventional and recycled concrete is determined.

The amount of outflow from the building stock can also be moderated as not all material can realistically be converted due to a recycled aggregates market that is still under-developed and other market/policy inefficiencies. We assess two explorative scenarios from a stock model perspective:

First, we assess a scenario where there would be no limit to market shares, i.e. everything that can be recycled will be recycled. We name this scenario *'Maximum'*. Secondly, we assess a scenario where the market share of recycling increases over time, from 0% in 2025 to a maximum of 50% in 2050. We name this scenario *'up-to 50%'*.

We stress that both scenarios are meant as an exploration of the potential for recycling aggregates, and do not reflect expectations with regards to market adoption of ADR and HAS. After assessing how much sand and gravel can come from recycled sources –the substitution rate- in both scenarios, we will only use the 'up-to 50%' scenario going further. We assess this scenario in more detail as it is the more realistic one of the two. We will show how much aggregates are produced from conventional and recycled sources in aggregated regions.

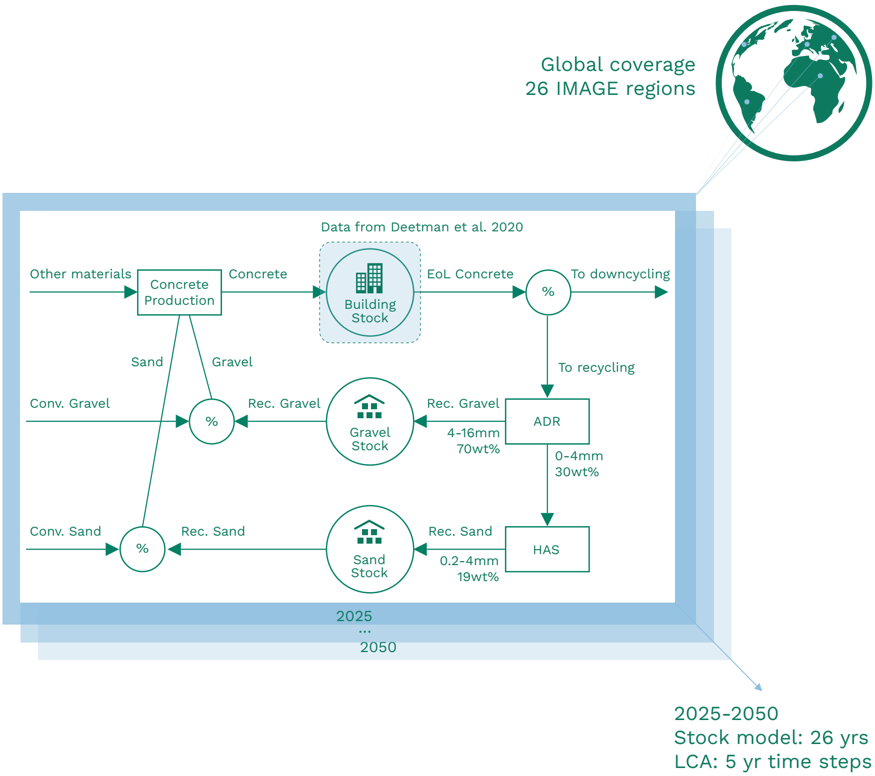


Figure 5.1 - Recycling material flow analysis model. Starting from the top-middle, EoL concrete is partially recycled (amount depending on the scenario) and converted to recycled gravel by ADR and recycled sand by HAS. Depending on the demand for concrete (top left), gravel and sand are supplied, first by recycled sources and supplemented by conventional sources. The model is calculated from 2025-2050 and the 26 IMAGE regions.

5.2.2 Life Cycle Assessment

Goal and Scope

Our goal with the LCA is twofold: First, we want to compare environmental impacts between conventional and recycled aggregate production, and what contributes to those impacts. For this, we will assess a 'cradle-to-gate' production of aggregates. For the recycled aggregates, this means production from recycled EoL concrete. Secondly, we want to assess whether a shift to recycled aggregate production would pose any trade-offs compared to conventional aggregate production, which is why we combine it with Prospective LCA and our stock model to assess potential impacts up to 2050.

The scope of our assessment is the production of aggregates as described above, which will be integrated into a prospective version of the ecoinvent database (Wernet et al., 2016) using *Premise* (Sacchi et al., 2022). This integration means that other processes that require sand and gravel (e.g. concrete production) make use of both the conventional and recycled aggregates, immediately affecting all processes in the database that would make use of sand or gravel somewhere in their supply chains. Other database changes like the changes in the generation of electricity, transport and steel sector as made by *Premise* are also included. We assess the regionalized production of aggregates in all 26 IMAGE regions, making use of the ecoinvent market mixes if multiple conventional production routes exist, to which we add the recycled shares from our stock model. The script to generate the prospective database is included as SI in van der Meide (2025).

For our assessment, we consider a functional unit of 'aggregates needed for 1 ton concrete', which is 373 kg sand and 461 kg gravel, based on ecoinvent inventory data. We compare conventional and recycled aggregates to each other and compare the process contributions, grouped by product names, we apply a cumulative cut-off of 80% to show the most important contributors, the full method is described by van der Meide et al. (2025).

To keep this assessment in the context of the most important use of aggregates, concrete production for this we use concrete production in Switzerland (in the IMAGE region Western Europe (WEU)). We show the product contributions of sand, gravel and cement as described in van der Meide et al. (2025). For this assessment, compare three alternatives:

100% conventional production in 2025, the market mix of 2050 with 20% recycled sand and 50% recycled gravel and a 100% recycled production. Finally, based on the original LCA model and market shares between conventional and recycled aggregates from our stock model we model, we assess how impacts change over time. We use the 'up-to 50%' scenario to assess impacts. We assess impact of aggregate production in five year time steps from 2025-2050 and show how the impacts change for the world average, highest and lowest regions on a per-unit basis. Lastly, we combine the demand from the stock model and the per-unit impacts to assess the potential total impact of aggregate production.

Advanced Dry Recovery (ADR) and Heated Air Classification System (HAS) Life Cycle Inventory

For the LCA of recycled aggregates, we use updated inventories from Lotfi et al. (2017) for ADR and Gebremariam et al. (2020) for HAS. We provide the exact inventories in the SI in van der Meide (2025) but do discuss the technologies here from a Life Cycle Inventory perspective. Advanced Dry Recovery (ADR) is meant to separate a stream of crushed end of life (EoL) concrete (0-16mm) into two streams. One stream can be used to replace gravel and is 4-16mm in size and the other is an intermediate of 0-4mm size that needs to be processed further. ADR works by physically separating particles based on density (see also Lotfi et al. (2017)). The machine can be installed locally on a deconstruction site, is filled and emptied by excavators and requires only electricity to run.

Heated Air Classification (HAS) is meant to separate the 0-4mm stream further into another two streams. One stream can be used to replace sand and is 0.125-4mm in size and the other is 0-0.125mm. In the future the latter stream may be used as a useful filler material in clinker, but we do not consider this stream further in this study. HAS works by rapidly heating and cooling the particles, fracturing them on weak points in their physical structure, splitting them into two stable fractions (as explained in more detail by Gebremariam et al. (2020)). The machine can be installed locally on a deconstruction site, is again filled and emptied by excavators and requires diesel to run. While Zhang et al. (2023) assessed the potential for biodiesel use in HAS, we use conventional diesel in our inventory to make for a fairer comparison to conventional aggregate production. We provide the ADR and HAS LCI in van der Meide (2025).

We consider both ADR and HAS multifunctional processes, producing two sizes of recycled aggregates. We apply mass-based allocation to the fractions, price-based allocation would not be possible as there is no openly available pricing on aggregates globally nor for the ADR and HAS products. The mass fractions of each stream are shown in Figure 5.1. We do not consider the processes as waste treatment processes, this happens at an earlier step of concrete crushing, which happens for all waste treatment options of EoL concrete, whether it is landfilled, used as road base or recycled with ADR and HAS. We consider the crushing step cut-off for two reasons, this is consistent with the cut-off model from ecoinvent (Wernet et al., 2016) and it is the same for all waste treatment options.

Conventional aggregates and concrete production Life Cycle Inventory
In our LCA we compare ADR and HAS to conventional production of aggregates, for this we use the inventories available in ecoinvent:
- ‘Gravel and Sand quarry operation’ for ‘sand’ and ‘gravel, round’
- ‘Sand quarry operation, extraction from river bed’ for ‘sand’
- ‘Zinc mine operation’ for ‘sand’
- ‘Gravel production, crushed’ for ‘gravel, crushed’

Some regions have multiple processes available, while others have only one source available, e.g. ‘India’, which –according to the ecoinvent data- only produces sand from riverbed mining. We make use of the market processes in ecoinvent so we use regional mixes for conventional production. For other regions, we use the market shares from the global market in ecoinvent. While market shares between these conventional routes could change, there currently is no information about these market shares and we assume no change. The integration into the LCI database through *Premise* (Sacchi et al., 2022) ensures that all consumers of aggregates in the database would consume from this modified market, making use of both conventional and recycled sand and gravel where applicable. The market shares between conventional and recycled aggregates differ per region and year based on our stock model.

Impact Assessment
We do a Life cycle impact assessment based on the Environmental Footprint (EF) 3.1 impact categories and characterization factors (EC, 2022). We focus on climate change, water use and land use, but provide the results for all 25 impact categories in SI 1.

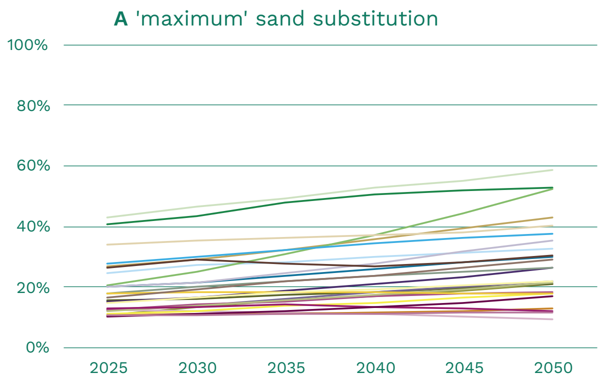
5.3 Results

5.3.1 Stock model

Our stock model shows how much sand and gravel can be substituted (indicated in percent relative to the total demand in Figure 5.2). We modeled this for both the *‘maximum’* scenario without technological limits to recycling and the *‘up-to 50%’* scenario where a maximum market share grows from 0% in 2025 to 50% in 2050.

In the maximum substitution scenario, we find that for sand the recycling depends mainly on the region and does not grow over 60% for the highest region (Figure 5.2 A). For gravel, we find substantially higher rates, even reaching a potential 100% substitution in some regions (Figure 5.2 B), suggesting that no further production of conventional gravel would be necessary in those regions to produce concrete.

In the ‘up-to 50%’ scenario, we find a maximum rate of 29% in 2050 and most regions not passing 20% (Figure 5.2 C). For gravel, we again find higher rates, though many regions still don’t surpass the 40% substitution (Figure 5.2 D).



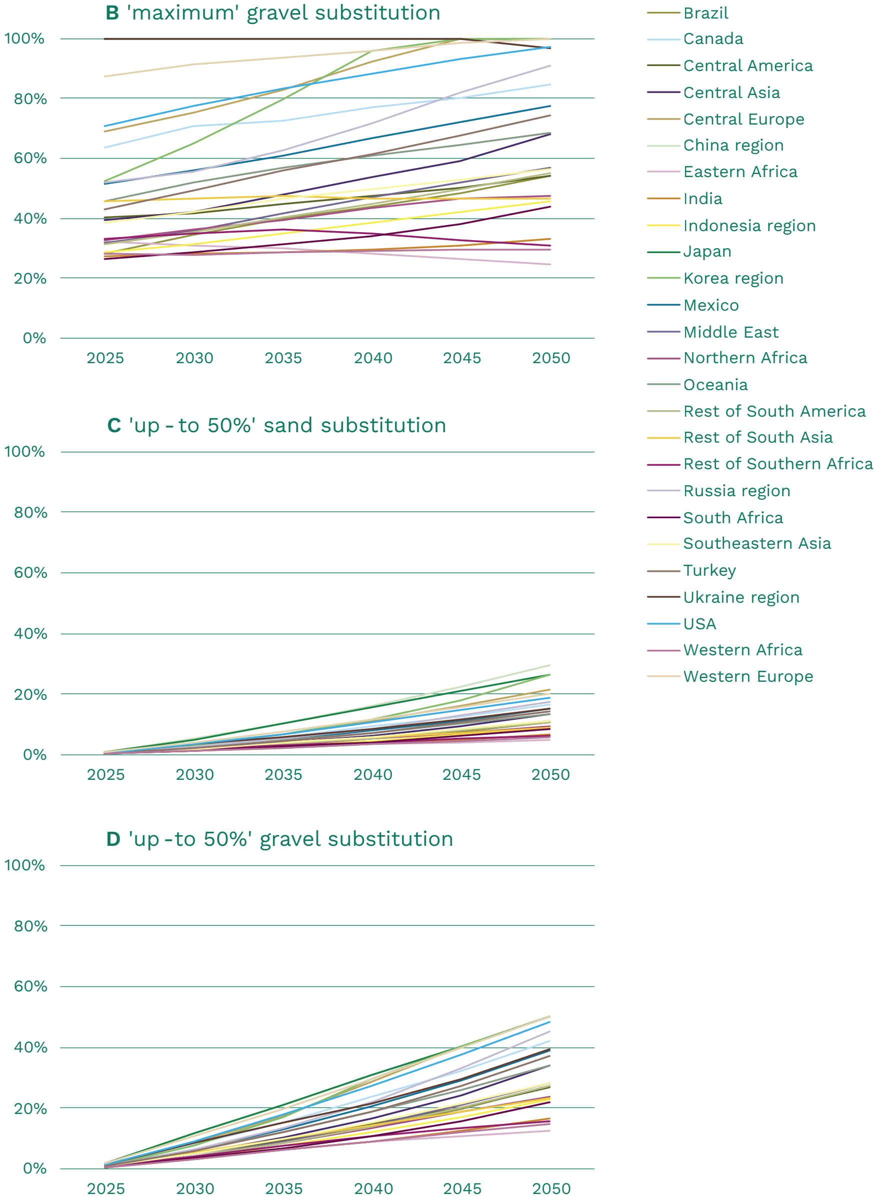


*Figure 5.2 - Substitution rate of recycled Aggregates over time. **A** 'maximum' scenario for sand, **B** 'maximum' scenario for gravel, **C** 'up-to 50%' scenario for sand, **D** 'up-to 50%' scenario for gravel*

For the ‘up-to 50%’ scenario we also show the aggregate demand for grouped regions (exact grouping presented in SI 1) in Figure 5.3. In the figure, we show the total demand for aggregates for concrete production in aggregated regions in five year steps and how much can be supplied from conventional and recycled sources in 2050. We find that in 2050, 26% of global aggregate demand could come from recycled sources, though about two thirds of this would be gravel.

Further, from Figure 5.3, we also find that demand in China is -and remains- the largest consumer of aggregates. While this is not surprising, we also see a strong growth in the availability of EoL concrete. In contrast, India also grows fast in total demand, but the end of life availability concrete remains relatively low. This is due to the fact that China has been developing its housing and infrastructure strongly for a longer period already, meaning that now already more stock reaches the end of life stage and needs to be replaced, providing significant amounts of EoL concrete.

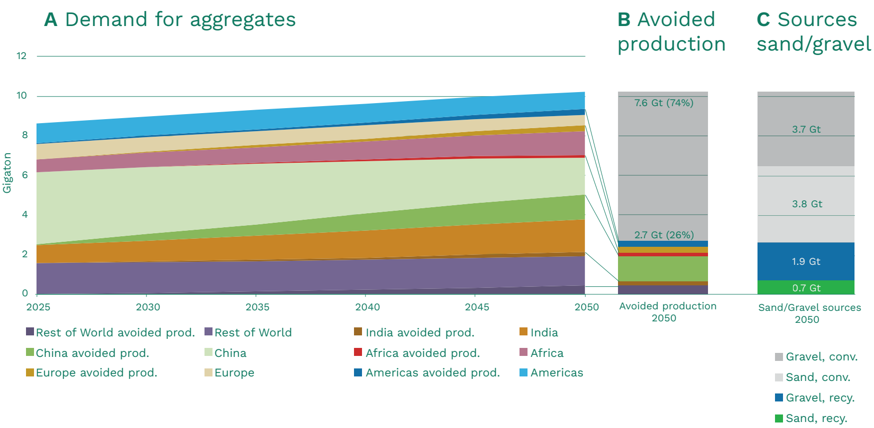


*Figure 5.3 - Demand for aggregates, **A** Demand in six aggregated regions between 2025-2050, **B** Avoided production of conventional aggregates in the same regions of **A** in 2050 based on 50% scenario, **C** Sources of sand and gravel in 2050 based on 50% scenario.*

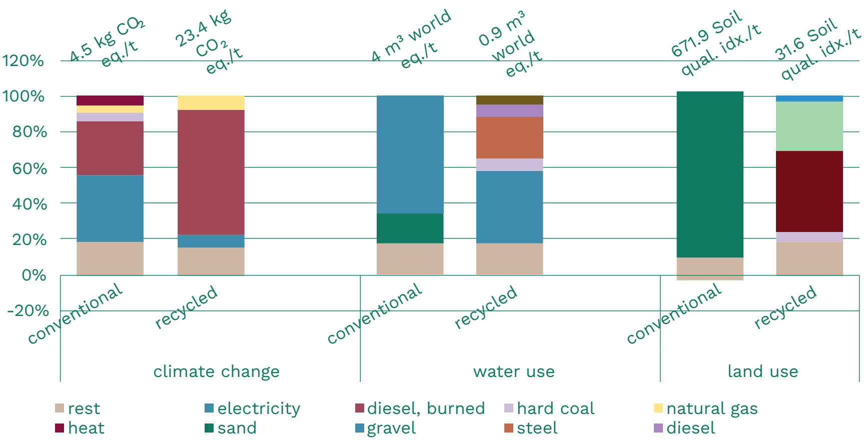
5.3.2 LCA ADR/HAS

We assessed the environmental impacts for conventional and recycled aggregate production for 1 ton of concrete for the world average. We show comparative process contributions in Figure 5.4 A. We show the relative process contributions, grouped by product names for three important impact categories. The per-unit results for all 25 impact categories for sand, gravel and combined as aggregates are provided in SI 1. We find that for climate change impact, the ‘diesel, burned’ group results in a much higher impact for recycled aggregates, this is due to the HAS requiring substantial amounts of fuel. Furthermore, we find that for water use, over 80% of the impact can be explained directly by sand and gravel production for conventional production. While the per-unit impact for climate change is ~5x higher for recycled aggregates, the impacts in water use is ~4x lower and land use is ~20x lower.

To keep aggregates production in context of its main consumer, concrete production, we also assess the product contributions of sand, gravel and cement to concrete production in Switzerland based on the Central EU aggregates production, we do this for 100% conventional aggregates in 2025, the market mix of aggregates in 2050 (20% recycled sand, 50% recycled gravel, Figure 5.2)and 100% recycled aggregates in 2025. We show this in Figure 5.4 B. For the market mix of aggregates in 2050 compared to a 100% conventional production in 2025, we find that the contribution of aggregates to climate change increases from 2.8% to 5.3%. We find a < 1% decrease in water use impact and Land use contribution changes 3.7%. When assessing 100% recycled compared to re, the main changes are in the contribution of sand to climate change and reduction of the total land use of aggregates from 71.8% to only 14.2%.

5

A Relative process contributions to aggregate production



B Relative product contributions to concrete production

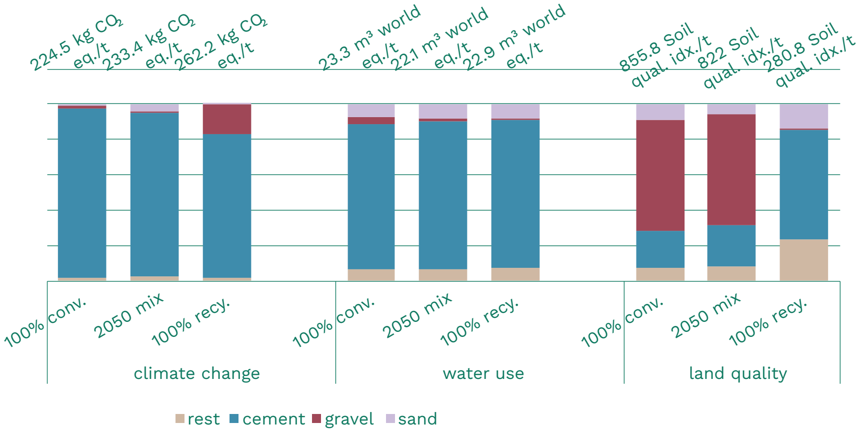
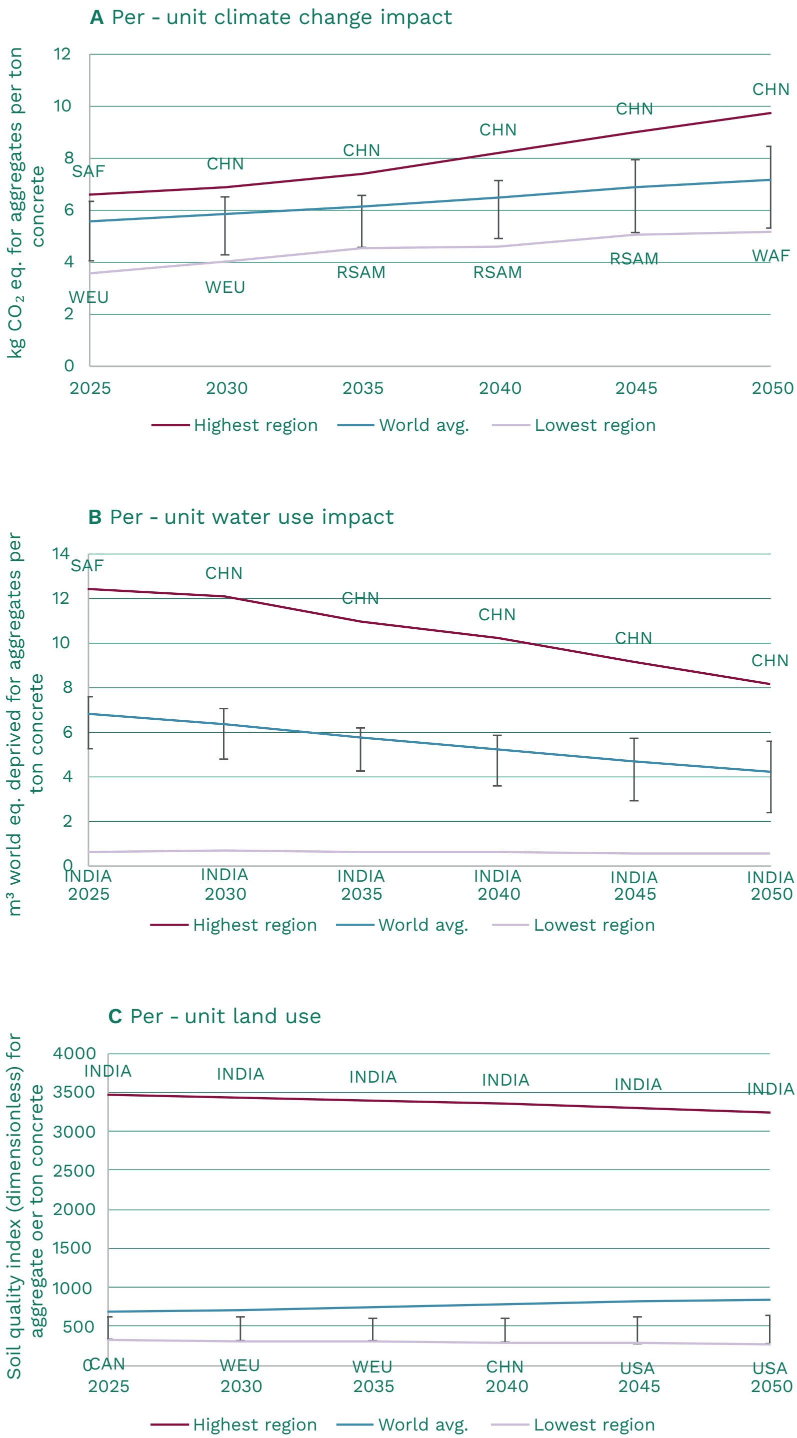


Figure 5.4 - Contributions to LCA results. A: Relative contributions of process groups to three major impact categories, cumulative to 80% of contributions. B: Product contributions to the production of 1m3 concrete with 100% conventional aggregates, the 2050 mix of conventional/ recycled aggregates and 100% recycled aggregates for 'sand', 'gravel', 'cement' and all other products.

5.3.3. Prospective LCA

With market shares between conventional and recycled aggregates known, environmental impacts per-unit can be calculated up to 2050. We show this for the 'up-to 50%' scenario in Figure 5.5. From this figure, we find a slightly increasing climate change impact, coinciding with increased market share of recycled aggregates. For water use, we find that 'Rest of South America' (RSAM) and India are outliers compared to the majority of the regions –5th to 95th percentile, between the error bars-, with most of the data slowly declining from ~7m^3 to ~4m^3. For land use, we find that India is again a major outlier, with most regions having much lower results. These outliers can be explained by regionalized ecoinvent market datasets that use only material from a single source. Finally, we find that per-unit of aggregates, China shows the largest decline, due to its high recycling share. Overall, tradeoffs per unit of production for aggregates appear limited.


A Per - unit climate change impact
kg CO₂ eq. for aggregates per ton concrete
12
10
8
6
4
2
0
2025
2030
2035
2040
2045
2050
SAF
CHN
CHN
CHN
CHN
CHN
WEU
WEU
RSAM
RSAM
RSAM
WAF
Highest region
World avg.
Lowest region
B Per - unit water use impact
m³ world eq. deprived for aggregates per ton concrete
14
12
10
8
6
4
2
0
SAF
CHN
CHN
CHN
CHN
CHN
INDIA 2025
INDIA 2030
INDIA 2035
INDIA 2040
INDIA 2045
INDIA 2050
Highest region
World avg.
Lowest region
C Per - unit land use
Soil quality index (dimensionless) for aggregate oer ton concrete
4000
3500
3000
2500
2000
1500
1000
500
0
INDIA
INDIA
INDIA
INDIA
INDIA
INDIA
CAN 2025
WEU 2030
WEU 2035
CHN 2040
USA 2045
USA 2050
Highest region
World avg.
Lowest region

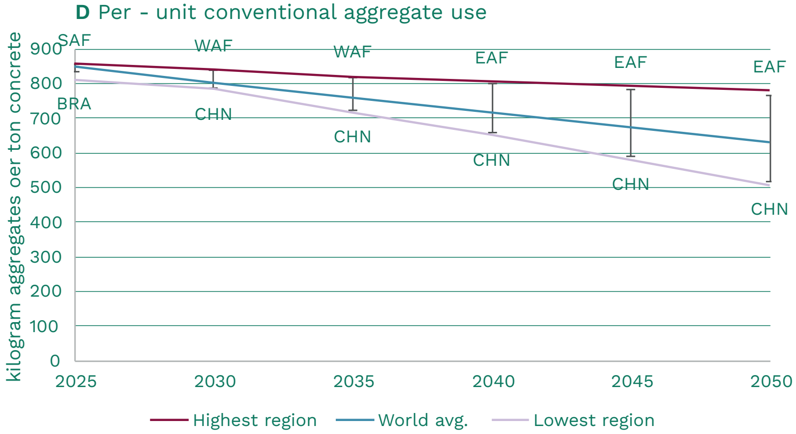
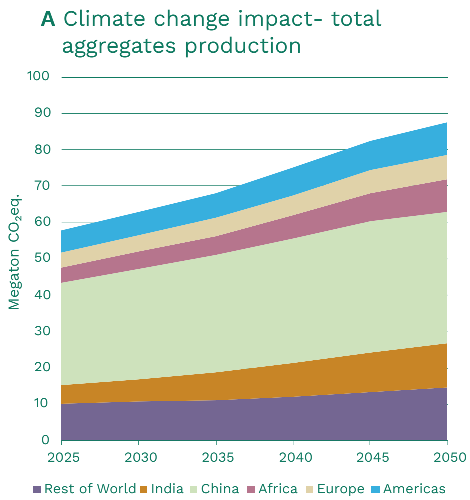
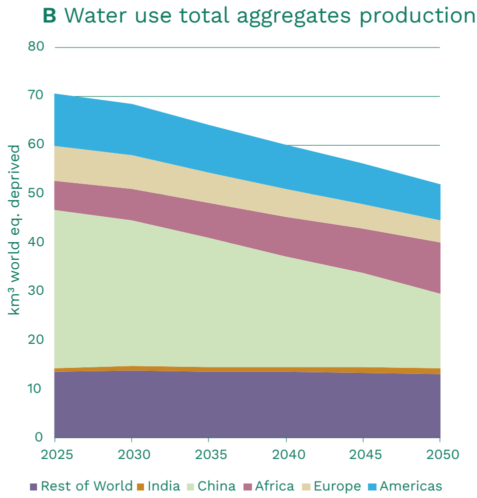


Figure 5.5 - Per-unit impact between 2025 and 2050 for aggregates, showing world average, the highest and lowest regions (labeled) and a 5th and 95th percentile as error bars. A: shows per-unit climate change impact, B: shows per-unit water use impact, C: shows per-unit land use impact, D: shows per-unit use of conventional aggregates.

Combining the per-unit impacts with the aggregate demand projected by the SSP2 scenario (as shown in Figure 5.3), we find that the total yearly climate change and land use impact from aggregates production would increase, while decreasing water use, as shown in Figure 5.6. Relating this back to concrete production, total land use could become a challenge, depending on the region.





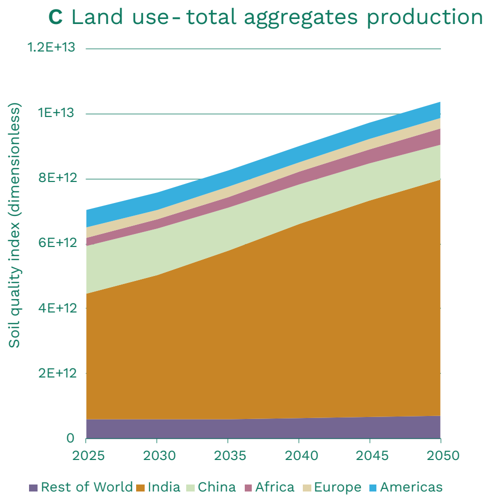


*Figure 5.6 - Impact of aggregate demand between 2025 and 2050 for aggregated regions. **A** shows climate change impact, **B** shows water use impact, **C** shows land use impact.*

5.4 Discussion

With our study, we have shown for the first time the potential of recycling aggregates from EoL concrete in a future scenario with a stock model and how this would affect environmental impacts with prospective LCA. We modeled the future potential of EoL concrete recycling to reduce sand and gravel scarcity with a dynamic stock model. We coupled this data to a prospective LCA to assess potential trade-offs of recycling with environmental impacts. From our assessment we found that up to 16% of sand demand and 34% of gravel demand for concrete production could be substituted with sand and gravel recycled from EoL concrete assuming a scenario where EoL concrete recycling reaches 50% market share.

These relatively low substitution rates –especially for sand- can be explained by a combination of two reasons: First, even if the ADR/HAS technologies would recycle all EoL concrete, the output is still only 19% recycled sand due to how ADR and HAS are currently used. This, combined with the fact that the concrete types we assessed require 37%wt sand, means that not all sand could be from recycled sources if the demand were the same as supply from EoL concrete. Secondly, many regions have a mismatch between their demand for concrete and supply of EoL concrete. If more material is required for new construction than becomes available for recycling, not all material can be recycled by definition –a circularity gap (Krausmann et al., 2017)-, we see this back in our comparison between the China and India regions in Figure 5.3.

While this circularity gap between demand for new concrete and supply from EoL concrete cannot be closed entirely, it can help significantly reduce demand for conventional sand and gravel. Recycling can especially help in regions where there is low growth, while regions like India and Africa would still need to supply a major share of their production from conventional sources.

In terms of environmental trade-offs with increases in supply from conventional sources, impacts can be expected to increase, though in the context of environmental impacts of concrete production, the increase would be rather limited. Specifically for climate change, the contribution of sand and gravel to concrete production would still only account for <5% if the total impact, with the majority of the impact still caused by clinker production. Despite this, ADR and HAS still have a high energy cost, making the cost-effectiveness of HAS largely dependent on the cost of energy. Technology developers should attempt to improve this in the future.

One major challenge for the production of sand and gravel is that the production is often limited to local production and consumption –though exceptions like Singapore exist, which imports significant amounts of sand (Peduzi, 2014)-. The low value of sand and gravel per unit weight makes it often uneconomical to transport over large distances, making scarcity of sand and gravel a local problem, requiring local solutions. We represented this in our model by only considering the balance between EoL concrete availability and consumption per region.

A main problem with recycling is that it can only partially help resolving current scarcity issues. It helps to reduce demand for conventional sand and gravel, but due to a still rising demand for concrete in many regions and imperfect collection and recycling, recycled aggregates can cover the needs for aggregates only for 26% (Figure 5.6). Recycling must be combined with other measures like reducing demand for aggregates e.g. like Zhong et al. (2022) modeled. Specifically for regions that have had strong growth in the past, this may be effective now, as there would still be a major amount of stock from the built environment, reducing the circularity gap in the future. For regions that do currently not have a large stock of materials in the built environment, this would not help reduce the circularity gap much as the ratio of demand and availability of EoL sand and gravel would not change much.

We identify one main limitation to our study: We modeled ADR and HAS while there are more technologies to recycled EoL concrete (Ren et al., 2021; Zhang et al., 2019). We used ADR and HAS due to availability of data and it's promising cost-effectiveness and market readiness. Our stock model can be adjusted with different recycling parameters and the Life Cycle Inventories could also be changed to apply our models to different technologies to assess their potential.

While we assess the potential to reduce sand and gravel demand and its associated environmental impacts, we do not know how these values relate to actual aggregate availability and scarcity problems, this would be a topic that needs to be investigated in the future. This needs to be studied both a level of local impact, but also globally.

Chapter 6

An analysis of the effects of changes in the *Premise* database on the environmental impacts of key products

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The Supplementary Information (SI) to this chapter is available at the website of the publisher.

Abstract

Purpose: *Premise* has been quickly adopted as the state-of-the-art for performing prospective LCAs (pLCA). *Premise* databases are generated by combining the ecoinvent database and data from climate change (CC) scenarios implemented in Integrated Assessment Models (IAMs). Both the extent of changes and the focus on CC raise a question on how they affect LCA results. We evaluate 9 representative products in three scenarios to assess how impacts change and what contributes to those changes.

Methods: Our analysis of *Premise* consists of several steps. We begin by generating three *Premise* databases, one for 2020, and two for 2050 assuming different future changes one that represents a continuation of current trajectories and policies (Base) and one that represents assuming ambitious decarbonization strategies (RCP 2.6). We analyze *Premise* based on 9 representative products: Electricity, Heat, Road Transport, Steel, Aluminium, Copper, Concrete, Organic Chemical and Inorganic Chemical. We calculate results for each of the 9 products for 16 impact categories, although we focus on CC. We then assess impact change between different scenarios for every product. We do a contribution analysis where we analyze the contribution of 15 overarching product groups to each product.

Results & Discussion: For CC, we find that impact changes for most products are related to impact reductions in electricity production and increased use of biomass and Carbon Capture and Storage. We find that Electricity, Heat, Road Transport, Steel and Concrete are primary contributors to their own respective impacts. Other products are instead mainly affected by these groups. Furthermore, the contribution from the Ore & Minerals, Energy resources, Chemicals and Transport product groups is much higher when we include Indirect contributions (contributions 'connected through' another group, e.g. production of fuel for Transport), these product groups connect to impacts elsewhere in the system. In other impact categories we find much more varied results, though the uncertainty around these results is high, specifically 'land use' shows large changes in impact.

Conclusions: Our approach can highlight products or product groups of interest in large databases like *Premise*, which can aid in modeling and finding errors. We suggest *Premise* to be used primarily for assessments of climate change impacts and practitioners clearly communicate versions and settings to make their work reproduceable. Despite us taking a critical stance toward some aspects of *Premise*, we still recommend using it for pLCA.

6.1 Introduction

Life cycle assessment (LCA) is a method to assess the impacts of a product over its life cycle. LCA became more useful and relevant for policy when the scientific community started to explicitly assess possible impacts of new technologies in the future (Azapagic, 1999; Hirschberg et al., 2009; Hummen & Kästner, 2014; Villares et al., 2017). While modeling changes to future foreground systems (the core part of a supply chain for a reference flow, usually modeled by the practitioner) is important, it is important for consistency to also model changes to background systems (all other processes used, usually taken from large scale Life Cycle Inventory (LCI) databases such as ecoinvent (Wernet et al., 2016)) as well (Arvidsson et al., 2018, 2024; Bergerson et al., 2020; Cucurachi et al., 2018; Miller & Keoleian, 2015; Steubing et al., 2023; Thonemann et al., 2020). For example, Mendoza Beltran et al. (2018) showed the influence of changes in the climate change effects of electricity generation in future scenarios for electric vehicles compared to internal combustion engine vehicles. Sacchi et al. (2022) continued the work of Mendoza Beltran et al. (2018) and embarked on changing the ecoinvent LCI database based on future scenarios informed by Integrated Assessment Models (IAMs) and created the open-source library *Premise* to create such LCI databases and fill this gap. Since its introduction, *Premise* was quickly adopted as a major tool used to generate prospective LCI (pLCI) databases.

Premise enables LCA practitioners to adapt the background ecoinvent database to different future scenarios, facilitating the assessment of product impacts under changing technological and socioeconomic conditions. It translates scenario assumptions, such as shifts in electricity generation technologies or energy mixes, into corresponding modifications of LCIs by updating existing data or introducing new inventories where needed. *Premise* is most commonly linked to scenarios from IAMs such as IMAGE (Stehfest et al., 2014) or REMIND (Baumstark et al., 2021), though its scope is expanding to include other IAMs and scenario sources.

Initially limited to five sectors (electricity, steel, concrete, fuel, and road transport) (Sacchi et al., 2022), *Premise* now modifies around ten sectors (Sacchi, 2025b) and adds over a thousand new technology-specific inventories, resulting in well over ten thousand additional processes when regionalized. These databases intended as consistent, scenario-based projections derived from IAM outputs that combine Shared Socioeconomic Pathways (SSPs) (O'Neill et al., 2014) with Representative Concentration Pathways (RCPs) (Van Vuuren et al., 2011). Together, these scenarios reflect both how challenging it is to mitigate and adapt-to climate change (the SSP scenarios), and how much climate change occurs (the RCP scenarios) far into the future. Each IAM provides distinct trajectories toward the same SSP–RCP combinations, reflecting differences in assumptions about economic growth, population, energy systems, and material demand. *Premise* translates these IAM-specific outputs, using its own detailed technology assumptions, into prospective versions of ecoinvent (Wernet et al., 2016), enabling transparent and comparable LCA studies across a range of plausible future scenarios.

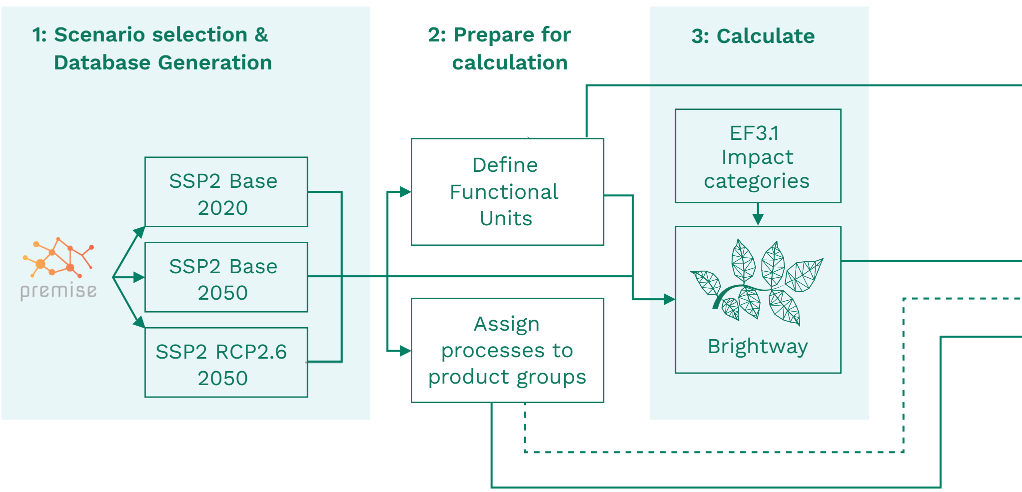
The IAM input data used in *Premise* revolves around climate change. This is thus the main focus of changes for pLCI databases generated with *Premise*. While LCA is arguably the best-positioned method to assess trade-offs with other impact categories within these scenarios, a requirement for an accurate assessment of these other impact categories is that they are properly modeled with the changes *Premise* makes. Sacchi et al. (2022) warn specifically that "toxicity related indicators [..] should be regarded as highly uncertain". Furthermore, *Premise* makes additional LCI changes that are not explicitly modeled in IAMs such as specific battery type market shares in electric vehicles or ore grade changes in mining. This increases completeness of 'future changes' at the cost of consistency with the underlying scenario data. *Premise* may not accurately model changes in elementary flows. *Premise* was further criticized on its IAM input data based on SSP based scenarios which embed optimistic technological assumptions, can neglect finance or biophysical limits and can have opaque ethical choices, this produces scenarios that could be technically implausible, ethically biased and thus misleading as inputs for pLCA (de Bortoli et al., 2025).

Both the focus of *Premise* source data on climate change and additional changes *Premise* makes to LCI data raise a question on how these changes affect LCA results from these pLCI databases. While it is documented clearly what changes are made on the inventory level by *Premise* (Sacchi, 2025b), because of the networked relationships between processes, it remains unclear what effects these changes have throughout *Premise* databases on the LCIA level, and how this can affect LCA results for both climate change and other impact categories.

In this study, our goal is to systematically analyze the effects of changes between several pLCI databases generated with *Premise* on LCIA results for practitioners. We assess the effects on impact results for important industrial products from these databases in various impact categories and which product groups (e.g., electricity, steel, transport) contribute to these changes. Through our analysis, we aim to give practitioners better insight into what kinds of changes they may expect when using *Premise* databases and how those may affect their own results.

6.2 Method

We first explain more about the workings of *Premise* where relevant to this study in section 6.2.1. We begin by generating three *Premise* databases (section 6.2.2). We choose nine products as functional units (FUs) to assess impact changes between the databases (section 6.2.3) and calculate LCA results for 16 impact categories (section 6.2.4). Next, we assess changes in results between the databases (section 6.2.5) and finally we assess what contributes to those changes (section 6.2.6). We show an overview of our approach in Figure 1. We provide more detail in SI 1.1.



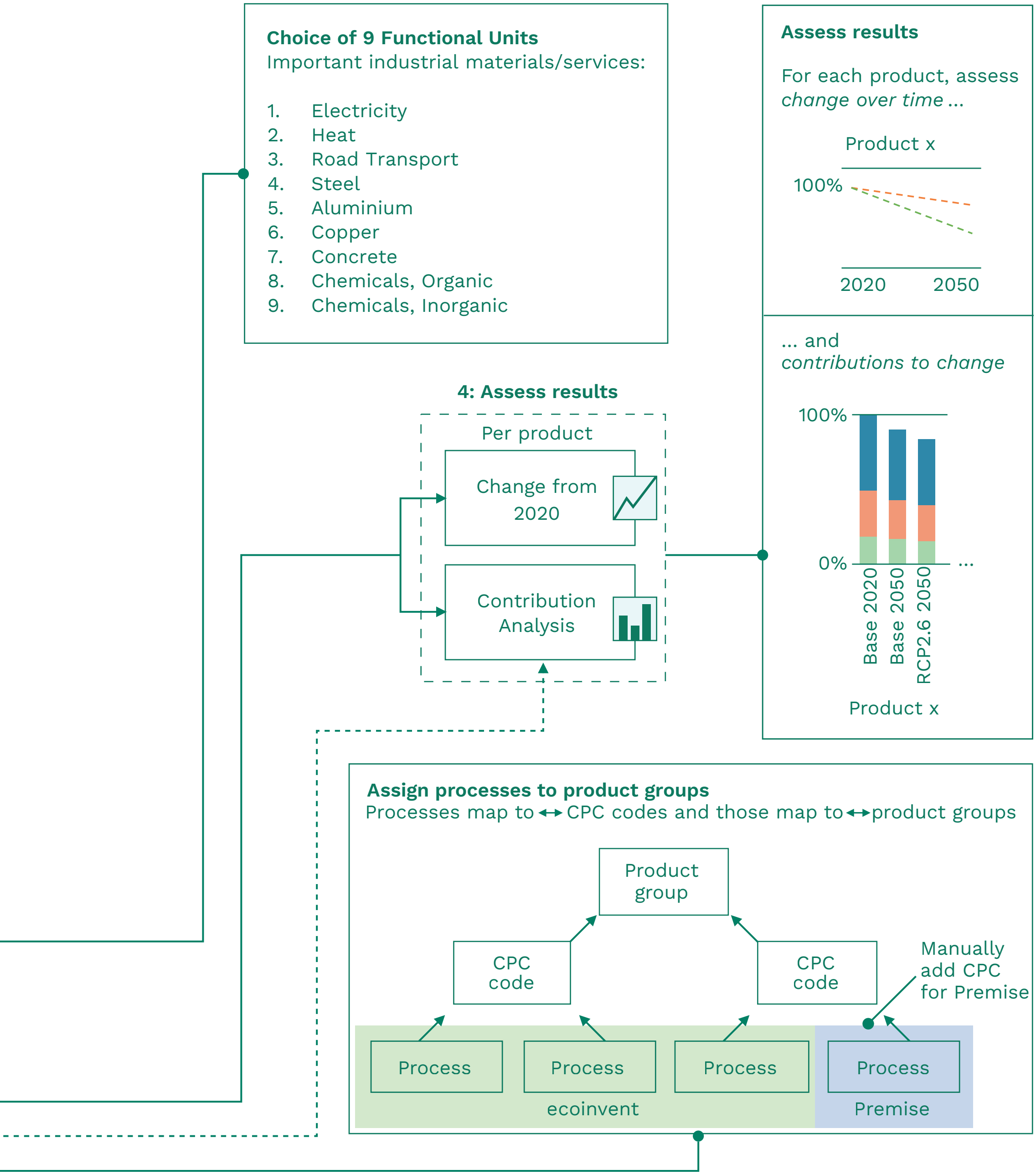


Figure 6.1 - Overview of our approach. We 1: choose scenarios and generate three scenario databases (section 6.2.2), 2: we define which processes serve as FU and their amount (section 6.2.3) and 3: choose impact categories (section 6.2.4), then we calculate LCA impact results and analyze 4: for each product group the change between scenarios (section 6.2.5) and what product groups contributes to those changes (section 6.2.6).

6.2.1 Workings of *Premise*

We shortly describe here some aspects relevant to how *Premise* works for this specific study, for more general information we recommend reading Sacchi et al. (2022) and the documentation (Sacchi, 2025b).

We make a distinction between the following (Steubing et al., 2023):

- *Premise* as a software library: If no other distinction is given we are discussing the software,
- *Premise* scenarios: The data from IAM-SSP-RCP combinations plus data from other sources for additional changes made by *Premise,*
- *Premise* databases: The resulting pLCI databases LCA practitioners can use generated by *Premise* from a *Premise* scenario and ecoinvent.

Premise takes input data from different IAMs such as shifts in electricity generation technologies or energy mixes from IAM-SSP–RCP scenario combinations. *Premise* then translates this into changes on the inventory level based on those scenarios. These changes are made either to existing processes, or to newly added processes. IAMs provide general information, which needs to be made specific to be used in LCA, for example, an IAM may prescribe a certain market share of 'electricity from solar' in a given scenario and year, but which specific technologies to generate that solar electricity is not provided. *Premise* developers need to make assumptions, either based on their own expertise or literature to map these high-level changes to inventory-level data. Furthermore, *Premise* makes other changes as well, which are not directly linked to the scenario data, like adding new battery chemistries, or ore grade decline data to alter mining processes. All *Premise* scenario data is eventually mapped to inventory data that practitioners can use in a *Premise* database. *Premise* generates reports on the changes that have been made to an underlying ecoinvent database with a *Premise* scenario to generate a *Premise* database and the documentation (Sacchi, 2025b) provides more information about additional changes.

6.2.2 Scenario selection & Database generation

We assess two *Premise* scenarios, the IMAGE SSP2 Base scenario and the IMAGE SSP2 RCP2.6 scenario, we assess these scenarios for 2020 and 2050. The IMAGE SSP2 Base scenario assumes global society follows current emission trajectories without major changes (thus base), which results in RCP6, suggesting >3 oC warming in 2100, the IMAGE SSP2 RCP2.6 scenario assumes a scenario where warming in 2100 is limited to below 2 oC (Van Vuuren et al., 2011). The year 2020 is a common point from which the two scenarios diverge, thus we create three *Premise* databases: The 2020 SSP2 Base database, the 2050 SSP2 Base database, and the 2050 SSP2 RCP2.6 database. As the goal of this study is to assess the effects of scenario changes from *Premise*, the ecoinvent database itself is not used in this study directly. Furthermore, not all FUs we assess exist in ecoinvent (FUs are presented in the next section).

We make use of the IMAGE (Stehfest et al., 2014) implementation in *Premise*. We use Brightway v2.4.6 (Mutel, 2017) and *Premise* v2.2.9 -the most recent version of *Premise* at the time of writing- and ecoinvent v3.10.1 cut-off (Wernet et al., 2016) for our analysis, the most recent compatible ecoinvent version compatible with this version of *Premise*.

6.2.3 Choice of Functional Units

With well over 30000 processes in each scenario database it becomes impossible to comprehensively show the impact change and contributions to those changes for all processes. Instead we choose a small subset of nine products which are (directly or indirectly) important to industry to assess the changes *Premise* makes. Where possible, we use high-level processes like markets. Doing this allows *Premise* to make changes to production mixes and production processes in different regions where relevant for the scenarios we use.

We define a set of FUs focused on industrial goods, utilities and services. The focus is on industry as ecoinvent and additional inventories in *Premise* represent these relatively well. Furthermore, this set of FUs is responsible for considerable climate change impacts, is produced in large volumes or has major expected increases in demand. We attempt to strike a balance between showing wide coverage of important industrial products while limiting the total amount to allow more in-depth assessment of results.

We make use of the following nine FUs presented in Table 6.1.

#	FU	Name	Database identifier	Relevance
1	1 kWh	**Electricity**	Market group for electricity, high voltage, World	Direct contribution to global climate change impacts *Sources:* • *Climate Watch, 2024* • *Gütschow & Pflüger, 2023* • *Harpprecht et al., 2024, 2025* • *UNEP, 2023* • *UNFCCC, 2022*
2	1 MJ	**Heat**	Market for heat, from steam, in chemical industry, World	
3	1 tkm	**Road transport**	Transport, freight, lorry, unspecified, long haul, World	
4	1 kg	**Steel**	Market for steel, low-alloyed, hot rolled, GLO	
5	1 kg	**Aluminium**	Aluminium ingot, primary, to aluminium, cast alloy market, GLO	Major metal with large dependence on electricity for production *Sources:* • *Harpprecht et al., 2024, 2025* • *UNEP, 2023* • *Watari et al., 2022*
6	1 kg	**Copper**	Market for copper, cathode, GLO	
7	1 m³	**Concrete**	Market group for concrete, normal strength, GLO	Major construction material with large contribution to global climate change through cement *Sources:* • *Climate Watch, 2024* • *Gütschow & Pflüger, 2023* • *UNEP, 2023* • *UNFCCC, 2022*
8	1 kg	**Chemicals, Organic**	Market for chemical, organic, GLO	Major contribution to environmental impacts through dependence on energy and fossil feedstocks *Sources:* • *Climate Watch, 2024* • *Gabrielli et al., 2023* • *Gütschow & Pflüger, 2023* • *UNFCCC, 2022*
9	1 kg	**Chemicals, Inorganic**	Market for chemical, inorganic, GLO	

Table 6.1 - Functional Units used in this study. The columns show from left to right: the FUs numbering, the functional unit amount, the name we use in this study is marked in bold, the name in Premise databases is given and relevant sources as to why they are important are given.

One category of product that may seem to be obviously missing is agricultural products. Despite the substantial environmental footprint of the agricultural sector, we omit these as there is not one single or a few obvious products that could well represent this sector in our assessment. However, we still assess the contribution of the Forestry and Agriculture sector to the products above, as explained in section 2.6 below.

The above process names listed in brackets are the names and regions in the scenario databases. Any time we refer to one of these FUs in the further text, its name will be written in **bold**. Some of these processes are part of sectors directly changed with *Premise* (**Electricity, Heat, Road Transport, Steel, Concrete**), though the others will also be affected by changes in other sectors.

6.2.4 Choice of Impact Categories

Despite the primary focus of IAMs on climate change resulting in that same focus on climate change related changes by *Premise*, we will be using the EF 3.1 (EC, 2022) impact categories, to demonstrate the effects of changes in *Premise* in a broad range of impact categories. That said, we will mainly highlight climate change results to assess how this focus affects impacts to climate change. We also assess the impact changes to 15 other impact categories to demonstrate how this focus on climate change affects other impact categories. Full results for all impact categories are available in SI 1.2. For Climate change, we account for biogenic carbon flows (e.g., CO_2 uptake has a -numerically-negative impact, and burning biogenic CO_2 will have a positive impact) as prescribed by *Premise*[1].

6.2.5 Assessing impact changes

To assess the differences between scenarios, we calculate the impact score of each FU in each database and compare the relative change in score for each FU compared to the 2020 SSP2 base database, calculated as 'new' divided by 'old': ***2050 Scenario / 2020 Base***. Sacchi et al. (2022) already compared the total impact change between databases

[1] *https://github.com/polca/premise_gwp*

for some combinations of their original 5 sectors in their original introduction of *Premise* (2022), but assessing in this manner allows us to see the change in impacts of individual FU as opposed to a general idea of impact change throughout a *Premise* database.

6.2.6 Assessing contributions

To gain deeper insight into the effects changes of *Premise* have, we next assess the contributions from large product groups to each product.

Product groups
With well over 30000 processes in each scenario database, it becomes infeasible to assess the contribution of single processes, instead, we assess the contribution of fourteen product groups and one *Other* group for any remaining processes.

1 *Forestry & Agriculture**	6 *Steel & Iron**	11 *Cement & Clinker**
2 *Ores & Minerals**	7 *Aluminium*	12 *Construction*
3 *Energy resources**	8 *Copper*	13 *Transport**
4 *Electricity**	9 *Other Metals**	14 *Waste*
5 *Heat & Steam**	10 *Basic Chemicals**	15 *Other*

We map each of the processes to a product group in two steps as shown in Figure 1: First, processes in our scenario database are mapped to Central Product Classification (CPC) V2.1 (UN, 2015) codes, for ecoinvent, all processes are already assigned a code, for processes added by *Premise*, we add CPC classifications. As the CPC scheme does not completely match our groups of interest, we further aggregate CPC codes into the fifteen product groups shown above. We explain this mapping procedure in more detail in SI 1.1.

Any time we refer to one of these groups -and to avoid confusion with FUs- in the further text, product groups will be written in italic. The groups marked with * are (partially or completely) altered by the *Premise* scenarios. We refer to the *Premise* documentation (Sacchi, 2025b) for an overview of exact changes. As an example for Other Metals; this would be production of battery metals, e.g., Lithium and Cobalt. Additionally, *Premise* implements CCS, but it does so in different ways depending on the sector where it is implemented, effectively meaning CCS cannot be assessed as a single product group in our approach.

In addition to the product groups that *Premise* directly changes, we also assess some other relevant groups; we add the metals product groups (*Aluminium*, *Copper* and *Nickel*) as these are often of interest in prospective LCA (Harpprecht et al., 2024). We add Construction as it is deeply integrated into LCI databases, despite often not being in the foreground (Frischknecht et al., 2007). Finally, we add Waste as it is relevant from a life cycle perspective.

Contributions from product groups
We assess the Direct contributions (direct contributions are the contributions caused by the elementary flows (EFs) from a process where those flows occur Srocka & Montiel, 2021; van der Meide et al., 2025) of the product groups, e.g., the climate change contribution of Energy resources to Electricity could be the effects of mining coal, gas, and other fossil fuels for electricity production.

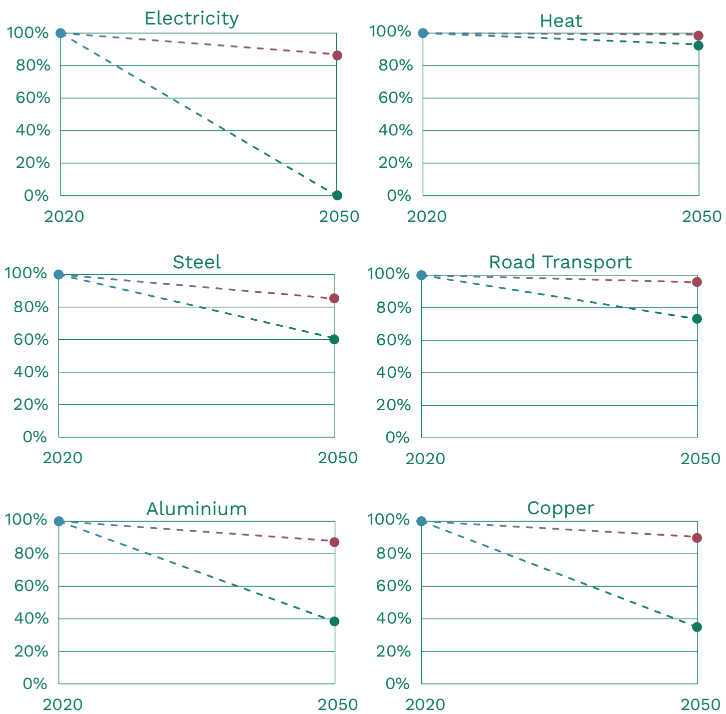
We do process group contributions (van der Meide et al., 2025) based on the 15 product groups we defined above.

Additionally, in SI 1.2, we also assess the combination of Direct+Indirect contributions. Indirect contributions are from all EF of processes contributing to the intermediate flows (products) (van der Meide et al., 2025). An example of this could with the contribution from the *electricity* group to **Steel**. Here, all impacts to produce the electricity for steel production would be included in the electricity group, the CH^4 released during the mining of coal (in the energy resources group) for the production of electricity (in the *electricity* group) would be included as contribution from electricity to **Steel**. This is explained in more detail in (van der Meide et al., 2025). With the combined Direct+Indirect approach, we assess how contributions propagate through different sectors, providing a 'connector' role (Reinhard et al., 2016) for some sectors. We adopt the Hypothetical Extraction Method from Input Output Analysis (van der Meide, 2025a) for this combined perspective and explain this approach in more detail in SI 1.1. By using both a Direct and Direct+Indirect approach, we can take multiple complementary perspectives on the contribution of each product group to the FUs.

6.3 Results

6.3.1 Impact changes in different scenarios

For Climate Change, we show impact changes for each product in Figure 6.2 and provide results for all impact categories in SI 1.2. We go deeper into the causes of our observations in the section after this with our contribution analysis. Overall, we see the expected result that the 2050 Base database has lower climate impacts compared to the 2020 Base database, and that the RCP2.6 2050 database has lower climate impacts compared to both scenarios. We also see that the 2050 Base database does not have major changes (max 15% reduction) in climate change impact compared to the 2020 Base database. One notable product is **Heat**, where impacts change very little between the different *Premise* scenarios compared to the other products, despite this being a sector that is changed by Premise. However, it should be noted that this result excludes a possible larger difference with ecoinvent, which was not assessed.



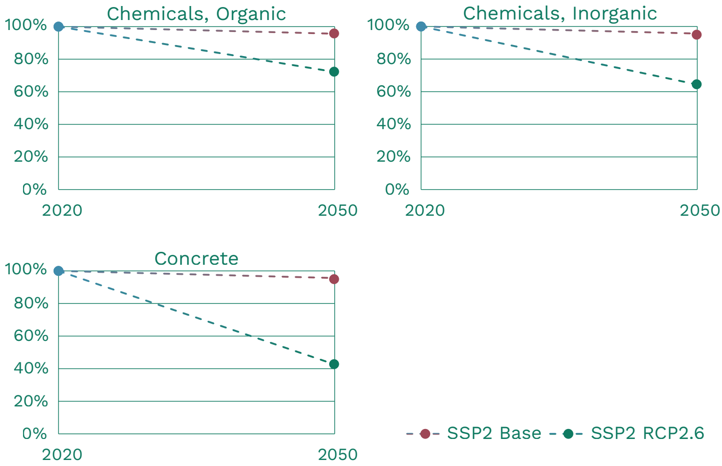


Figure 6.2 - Overview of the relative change of the Base 2050 (orange) and RCP2.6 2050 (green) scenarios from the Base 2020 scenario in Climate Change impacts for each of the 9 products. Note that the dotted line does not represent data points between 2020 and 2050 but is a visual aid to show the direction of change.

6.3.2 Direct contributions

In Figure 3 below, we show the Direct contributions from each of the product groups to each product in each of the 3 scenarios for Climate Change. Contribution results for all impact categories are presented in SI 1.2. Each stacked bar shows the contributions from a product group in a specific scenario, normalized to the SSP2-Base 2020 database; the black diamonds show the total change compared to the SSP2-Base 2020 database, similar to Figure 2 above. We find that total impact results are decreased through carbon uptake causing negative contributions from agriculture, though this result is skewed through our cradle-to-market approach, that biogenic carbon is generally emitted later, unless it is compensated for with CCS. For example, the Climate Change result for **Electricity** would still be low in the RCP 2.6 2050 database without the biogenic carbon contribution (~15% of 2020), though notably less with it included (~1% of 2020).

Also shown in Figure 3 is that the product groups *Electricity, Heat & Steam*, *Transport, Steel & Iron, Cement & Clinker* and *Chemicals* are primary direct contributors to their own respective FUs (**Electricity, Heat, Road Transport, Steel, Concrete** and both chemical products:

Chemical, organic and **Chemical, inorganic**). This means that these products are strongly affected by their own Direct contributions. Of these, only *Electricity, Steel & Iron* and *Cement & Clinker* show major changes. One other major product group contributing to all products is *Energy Resources*. The other products (A**luminium** and **Copper**) are also mainly affected by the previously mentioned product groups, primarily *Electricity* and *Heat & Steam*, though to a lesser extent than the product groups above.

Changes in impact for the FU **Electricity** are mainly affected by reductions in direct contributions from itself and *Forestry & Agriculture*. Changes in impact for **Road transport** are mainly from *Electricity* and *Forestry & Agriculture*, with little change in direct contributions from itself. Changes in impact for the metals (**Steel**, **Aluminium** and **Copper**) are mainly affected by reduced contributions from *Electricity* and *Energy resources*. This confirms that the product group *Electricity* is a major contributor in reducing climate change impacts. Finally, we see that changes in impact for **Concrete** are mainly affected by *Cement & Clinker*.

When we look more in-depth at the change in contribution from the product group *Electricity*, in Figure 3 we find that **Road transport, Concrete** and **Chemical**, **Organic** have a much higher relative impact from *Electricity* in the RCP 2.6 2050 database compared to Base 2020, this means these products make more use of electricity in the given scenario.

6.3.3 Direct and Indirect contributions

We also include a perspective of both Direct+Indirect contributions from each sector to each sector in SI 1.2. Contrasting to the Direct-only perspective for all databases for Climate Change above, we find that *Energy Resources* becomes more relevant in contribution for all FUs and scenarios, especially for **Chemical**, O**rganic** (45% - 57% of total impact). Transport also has a higher contribution for most FUs (from 10% to 17% avg.). Ore & Minerals becomes has a higher contribution for metals (**Steel, Aluminium**) but especially **Copper** (from 1% to max. 38%). Ore & Minerals also becomes more relevant for **Concrete** (from <1% to max. 9%) and **Chemical**, **inorganic** (from 2% to max. 22%). Chemicals also has a higher contribution for the metals, especially **Aluminium** (from <1% to max. 19%). This indicates that the product groups *Ore & Minerals*,

Climate Change Direct contribution from product groups to products in different scenarios

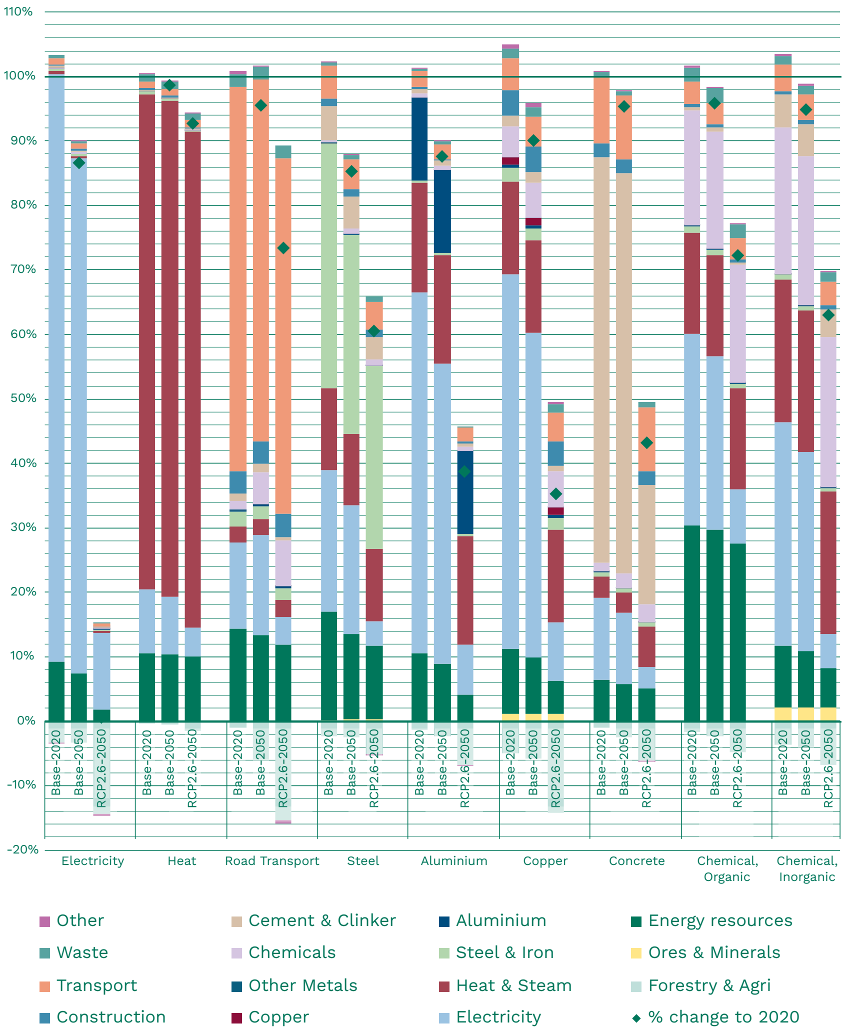


Figure 6.3 - Direct contributions for Climate Change of product groups to products. Each column represents Direct contributions from product groups to that specific product/scenario combination using SSP2-Base 2020, SSP2-Base 2050, and SSP2-RCP2.6 2050 databases. Each result is normalized to the Base-2020 database result of that product group, with a green diamond showing the percentage of the 2020 impact (e.g. a diamond at 80% implies the impact is 20% reduced). Due to (numerically) negative contributions, bars can total over 100%, as negative contributions offset all contributions >100%, the total will be 100%. For the exact values for this graph, see SI 1.2

Energy resources, *Chemicals* and *Transport* have strong connector roles, despite not always having high direct contributions themselves in each of the databases. Finally, specifically between the Base 2020 and RCP2.6 2050 databases, we also see that *Electricity* decreases in importance as a product group (37% avg. decrease), more so than we see with just Direct contributions (30% avg. decrease), due to the additional use of biomass (in the *Forestry & Agriculture* group) and CCS (of which a part happens directly in the *Electricity* group).

6.3.4 Impacts in other impact categories

We show an overview of our most relevant findings for all impact categories in Figure 6.4. This figure shows for each impact category the change in impact compared to the 2020 Base database for both 2050 databases. In SI 1.2 we show the Direct and Direct+Indirect contributions for each product group for each impact category.

In general, the trend we see is that impacts decrease the most in the RCP2.6 2050 database, in line with the storylines for both scenarios. We find that **Electricity** is generally a product with larger changes (Base 2050: 19% avg, RCP 2.6 2050: 70% avg.) than average (Base 2050: 10% avg, RCP 2.6 2050: 26% avg.), additionally, **Road Transport** and **Aluminium** are often found to have high changes (max. 47% and 151% increase compared to Base 2020 respectively). Of these, changes in impacts from Aluminium impacts are primarily driven by changes in the *Electricity* product group, as shown in SI 1.2.

With regard to impact categories, the following show the least change overall: 'Ecotoxicity, Fresh water' (Base 2050: 5% avg, RCP 2.6 2050: 19% avg.), 'Human Toxicity, Carcinogenic' (Base 2050: 3% avg, RCP 2.6 2050: 11% avg.), 'Ozone depletion' (Base 2050: 8% avg, RCP 2.6 2050: 13% avg.) and 'Water use' (Base 2050: 9% avg, RCP 2.6 2050: 12% avg.). Contrastingly, specifically in between the Base 2020 and the RCP 2.6 2050 database, 'Climate Change' and 'Eutrophication, freshwater' show major decreases overall (with -47%, -42% avg. respectively). Furthermore, 'Ionising Radiation: Human Health' shows the largest difference between the two 2050 databases, with major decreases in the Base database (with -56% max.) and major increases in the RCP2.6 database (with 151% max.). 'Land Use' is variable with major increases or decreases depending on the product with no obvious pattern. We

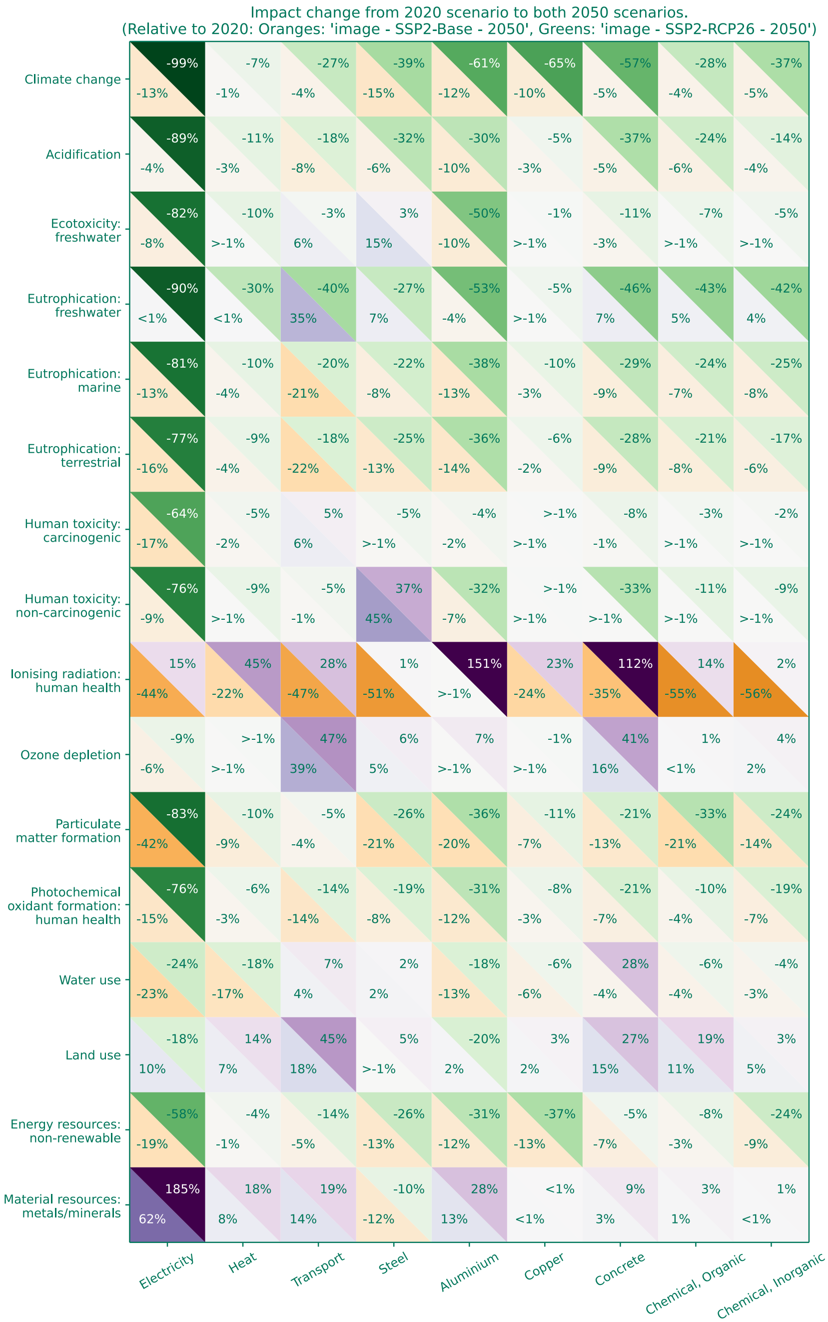


Figure 6.4 - Combined heatmap showing relative change in impact from 2020 scenario to both 2050 scenarios. Lower-left triangles in Orange for SSP2 Base 2050. Upper-right triangles in Green for SSP2 RCP2.6 2050. Columns show FUs, rows show impact categories. Note that purple triangles mean impact is increased compared to 2020.

6

also see a substantial increase in 'Material resources, Metals & Minerals' impact for **Electricity** (Base 2050: 62%, RCP 2.6 2050: 185%), this comes from increased material intensity from use of batteries and solar generation, conversely, we find decreases for **Steel** (Base 2050: -10%, RCP 2.6 2050: -12%), which comes from increased steel recycling.

6.4 Discussion

6.4.1 Key findings

We find that the product group *Electricity* is singularly the most important contributor to decrease future climate change impacts. *Forestry & Agriculture* is also a major contributor to decrease climate change impacts. Only the use of biogenic carbon when combined with CCS can be a source of CO^2 removal for the *Forestry & Agriculture* sector. We have also found that product groups like *Ore & Minerals*, *Energy resources*, *Chemicals* and *Transport* have strong connector roles (meaning they have relatively low direct contributions but link to processes with high impacts (Reinhard et al., 2016)) and can help reduce climate change impacts if used differently or less (e.g. switching ore types, or switching to electrified transport). Furthermore, we find that *Heat & Steam* is another important contributor to climate change impacts, with almost no change between databases in the FUs studied. While the *Heat* product group is currently changed by *Premise*, it is confirmed to be re-evaluated a future version of *Premise* (Sacchi, 2025a).

CCS is an important driving factor for decarbonization in *Premise* scenarios -specifically in the IMAGE IAM model (Stehfest et al., 2014)- but the implementation of CCS on the inventory level in *Premise* makes it challenging to assess the effects of CCS properly. Depending on whether CCS is modelled directly within a production process (e.g., clinker production) or indirectly via a separate CCS process (e.g., direct air capture), the flow of captured CO_2 may not be modeled as an elementary flow. While both implementations can technically be correct depending on the context, the use of different approaches makes it challenging to assess the effects of CCS at the scale of our assessment and impossible to create a single 'CCS' product group to assess contributions from.

We have shown that while climate change impacts can be expected to go down over time, depending on the specific scenario, we also see trade-offs between impact categories. These findings are in-line with recent work from Harpprecht et al (2025, Fig. 9) and Müller et al. (2024, Fig. 8) who studied steel and cement respectively. However, they do find that these trade-offs occur with different impact categories. While we cannot make direct quantitative comparisons, this still indicates that small modeling changes could contribute to high uncertainties in other impact category results than climate change.

As we shortly discuss in our results and more completely in SI 1.2, 'Land use' is an impact category with large changes in impact scores and large contributions from some product groups. We also see exceptional -but less large- land use impact changes in other recent work from Harpprecht et al. (2025) and Müller et al. (2024) who both use *Premise* as well. We discuss potential data problems in *Premise* based on our findings further in SI 1.2.11.

While *Premise* implements many different changes in different sectors, many are focused on improved technologies related to the energy transition or reduced climate change impacts. More negative potential changes have received less attention so far. For example ore grade has been established as an important variable for the environmental impact of many metals, (Aramendia et al., 2023; Harpprecht et al., 2021, 2024; van der Meide et al., 2022), inventories in *Premise* in product groups like Copper and many metals in the Other Metals product groups are often not changed to account for this. Not considering ore grade decline and other potential negative developments could mean impacts for metals production and other processes could turn out to be higher than found with current *Premise* databases. Such future developments should ideally also be included in pLCI databases for completeness, though attention should also be paid to keeping such work consistent with existing scenario story lines.

Our assessment shows that while *Premise* is a useful tool for the Prospective LCA community, there could be many specific details and nuances that practitioners need to be aware of, depending on the application. How representative the changes *Premise* makes are for other impact categories besides climate change, and how accurate these are, remains a question that is hard to answer. Though efforts are being made to make future scenarios more accurate for other impact categories as well, for example, changes to Ozone depletion (Van Den Oever et al., 2024). While some practitioners are aware of the additional uncertainty in interpreting LCA results for other impact categories besides climate change, this awareness may not be present in some parts of the *Premise* user community. Considering the advice Sacchi et al. (2022) give that “toxicity related indicators” should be considered to have high uncertainty and our findings for ‘Land use’, we advise practitioners to be very cautious with interpretation of any impact categories besides climate change.

6.4.2 Limitations

We identify two limitations to our work, both specifically relate to our choice of FUs.

First, we only assess the nine FU from over 30000 processes in *Premise* databases. While it is not reasonable nor feasible to assess each of those processes, we made a choice to limit our assessment to only nine processes. This is a result of balancing a ‘broad and shallow’ approach versus a ‘narrow and deep’ approach. Where the former assesses many processes superficially and the latter assesses a small set of processes in more detail. An example of a more ‘broad and shallow’ approach could be the work of Reinhard et al. (2019) on the ecoinvent database or the original presentation of results from *Premise* databases by Sacchi et al. (2022). We instead chose a ‘narrow and deep’ approach to gain deeper insight into the causes of changes, which may be missed with a more shallow approach.

Secondly, our specific choice of processes could also be considered a limitation. We chose these processes specifically for several reasons: They have global coverage (either the ‘GLO’ or ‘World’ regions) with many processes from each region feeding into those processes. They are often-used products by other processes, either directly or indirectly and contribute to global climate change impacts substantially. In our assessment, the product groups our FUs belong to contribute over two thirds of the climate change impact on average. Additionally, we chose a mix of products that are changed by *Premise* so we could thus assess the sectoral changes that affected these processes, but also processes that have no direct changes, so we could see to what level they were still affected by changes. As each practitioner could have different interests in processes, we encourage practitioners to critically inspect processes relevant to them in *Premise* databases themselves by for instance making use of our code supplied in van der Meide (2025b) to investigate processes they find of interest.

6.5 Conclusions

In this study, it was our goal to systematically analyze the effects of changes between several pLCI databases generated with *Premise* on results for practitioners, with the aim to give practitioners better insight into what kinds of changes they may expect in *Premise* databases and how those may affect their own results. We have shown with our approach that the effects of changes made by *Premise* have a wide reach within a database in terms of impact changes. We find that while climate change impacts for all products that we investigated decrease over time, they may cause substantial trade-offs in other impact categories, yet the quantification of these trade-offs is highly uncertain.

Our approach can help practitioners find potential errors -or otherwise product groups/processes of interest- in an LCI database, it could be useful for practitioners to adopt similar checks into product groups or processes to gain a deeper understanding of their results or find potential problems with inventory modeling or data. We also show that including an 'Indirect' perspective is important to highlight product groups connecting impacts from other product groups, an insight that a "Direct-only" perspective cannot provide, in line with findings by Reinhard et al. (2019). Though the approach of Reinhard et al. only allows the investigation of single processes, ours can assess groups of processes.

For practitioners, we recommend *Premise* be used primarily for assessing Climate Change impact and that practitioners emphasize the additional data uncertainty for other impact categories compared to e.g. the use of ecoinvent. Practitioners should explicitly mention which version of *Premise* databases and other software they use as continual development of the tool is likely to make their work irreproducible otherwise. While continuous improvement has advantages, it is also important for practitioners to realize this can lead to changes in results and to be explicit about what software versions they use to maintain replicability. Another option is to slow down the update cycle of *Premise*, e.g., aligning it with yearly updates from ecoinvent, this would give more time for quality assurance and fewer different versions used by practitioners, making studies using *Premise* more consistent with each other and more comparable. We discuss this in more detail in SI 1.2.11. We strongly recommend practitioners to review other recent work aimed at helping practitioners make correct use of *Premise* like that from de Bortoli et al. (2025) and Paris et al. (2026).

While we have taken a critical stance toward some aspects of *Premise* as a tool and the data it uses, we still recommend using it for prospective LCA and we encourage its developers to continue improving the tool. However, we suggest newly added LCI data to be peer-reviewed by experts in relevant fields to reduce inaccurate sources and mistranslation, we discuss this in more detail in SI 1.2.11.

6.6 Data Availability Statement

All data used in this manuscript is available in the Supplementary Information and code repository.

6.7 Funding declaration

The authors declare no external funding was used for the creation of this manuscript.

6.8 Competing Interest statement

Nils Thonemann serves as Guest Editor for this ‘Collection’ to which this paper was submitted but was not involved in the editorial handling of this manuscript.

6.9 Author Contributions

The authors contributions according to the CRediT taxonomy are:

	M. van der Meide	M. Hu	B. Steubing	N. Thonemann	A. Tukker
Conceptualization	●		●	●	
Data curation	●				
Investigation	●				
Methodology	●		●	●	
Software	●				
Supervision		●	●		●
Visualization	●				
Writing - *Original draft*	●	●	●	●	●
Writing - *Review & editing*	●	●	●	●	●

Chapter 7
Conclusions

7.1 Introduction

Life Cycle Assessment (LCA) is widely used to assess environmental impacts. Yet methodological advances remain necessary, particularly in Contribution Analysis (CA), which requires clearer structuring and where missing, formalization. Specifically, the field would benefit from an overarching definition of CA that accommodates current practice and from consistent terminology that enables practitioners to communicate and interpret results more reliably.

In addition, while some current CA approaches can assess both Direct contributions (e.g. CO_2 emitted from electricity production) and Indirect contributions (e.g. the CH_4 released during the mining of coal for electricity production to be included as contribution for electricity production), the analysis of both these perspectives together for large groups of processes could not be done effectively. This could be useful for the analysis of the contribution from industry sectors or countries. It is important to investigate if this problem could be resolved with an additional CA approach. To this end, this thesis investigated if the Hypothetical Extraction Method (HEM) from Input Output Analysis could be used for that purpose.

CA is especially important in the context of prospective LCA (pLCA), where scenario-driven change makes it harder to interpret results. In pLCA, the most used tool to generate future versions of background databases is *Premise* (Sacchi et al., 2022) currently. This tool allows the generation of prospective LCI databases based on storylines that prescribe combinations of global warming in Representative Concentration Pathways (RCPs) (Van Vuuren et al., 2011) and how well global society adapts to and mitigates climate change in Shared Socioeconomic Pathways (SSPs) (O'Neill et al., 2014). These storylines are implemented in Integrated Assessment Models (IAMs) which project quantitative results from these scenarios into the future. *Premise* finally makes use of these IAM outputs and maps them to changes in the ecoinvent LCI database. With the numerous scenario changes *Premise* can include, it becomes more important to deeply understand what contributes to impact changes.

To evaluate and assess the specific challenges different approaches to CA pose and learn how they could be overcome, this thesis applied CA in three pLCA cases.

These cases were chosen for the following reasons: 1) cobalt production given its low production scale but high expected change in demand; 2) sand and gravel production, given concrete demand and the vastly larger production scale relative to cobalt; and 3) evaluation of the pLCA tool *Premise* via analysis of nine commonly used industrial products to clarify drivers of future impacts. Overall, the real-world application of CA in pLCA is a necessary step to improve understanding of CA.

Via this, this thesis aimed to realize the following main objective: to structure and -where necessary- formalize CA and to learn from practical cases so that this toolbox of approaches becomes more useful to LCA practitioners. So, based on the above, this thesis investigated the following Research Question and sub questions:

How can Contribution Analysis be structured and utilized to better analyze environmental impacts in Life Cycle Assessment?

1. How can Contribution Analysis be structured and formalized?

2. How can indirect contributions from groups of processes be better quantified and understood in LCA?

3. What can we learn from Contribution Analysis results in practice, applied to prospective LCA of 3 cases?
   - Prospective LCA of Cobalt production
   - Prospective LCA of Sand and Gravel production
   - Prospective LCA of Nine commonly used products from *Premise*

The following sections provide the key findings and conclusions to this thesis. In section 7.2, the three sub-questions posed in the introduction are answered which lead to the answer to the research question. Next, other contributions from this thesis are discussed in section 7.3. Next, some of the limitations and potential future work related to this thesis are presented in section 7.4. Finally, section 7.5 discusses some reflections and implications of this thesis.

7.2 Answers to Research Questions

7.2.1 Sub Question 1: How can Contribution Analysis be structured and formalized?

Chapter 2 answered this question through reviewing existing literature on the theory of CA and analyzing how CA was applied in literature. Each of the existing approaches was structured into five Direct and three approaches where Direct and Indirect perspectives are combined (Direct+Indirect). This led to eight approaches which were discussed and compared both following a single simplified case study designed to highlight differences and through their mathematical formulation. Furthermore, when CA is used, it should be described as contributing *from* something (e.g. a process or EF) *to* something (e.g. LCI or a characterized result).

To start with, while many similar definitions or descriptions of CA existed, none of them accurately and fully described CA. Chapter 2 therefore proposed a new definition which should better cover most cases. This definition was extended from the definition given by ISO 14044 (2006) and Guinée et al. (2002): *A step of the Interpretation phase to assess the contributions from entities like individual life cycle stages, (groups of) processes, elementary flows and indicator results to the overall (or a partial) LCI or LCIA result (e.g. as a percentage).*

Furthermore, Chapter 2 identified eight approaches to CA and defined them carefully. allowing for easier comparison and understanding. A main differentiation between approaches being either Direct or combined Direct+Indirect perspectives is used. Direct contributions are the contributions caused by the elementary flows (EFs) *from* a process where those flows occur (Srocka & Montiel, 2021). For instance, the CO^2 emitted *from* electricity production by burning coal in a power plant is a Direct contribution from the process 'electricity production with coal'. In contrast, Indirect contributions are the contributions caused by the production *from* an intermediate flow (e.g. a product) from a process, this would include the contributions *from* all EFs of all processes *Indirectly* needed to produce that product in the required amount (e.g. the CH^4 released during the mining of coal for electricity production to be included as contribution for electricity production).

The five Direct approaches are:

- **Individual Elementary Flow (EF) CA** from specific individual EFs from single processes (Individual EF CA),
  - e.g. the contribution from CH_4 emission from a single process 'coal mining'.
- **EF CA**, from one EF across all processes,
  - e.g. the contribution from all CO_2 flows from all processes in the system.
- **Process CA**, from all EFs per process,
  - e.g. the contribution from all EF (CO_2, CH_4 etc.) from the process 'electricity production from coal' to Climate Change impact.
- **EF group CA**, from groups of EF,
  - e.g. the contribution from a group of all carbon containing flows.
- **Process group CA**, from groups of processes,
  - e.g. the contribution from all 'electricity production' processes.

Three combined Direct+Indirect approaches have also been introduced:

- **First-Tier CA**, measuring the Direct contribution from the Functional Unit (FU) process and Direct+Indirect contribution from each intermediate flow of the FU,
  - e.g. the contribution from 'aluminium production' and contribution from all intermediate flows needed for 'aluminium production' like 'electricity' and 'bauxite'.
- **Life Cycle Stage CA**, from life cycle stages,
  - e.g. the contribution from life cycle stages like 'production', 'use' and 'end of life'.
- **Path CA**, contributions from a path (e.g. value chain) of processes, often visualized in Sankey diagrams,
  - e.g. the contribution *from* intermediate flows throughout the product system lead to the final LCA score, showing the 'path' of contributions.

Each of these approaches provides a unique perspective into results of an LCA. Combining approaches can provide deeper insights into results as well.

Finally, guidance was formalized for practitioners on how to report and present their CA methodologies and results, such that LCA studies could become more replicable and interpretable.

In total, the work in Chapter 2 should contribute to higher quality and more reproducible CA's in LCA literature and by this, result in better founded conclusions of LCAs.

7.2.2. Sub Question 2: How can indirect contributions from groups of processes be better quantified and understood in LCA?

Chapter 3 answered this question by investigating if and how the Hypothetical Extraction Method (HEM) earlier developed and applied for Input Output Analysis (IOA) (Hertwich et al., 2024; Miller & Lahr, 2001) could be used in LCA. When used in an LCA context, HEM could be described as 'assessing the Direct and Indirect contribution from processes -or groups of processes- to the impact of other processes'. While other CA approaches could show the Direct and Indirect contributions of single processes or life cycle stages, the HEM allows practitioners to assess the Direct and Indirect contribution of groups of processes, such as industry sectors or regions. With HEM, groups of processes are not necessarily connected through their flows such as with life cycle stages. For example, in an LCA of steel production, the HEM approach could be used to assess the Direct and Indirect contribution of transport, independent of which production step the transport is related to. The HEM approach was demonstrated in this chapter through introducing four steps to perform HEM in LCA and formalizing the mathematical approach for these steps and showing these results in a simple case study comparison with other CA approaches.

Making use of HEM in LCA specifically provides more insights in cases where an Indirect perspective is required on groups of processes such as industry sectors or regions. While other existing CA approaches have their own advantages, they could not provide this perspective. With direct process group CA, only Direct impacts were included. With First Tier CA, only the FU and flows to the FU could be assessed. With Life Cycle Stage CA, processes need to be connected through their intermediate flows to form stages (e.g. if we consider the last example, a single life cycle stage could not encompass all different 'transport' instances). Path CA can show contribution paths through intricate supply chains, but cannot combine groups of processes. As each of these approaches helps take a different perspective and answer different questions, HEM is not a replacement of any approach but rather an additional approach to take a different perspective on results.

The approach was not only introduced as a theoretical concept but also in terms of mathematical steps to follow the procedure and includes examples in Excel to reproduce results and contains Brightway2 compatible code so practitioners may re-use this approach in their own work.

7.2.3. Sub Question 3: What can we learn from Contribution Analysis results in practice, applied to prospective LCA of 3 cases?

Three case studies were conducted:

- Prospective LCA of Cobalt production
- Prospective LCA of Sand and Gravel production
- Prospective LCA of Nine commonly used products from *Premise*

This question was answered by making use of CA in three separate case studies, each with different topics. The first was a pLCA study on the production of cobalt, in this study, process group contributions were used to assess the contributions to cobalt production impacts. The second was a pLCA study on the production of sand and gravel for concrete production, in this study process group contributions and first-tier (product) contributions were used. In the third study, nine different products from *Premise* were assessed, process group contributions and HEM from the same fifteen groups were applied.

Findings from a study on cobalt production (Chapter 4)
Cobalt production was assessed with pLCA under two different scenarios from 2020-2050 and with four combinations of production variables like ore grade decline and market shares in each of the two scenarios. Process group CA was used to assess what the main contributing process groups were in each of these variable-scenario combinations. The processes were grouped based on the products they produce (e.g. all processes producing ‘electricity’ were grouped together).

This case study provided the main learning that led to the structuring of CA. This study showed that CA should be executed in a more structured manner, to avoid findings that are less-replicable and with less insight into the contributions to impacts. Firstly, the methodology section did not discuss how CA would be performed -though the code in the Supplementary Information was provided-, this made replication more difficult. Furthermore, process group CA was used, though the groups were not well defined and the approach was mis-named as process

CA. Together, these reflections lead to the realization that CA needs to be better structured and approaches need to be communicated clearly.

Findings from a study on sand and gravel production (Chapter 5)
The impacts of sand and gravel production were assessed with pLCA in two scenarios from 2025-2050 assuming different amounts of recycling. The study integrated new recycling processes into the pLCI database and connected this to sand and gravel markets in 26 regions globally, meaning all processes making use of those products would consume the recycled materials. Process group and First-Tier contributions were assessed. These CA approaches were used to assess how conventional production and production from recycling lead to different contributions and to show the effect of sand, gravel and cement on concrete production.

This case study provided as a main learning that current combined Direct and Indirect approaches cannot effectively be applied to large groups of processes. While the First-Tier CA approach is useful to assess the contribution sand and gravel have on concrete production, the focus was on a single 'concrete production' process. This analysis could have been performed on all concrete production processes and all sand and gravel production processes in unison with an approach that could measure the Indirect contribution of groups of processes. Other existing approaches like Life Cycle Stage CA would also not be effective here, as there are many different parallel production routes that could not be mapped to a single stage, however, this might have been possible by grouping life cycle stages. Path CA was not possible for a similar reason, since it requires the analysis of many processes, which cannot be counted together in this approach. These conclusions have led to the implementation of the Hypothetical Extraction Method in LCA presented in Chapter 3.

Despite the limitations of First Tier contributions, it was still possible to provide deeper insight into the total contribution of sand and gravel to the total impact of concrete production. Furthermore, the CA approach was described in the methodology section, making the study more replicable. Providing these insights and methodological structuring were made possible through the work presented in Chapter 2.

Findings from an analysis of several Premise products (Chapter 6)
Nine different products from *Premise* were assessed. Three pLCI

databases were generated with *Premise* to model one base 2020 scenario and two future scenarios for global warming for 2050 from the IMAGE IAM (Stehfest et al., 2014). While it is clear *what* changes *Premise* makes to LCI databases, it remains unclear *what effect* these changes have on environmental impacts and what the main contributions to those impact changes are. A range of products relevant for industry (Electricity, Heat, Road Transport, Steel, Aluminium, Copper, Concrete, Organic Chemical and Inorganic Chemical) were used to assess these impact changes. Process group CA and HEM were used to assess the contribution from fifteen large product groups representing industry sectors producing similar products. These CA approaches were used to assess the Direct and combined Direct+Indirect contribution of these groups to the nine products.

This case provided as main learning that when the contribution from large groups of processes is assessed, it is important to include both a Direct and combined Direct+Indirect perspectives. With the growth of use of tools like *Premise*, the analysis of changes to an LCI database is important and must be assessed. Process group CA is essential in this assessment to show where contributions (or changes in contribution) originate, however, the use of HEM allowed the finding that some sectors play an important role as 'connecting' sectors. These connecting sectors/processes don't necessarily have high contributions themselves, but 'connect' to other processes in the product-system that do through a causal link, e.g. one finding from this study could be the sector 'ore mining and processing' for copper production, which has a low direct climate change contribution, but connects to other sources of impacts such as electricity needed during the mining and processing. If in this case the mining and processing would use less electricity, or from different sources, the impacts may change substantially, this only becomes apparent through including an Indirect perspective. This analysis of Indirect contributions from large process groups was possible through adapting HEM from IOA into LCA in Chapter 3.

Summarizing the learnings from all three cases; the cases show it is important to define clear categories of CA approaches and develop a new approach to analyze the Indirect contribution of large groups of processes in the form of HEM. The practical insights given through performing pLCA in a variety of case studies and critically assessing the possibilities and limitations of CA made it possible to develop this structuring and convert the HEM approach to LCA.

7.2.4. Answering the main research question

Through answering the sub-questions above, it now becomes possible to answer the Research Question:

How can Contribution Analysis be structured and utilized to better analyze environmental impacts in Life Cycle Assessment?

Through dividing CA approaches into two groups of perspectives, *Direct* and *Indirect* and clearly describing how these approaches should be applied *from* some entity *to* another entity CA has been better structured. Furthermore, other approaches may in the future be added into this framework, such as HEM, which was introduced in this thesis for LCA as well. This structure gives practitioners a common language to discuss CA approaches with and helps practitioners choose which approaches they need for their work.

What can be learned as well from this thesis is that it is highly important for a practitioner to understand what questions a specific CA approach can answer and how that may fit in the goal and scope of their LCA study, to describe the methodological approach of CA used in a study and finally to clearly interpret and describe their results. The relatively unstructured approach in the case-study in Chapter 4 (on cobalt) is a clear example of why this is necessary. Chapter 2 in this thesis suggests a clear and structured approach to CA that was used in Chapter 5 and 6 and can in the future be used by other practitioners in their work.

While CA is a large toolbox of approaches, the various approaches all come with limitations of their own. Practitioners should be mindful of these when they make use of CA. For example with the case-study in Chapter 5 (on sand and gravel) it became clear that existing approaches could not provide the entire insight into the contributions of sand and gravel to other products such as concrete, leading to the development of HEM in Chapter 3, which was utilized for this purpose in the case-study in Chapter 6 (on products in *Premise*).

Furthermore, it also becomes clear from this thesis that the use of multiple CA approaches in studies makes sense in many cases, as this can provide multiple perspectives on the same underlying results. Practitioners should carefully consider which approaches are useful on a case-to-case basis to answer their research questions. This was discussed in Chapter 2, but the benefit of taking multiple perspectives to the results of a study are also shown in the case-studies in Chapter 5 (on sand and gravel) and Chapter 6 (on products in *Premise*). The combination of different perspectives, especially combining Direct and Indirect approaches allows for a deeper understanding of LCA results.

7.3 Other contributions of this thesis

In addition to structuring and formalizing CA approaches and introducing HEM to LCA, other contributions have also been made to the pLCA field through the three case-studies from Chapter 4-6.

In the study on cobalt production (Chapter 4), a new ore grade decline model was developed, which models changes in inventory data based on the demand for cobalt. Previous approaches that modeled ore grade decline did so based on progression of time, while in future scenarios regarding the energy transition, it is important to consider the demand for such materials, as those are closely related to the scenario in which they are used. This ore grade decline model was later used in Xu et al. (2022).

In the study on sand and gravel production (Chapter 5), a dynamic stock model was developed to model the recycling of sand and gravel based on how much material becomes available from the building stock and how much demand there is for new buildings. While dynamic stock modeling is not new, this has not yet been applied to assess the recycling potential of gravel and sand in this manner. This recycling model determines the market share between conventional and recycled production. Furthermore, this was integrated into a 'community scenario' for *Premise* such that other LCA practitioners making use of *Premise* can import and use this scenario in their own studies.

Finally, other contributions that may be useful for the LCA community have been made for the work done in this thesis in the form of code contributions to enable CA in the Activity Browser (AB) software (Steubing et al., 2019). While these contributions may not be considered scientific contributions as such, they benefit the scientific community by enabling practitioners to do CA. Contributions relevant to this thesis were the following: Co-authoring the first implementation of CA in AB[3], adding

First-Tier contributions to AB[4] and adding new options for cut-off calculations, in line with PEF regulation (JRC, 2018)[5].

7.4 Limitations and Future Work

One limitation to this thesis, and primarily Chapter 2 and the case studies (Chapter 4-6) is that only CA approaches in literature were studied. LCA is an applied field, and many LCA software alternatives exist, each with their own features. With this spread of software options also come different approaches to CA that are not found in literature, for example a 'Path CA' alternative in SimaPro[6], for which no clear public documentation exists for this approach to be replicated or verified to be correct. Contrastingly, OpenLCA makes use of a modified version (M. Srocka, personal communication, May/June 2025) of the path CA approach (Srocka & Montiel, 2021). While the approach is not clearly communicated in documentation[7], the code is open source and can be reviewed.

The spread of different software implementations for different CA approaches is a risk for LCA practitioners as it may be unclear what approach is really performed 'behind the screens' and for practitioners to verify if the approach is correct. Future work could potentially review different approaches in software based on the same case study implemented everywhere such that results can be compared and the approaches could be 'reverse engineered'. An alternative solution could be for LCA software developers to open their algorithms so their working may be verified. LCA software is the 'lab equipment' of LCA practitioners and the ability to verify the functioning of this equipment is essential for trust in the findings generated in this field.

Another limitation in this study is that CA is only demonstrated to characterized results (e.g. after the conversion from CO_2 and CH_4 emissions to 'climate change impact'). While most studies currently are concerned with characterized results, the inventory, normalized and weighted results should not be forgotten in LCA. Chapter 2 and its Supplementary Information discuss these other entities somewhat, but future work should also more deeply consider CA approaches to other entities. This is also relevant for more complex assessments, such as the recently introduced TimeEx (Müller et al., 2025), where contributions from different time periods become relevant.

While this thesis is able to provide some generalized recommendations on CA approaches, a limitation here is that it is not possible to recommend a specific approach or combination that applies to all cases. A practitioner needs to determine based on the requirements of their cases which approaches to use to provide the insights they need. Future work could focus on more specific recommendations for e.g. specific sectors or product groups with similar requirements in their assessment.

7.5 Reflections and Implications

LCA has become an important method in understanding the environmental impacts of products and services and LCA is still gaining importance in the policy landscape, for example in the European Union with Product Environmental Footprint (PEF: JRC, 2018) and the Carbon Border Adjustment Mechanism (CBAM)[8]. When looking at PEF, it is recommended to make use of CA to identify important entities for sensitivity analysis. Among these entities, life cycle stages are mentioned, but it is never defined how these should be assessed. Furthermore, a cumulative cut-off of 80% (sorted by highest contribution, counting up to 80%) need to be used for sensitivity analysis, though it is never made clear how to manage negative emissions. While the PEF is certainly a step in the right direction for including such guidelines in the first place, it is also clear improvements still need to be made to improve the standard, e.g. by clarifying how to deal with negative contributions.

Prospective LCA specifically is also relevant to help steer technology development and decision making for future technologies and could help prevent lock-in effects where a sub-optimal technology is adopted. While not directly related to policy through standards like PEF or CBAM, results from pLCA studies can be important in the shaping of policies or regulations to steer industries in a cleaner direction. Results from pLCA studies can be used to assess possible futures and what actions need to be taken to steer toward desired future scenarios. pLCA must keep developing and the CA tools to understand results must keep developing as well.

Through the introduction of CBAM and other policies that require LCA, more LCA practitioners are needed and more decision makers are required to understand LCA results. ‘LCA literacy’ is therefore an important topic that must be expanded to these new groups of practitioners and decision makers. This thesis, but specifically Chapter 2, could help increase this literacy.

[3] *https://github.com/LU-CML/activity-browser/commits/Results_Analysis/*

[4] *https://github.com/LCA-ActivityBrowser/activity-browser/pull/1046*

[5] *https://github.com/brightway-lca/brightway2-analyzer/pull/326*

[6] *https://support.simapro.com/s/article/The-Network-Tab-in-SimaPro*

[7] *https://greendelta.github.io/openLCA2-manual/res_analysis/res_sankey.html*

[8] *https://taxation-customs.ec.europa.eu/carbon-border-adjustment-mechanism/cbam-legislation-and-guidance_en*

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Curriculum Vitae

Marc was born in Vlissingen, the Netherlands in 1992. Marc became interested in sustainability in his late teens. Somewhere during this time he saw a 'VPRO Tegenlicht' episode where one of the interviewees had studied 'Industrial Ecology', which sparked his interest.

During his studies for Bacherlor of Science in Mechanical Engineering at the Hogeschool Rotterdam (2013-2017) he did a minor in 'Sustainable Development' at Leiden University. There he learned about the Master of Science programme 'Industrial Ecology' at Leiden University that was also hosted there and decided to enroll (2017-2020). While the programme was intense, the sense of community and deep interests in sustainability of his peers made the effort worth it.

At the end of his masters programme, the Covid-19 epidemic happened, and he was forced to do most of his master thesis from home. Despite the added challenges everyone faced during this time, his thesis supervisor, Bernhard Steubing saw an opportunity to keep working together and Marc started a PhD with Bernhard, Mingming Hu and Arnold Tukker.

During his masters and PhD, Marc also worked on the development of the LCA software 'activity browser', which was quite rewarding in its own right.

After completing his PhD thesis, Marc will continue his academic work as a PostDoc working with Mara Hauck and working on prospective LCA of re-useable solar panels at the Technische Universiteit Eindhoven.

List of publications

First Author

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