Assessing the Environmental Performance of Sugar Beet Pulp-Derived Galactaric Acid in Applications: A Prospective LCA

Aron koning

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By

Aron Koning

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Student number:	5898188 (Delft)	S3666751 (Leiden)
Thesis committee:	Dr. Ir. N. Thonemann	Leiden University
	Dr. ir. J.A. Posada Duque	TU Delft
External supervisors:	Dr. ir. S.N. Moejes	Royal Cosun
	Dr. ir. W. Huijgen	Royal Cosun

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Abstract

This thesis evaluates the environmental performance of Galactaric Acid (Gal-A) derived from sugar beet pulp (SBP), as a potential eco-friendlier alternative to Chromium(III) and Disodium EDTA in industrial applications. Utilizing a prospective lifecycle assessment, the study forecasts the environmental impacts of Gal-A's use in the Netherlands by 2030, focusing on its application as a chelating agent (application 1) in shampoo formulations and as a surface coating for zinc-plated steel (application 2).

The data collection to produce Gal-A was conducted using a mass balanced bill of materials provided by Royal Cosun. A combination of literature data and stoichiometric calculations were utilized for other processes within the study. The literature offered insights into the design of value chains and process data, while stoichiometric calculations allowed for the detailed analysis of chemical reactions and compound formations.

The scaling of the Gal-A production foreground in the thesis is informed by input from process technologists at Royal Cosun, ensuring a realistic and industry-informed projection, with attention to the valorization of side streams and internal recycling flows. For the scaling of other processes, literature research plays a crucial role, particularly in understanding the restrictions on chemicals and the development of novel production processes.

The results indicated for application 1, that Gal-A as a chelating agent in shampoo formulations showed mixed results. While it demonstrated advantages in reducing toxicity impacts due to its biodegradability, it also presented trade-offs in eutrophication, soil use, and acidification. These trade-offs are linked to the agricultural origins of the sugar beet pulp and the enzymes used in Gal-A's production.

The Gal-A-based anti-corrosive coating scored superiorly across all impact categories compared to traditional coatings. The use of Gal-A showed significant environmental benefits, particularly in reducing climate change impacts. However, uncertainties remain regarding the application procedure and the long-term performance of Gal-A as a coating, which necessitates further research.

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Nomenclature

Abbreviation	Definition
Gal-A	Galactaric acid
Gal-UA	Galactorunic acid
SBP	Sugar beet pulp
DM	Dry matter
LCA	Lifecycle assessment
EPS	Emerging product system
CPS	Commercial product system
CrCl3	Chromium(III)chloride
Cr2O3	Chromium trioxide
EoL	End of life
STP	Sewage treatment plant

1 Introduction

The burgeoning field of environmental sustainability is increasingly focusing on the commercial viability of biobased products to transition to a biobased economy. Nowicki et al. (2008) state that the biobased economy is an orientation towards the substitution of biologically derived materials and processes to produce goods that seek to reduce the use of extracted minerals and petro-chemistry. They also identified additional attributes, such as reduced energy required in production processes or a more benign waste treatment channel for production residues or discarded products.

Royal Cosun, a farmer's cooperative, processes sugar beets and valorizes co-products for food and non-food applications in the Netherlands. Galactaric acid (Gal-A) is an example of promising biobased solutions from sugar beet pulp (SBP) currently developed by Royal Cosun. Royal Cosun has designed and validated on a small pilot scale a series of technological process steps that enable the extraction of Galacturonic acid(Gal-UA) from SBP, followed by its conversion into Gal-A. Gal-A is a platform molecule with applications for various industries, notably, in steel passivation and as a chelation agent (Protzko et al., 2018). Royal Cosun intends to have these applications commercialized by 2030.

As far as publicly available data shows, Royal Cosun boasts the furthest development for Gal-a from SBP. No evidence of commercial-scale application or lab-scale studies could be found in the literature for Gal-a production from SBP. Only one study, a master's thesis by de Almeida Romano (2020), could be found that specifically investigated Gal-a production from sugar beet pulp as its substrate. The author applied a theoretical socio-technical assessment of the conversion of sugar beet pulp to Gal-A on a commercial scale.

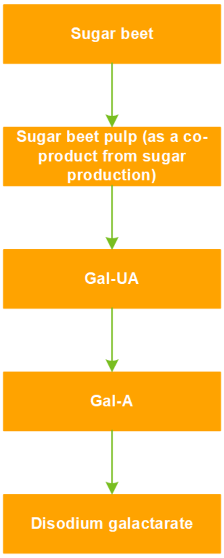
Despite the lack of literature available on Gal-A production from SBP as a substrate, there has been a significant scholarly exploration of the platform molecule from other substrates. Delving into the literature reveals a collection of lab-scale studies, ranging from 50 ml to 1000 ml batches, exploring the conversion of galacturonic acid using substrates other than sugar beets (e.g., orange processing waste). These studies employ various biotechnical conversion processes, as evidenced by the works of Mojzita et al. (2010), Kuivanen et al. (2016), and Barth & Wiebe (2017). Notably, Paasikallio et al. (2017) have surpassed the lab-scale quantities, conducting experiments in 250-liter batches.

Gal-A, with the molecular structure of C6H10O8, serves as a platform chemical with significant commercial potential and various applications. Gal-A has applications in a range of sectors such as the chemical industry, personal care, food, and steel passivation. High-purity Gal-A facilitates one-pot conversions to produce adipic acid (Li et al., 2014) and 2,5-furan dicarboxylic acid (FDCA) (Taguchi et al., 2008). Adipic acid is a key monomer for nylon-6,6 production, while FDCA is a versatile building block for various polymers, including polyethylene furanoate (PEF). PEF, recognized as a bio-based alternative to conventional polyethylene terephthalate (PET), displays environmental advantages, such as being 100% plant-based and recyclable, with improved gas barrier and mechanical properties (Eerhart et al., 2012). In the food industry, Gal-A shares applications with L-tartaric acid, serving as a leavening agent in self-rising flour when used with carbonate (Ortiz-Sanchez et al., 2020).

For this study, the two most promising applications have been selected in consultation with internal experts from Royal Cosun based on technical feasibility and marketability. The first application, referred to as application 1, is Disodium galactarate as a chelating and stabilizing agent. Disodium galactarate is produced through a chemical reaction of Gal-A and NaOH. Figure 1 represents a simplified representation of the different product stages leading to disodium galactarate. This application finds a use case for personal care products like skin moisturizers and shampoo. The second application, from now on referred to as application 2, is Gal-A, as a Disodium galactarate compound, as a surface coating for galvanized steel. Surface coatings are applied to increase the anti-corrosive properties of the substrate and in some instances to increase paint adhesion or for a decorative finish.

Figure 1

Simplified representation of the different product stages leading to disodium galactarate



Disodium galactarate, when compared with Disodium EDTA as a chelating agent, presents a promising alternative with one very apparent benefit. Disodium EDTA is difficult for sewage treatment plants (STPs) to treat and leaches into waterways as effluent from the plant (Fuerhacker et al., 2003; Nörtemann, 1999). Due to its persistence in nature and chelating abilities, it can bind to heavy metals, reintroducing them to the aquatic ecosystem and making them bioavailable and toxic to aquatic life, posing significant environmental risks (Yu et al., 2023). Gal-A is readily biodegradable according to a confidential study commissioned by Royal Cosun where biodegradation of >60% was observed within a week in the Closed bottle test for both river water and activated sludge.

In the context of chromium coatings, although Cr(III) is a less toxic alternative to Cr(VI), it is not without its own risks. The potential leaching of Cr(III) into the environment, particularly into industrial soil, can have significant implications for ecotoxicity and human toxicity, both carcinogenic and non-carcinogenic (Guillon et al., 2023; Qi et al., 2023). It is also possible that a portion of the Cr(III) present in coatings could oxidize to Cr(VI) (Rochester & Kennedy, 2007), exacerbating the toxicity risks. Gal-A on the other hand is non-carcinogenic as proven by the results of an externally commissioned test.

These properties of Gal-A applications are promising, but it remains crucial to critically assess their environmental performance. Although biobased products are generally perceived as more eco-friendly than their non-renewable counterparts due to their renewable origins and typically lower greenhouse gas (GHG) emissions, evaluating a product's environmental impact involves more than just these factors (Miller et al., 2007). According to Miller et al., (2007) often overlooked are the impacts of agriculture, such as nitrogen emissions, land use, ecosystem quality, and water consumption, when comparing the sustainability of bioproduction systems to those based on fossil fuels. Environmental assessments are particularly beneficial for applications still under development (Cucurachi et al., 2023). Analyzing the environmental performance of novel products provides valuable insights into its applications and production process offering the opportunity to make adjustments during development to enhance environmental sustainability (Cucurachi et al., 2023).

Prospective LCA is required to assess products that are under development. For several decades now, attributional LCAs have been used to quantify the environmental impacts of products and service systems across their full life cycle (from the cradle to the grave), from the extraction of raw materials up to the end-of-life (EOL), and across a wide range of impact categories (e.g., global warming Impact, ozone depletion). Prospective LCAs differ in that they include prospecting elements such as the development trajectories of relevant technologies involved scaled to a point in the future instead of the current situation, which is especially relevant when assessing an emerging product system (EPSs). These additional elements lead to increased uncertainty related to the accuracy of the results (Thonemann et al., 2020). A prospective LCA framework developed by De Souza et al. (2023) will be used as the methodological basis of this study.

There is a notable gap in the available knowledge concerning the environmental sustainability of applications for Gal-A derived from SBP at a commercial scale. The environmental performance of the production of Gal-a from SBP is unknown due to the relative novelty of the product. Its environmental performance for its intended applications has not been studied before. Subsequently, the comparative performance with industry standards is also not explored.

This leads to the following research question:

Main research question:

- *What will be the cradle-to-grave environmental impacts of SBP-derived Gal-A as a conversion coating and chelating agent compared to that of Cr(III) and EDTA respectively in the Netherlands in 2030?*

The thesis is structured as follows: Chapter 2, 'Methods and materials', outlines the research approach detailing and justifying the prospective LCA research steps taken, along with all the materials used such as life cycle inventory (LCI) databases and software. It provides the 'Goal and scope' specifying the functions functional units and the reference flows and the uncharacterized LCI results, along with LCI modeling assumptions and visual representation of the product systems. Chapter 3, 'Results', describes the 'Impact assessment,' which includes indicator results, normalization and weighting, a contribution and sensitivity analysis, and a completeness and consistency check. During the 4th chapter 'Discussion', the results of the LCA are interpreted and limitations are discussed. The thesis concludes with chapter 5, 'Conclusion and recommendations' where the research question is answered and its implications discussed, and future research recommendations are provided.

2 Method and materials

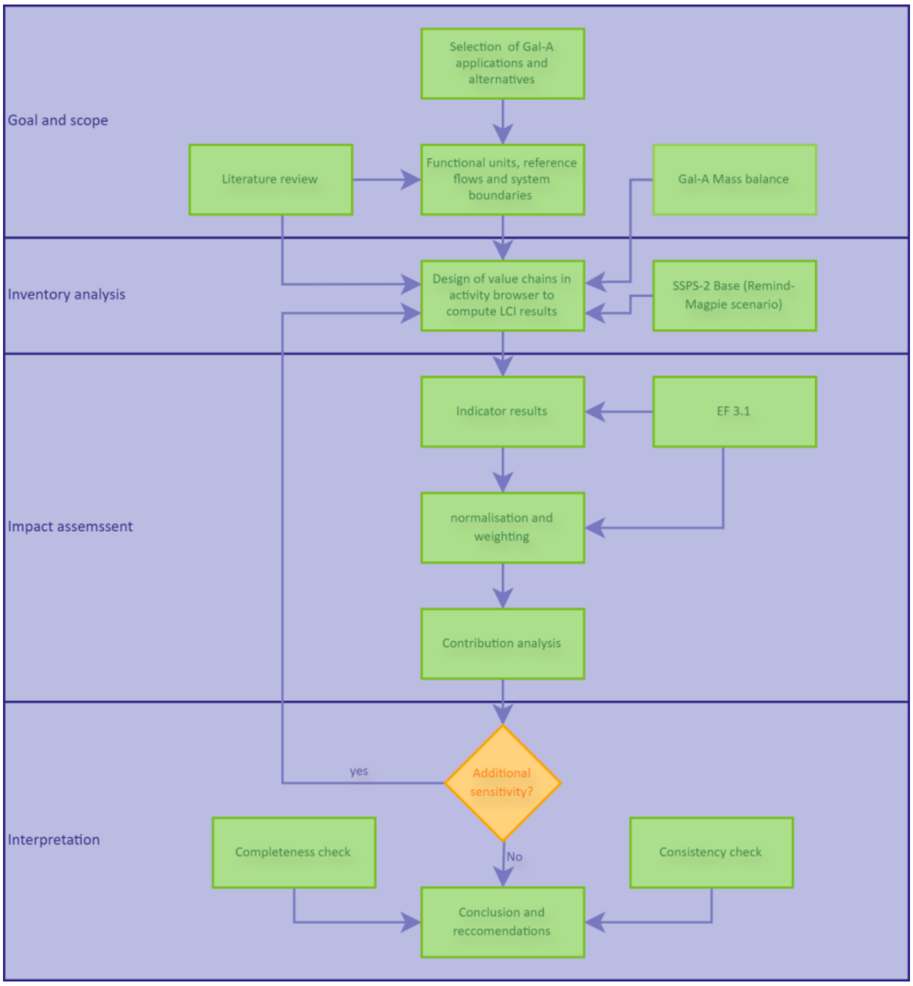
The first part of the method and materials section consists of a research framework in the form of a research flow diagram. It also includes the 'Goal and scope' section and the inventory results.

2.1 Framework

This section constitutes the research approach. Figure 2, the research flow diagram, provides a comprehensive overview of the research design, covering all elements mentioned in this section.

Figure 2

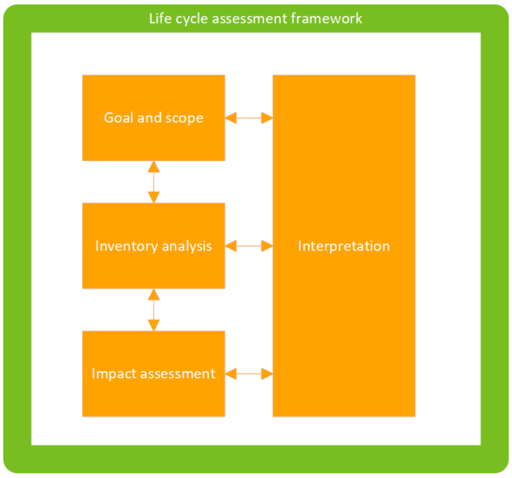
Research flow diagram



To capture the future environmental impacts of emerging product systems (EPS) and compare them on various impact categories with commercial product systems (CPS) a prospective LCA approach is needed. A prospective LCA has a comparable structure to that of an LCA: a goal and scope definition, inventory analysis, impact assessment, and interpretation as shown in Figure 3. Prospective LCA adds another layer of complexity by considering technological and temporal developments.

Figure 3

Phases of the methodological framework of LCA, according to ISO 14040



Note. Adapted from Guinee et al. (2002)

For a fair basis of comparison in a pLCA between two applications, consistency is crucial across their respective maturity and commercialization levels, and the assessment must be projected into the same future timeframe Thonemann et al. (2020). Figure 4 visually represents this concept. Instead of EPS and CPS, Emerging technology (ET) and commercial technology (CT) are used in the figure. The reason why it is decided to refer to EPS and CPS is because the technology is not novel, the products and how they are produced are novel.

Comparing the environmental performance of a Gal-A application from SBP to a commercialized non-Gal-A application without scaling to a comparable level of maturity and production scale would be an unfair basis of comparison. Gal-A applications and their product systems are still in development (TRL-5) comparing the environmental impacts on a TRL-5 scale of the EPS to a CPS would fail to represent the impacts of the EPS fairly as scale efficiencies and the effects of technological maturity are not considered (de Souza et al., 2023).

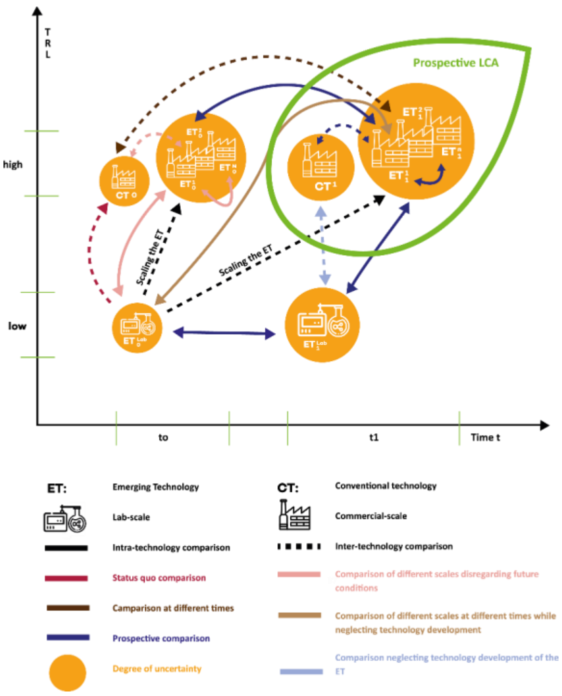
A large production capacity and high technological maturity decrease the environmental impacts of products per unit produced. An increased production scale allows in many cases for increased efficiency through more automation, and larger machinery making the per-unit impacts smaller (Piccinno et al., 2016). An increased production scale leads to larger output quantities making valorization of side streams more viable. Combining this with a high level of technological maturity allows us to explore process set-ups where byproducts are utilized and waste outputs are recycled decreasing the per-production unit impacts.

Comparing an EPS with a CPS at the current time is not an appropriate time horizon as the CPS might change in the future due to factors like regulatory developments and innovations (Langkau et al., 2023). Potentially hazardous chemicals and their use in the EU context are often increasingly restricted and less hazardous alternatives are introduced. The REACH regulation limits the use of shortlisted chemicals in the EU, like Cr(VI) compounds. The production process of products relying on the use of these restricted chemicals will have to be adapted in order to remain compliant.

Changes over time in the wider socio-technological system, in which the product systems are embedded, are important to consider. Changes in the electricity mix, even though not directly under the control of the organization producing the product, affect the (comparative) indicator results of its product system. For example, the electricity grid will make use of a larger percentage of renewables by 2030 in The Netherlands. When comparing two products for the year 2030, where one is highly reliant on the Dutch electricity grid, its comparative CO_2 eq. emissions will become favourable ceteris paribus.

Figure 4

Schematic illustration of the comparison possibilities within the application of prospective LCAs including temporal and technological development

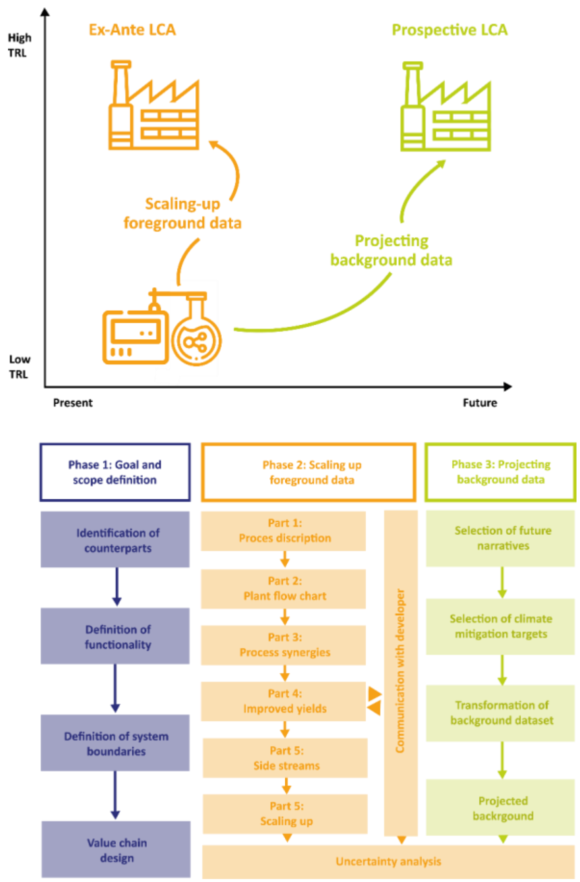


Note. Adapted from Thonemann et al. (2020)

A framework developed by De Souza et al., (2023) will be used as the main methodological basis to perform the prospective part of the LCA. The framework is depicted in Figure 5 and outlines how to integrate the effect of scaling up a product and scaling the background, while embedding it in the classical LCA framework. This allows to scale and mature the production of Gal-A and its application in a structured manner to 2030. Additionally, it gives guidance on how to approach the development of the prospective background, such as which Integrated Assessment Model (IAM) to use.

Figure 5

Prospective LCA framework



Note. Adapted from De Souza et al. (2023)

The goal and scope were set in line with the research question balancing accuracy and comprehensiveness. An extensive literature review of the applications was done. While comprehensiveness is important, stretching it to an extreme point increases uncertainty on the results of the study, due to complexity and unpredictability of the designed value chains. For each unit process, it was decided whether enough reliable data was available to keep it in scope and by doing so not compromise the quality of the study.

The production of Gal-A was scaled up in accordance with the framework from De Souza et al. (2023). The authors do a great job at distinguishing which elements to consider when scaling up and stress the importance of collaboration with the developer. Steps 1 to 6 of the scale-up process have been included, where the process technologist and project manager of Royal Cosun were in the lead. A plant flow chart was developed based on lab and subsequently pilot scale testing. The results of these tests have been extrapolated to a commercial-scale plant. The yield of processes that have only been tested at lab scale (plug flow reaction and crystallization) was set conservatively. Co-products were not valorized during the pilot study, each one is evaluated and an estimation was made which are valuable and which are to be considered as a waste stream. Water and heat integration were not tested at the pilot scale but are believed to be viable at the commercial scale. The resulting upscaled bill of materials, which includes improved yields, synergies, and side-streams, covers all economic flows in detail as can be seen in confidential Appendix C 'mass balance'. It is used as input LCI data to produce Gal-A.

The design of the value chains of the alternative product systems was based on publicly available literature and insights provided by LCI databases. Process data, final product properties, and available LCAs were used to construct the value chains. For processes with limited processing data available, LCI databases were used to get a better understanding of them and their embeddedness in the broader socio-technical system (e.g., downstream, and upstream processes).

Estimations for possible future changes in the alternative product systems including its up- and downstream processes were made. Langkau et al., (2023) stress the importance of considering future changes of production processes, even when they have already reached a high level of maturity. The scientific literature on the future production of these chemicals and applications was consulted for the year 2030. Regulatory developments, such as future bans on chemicals, were researched by analyzing information provided by relevant EU agencies, like The European Chemicals Agency (ECHA). For potential projected changes, it was assessed whether this was applicable already for 2030.

The unit process data for Gal-A applications by which the downstream processes after its production are meant, were estimated based on various types of information and in close collaboration with internal experts. The alternatives were used as a base scenario for unit processes, after which it is estimated how the Gal-A application might deviate from this based on the inherent properties of Gal-A, studies commissioned by Royal Cosun on Gal-A and its compounds, patents, and supplier feedback. This approach is taken because Gal-A applications are not established yet. Strong collaboration with experts was critical to ensure the quality of the estimations. To exemplify this approach, Disodium-EDTA is not readily biodegradable indicating that it does not effectively get treated in sewage treatment plants (STPS) and ends up in freshwater systems. If Disodium Galactarate were to replace Disodium-EDTA, it would in fact biodegrade based on studies commissioned by Royal Cosun.

The research adopted a predictive approach, focusing on a singular future state rather than an exploratory analysis involving multiple potential futures. This predictive stance is deemed acceptable when a plausible scenario is adequately justified (Langkau et al., 2023). The chosen timeframe for the study is 2030, significantly shorter than most prospective LCAs which prospect around 25 years in the future, which ensures decreased uncertainty.

Background data was scaled using the PREMISE approach, following the recommendations of De Souza et al. (2023), and is modeled using the Activity Browser built on Brightway2. Sacchi et al., (2022) cover the PREMISE approach in-depth in their article. In short, the PREMISE approach entails using an integrated assessment model (IAM), such as REMIND-Magpie or IMAGE to convert the Ecoinvent database to a superstructure database. IAMS are instruments that evaluate the environmental, economic, and social impacts of different scenarios such as the shared Socioeconomic Pathways (SSPs) by among others projecting and quantifying technological developments over time.

The selected scenario is based on SSP2-Base and was modeled using the REMIND-Magpie integrated assessment model. The background processes are structured around a singular cornerstone scenario type, aligning with the predictive scenario framework proposed by Langkau et al. (2023). SSP2-Base adheres to historical development patterns while transcending a simple extrapolation of recent trends. SSP2-Base offers an explicit dynamic pathway informed by historical patterns, maintaining consistency with middle-of-the-road expectations for future changes. This deliberate approach avoids extremes in possible outcomes, rendering SSP2 suitable for modeling the background data, as suggested by Reimann et al. (2018).

Ecoinvent version 3.9 allocation by cut-off was transformed into a superstructure database. The PREMISE approach uses Ecoinvent as the background basis. At the time of modeling, Ecoinvent 3.9 was the most recent Ecoinvent version supported in Activity Browser through the 'Scenario plug-in'. While the PREMISE approach is the most comprehensive approach to making the background perspective it is not complete. Currently, PREMISE covers 7 highly polluting sectors, such as electricity generation, steel and cement production, road transport, and liquid and gaseous fuels production. This applies only to the cut-off by allocation version of Ecoinvent (Sacchi et al., 2022). Hence, this system model was used. The system model determines how co-products are allocated and how the burden for waste/recycling processes is distributed. For co-products economic allocation is used, where when produced the economic value is determined by the co-products, and based on that, the upstream burden is allocated. This system model uses the principle 'polluter pays', where the further treatment of outflowing waste products without a positive economic value is burdened to the outflowing product(s) of that process.

While Ecoinvent version 3.9 for the superstructure database was used, the LCIA method was aligned with version 3.9.1 in the Activity Browser. Ecoinvent 3.9 has issues with some characterization factors for certain environmental flows. It was possible to update those to 3.9.1 without issues because the update only pertains to the characterization factors and not the addition or removal of environmental flows.

EF 3.1, a mid-point-oriented LCIA method, is the LCIA method that was used to compute the indicator results. LCIA methods classify and characterize environmental flows of which its aggregation constitutes the indicator results per impact category. EF 3.1 is the method recommended by the European Commission, hence it is selected. The respective impact categories, impact category indicators, and units are shown in

Table *1*.

Table 1

Impact categories, impact category indicators, and units of EF 3.1

Impact Category	Impact category indicator	Unit
Acidification	Accumulated Exceedance (AE)	mol H^+ eq
Climate Change	Radiative Forcing as Global Warming Potential (GWP100)	kg CO_2 eq
Ecotoxicity: Freshwater	Comparative Toxic Unit for Ecosystems (CTUe)	CTUe
Eutrophication: Terrestrial	Accumulated Exceedance (AE)	N eq (ter)
Eutrophication: Marine	Fraction of Nutrients Reaching Marine End Compartment (N)	N eq (Marine)
Eutrophication: Freshwater	Fraction of Nutrients Reaching Freshwater End Compartment (P)	P eq
Human Toxicity: Cancer	Comparative Toxic Unit for Humans (CTUh)	CTUh (Carc)
Human Toxicity: Non-Cancer	Comparative Toxic Unit for Humans (CTUh)	CTUh (Non-Carc)
Ionizing Radiation: Human Health	Human Exposure Efficiency Relative to U235	u235 Eq
Land Use	Soil Quality Index	Soil Index
Material Resources: Metals/Minerals	Abiotic Depletion Potential (ADP): Elements (ultimate reserves)	SB eq
Ozone Depletion	Ozone Depletion Potential (ODP)	CFC-11 eq
Photochemical Oxidant Formation: Human Health	Tropospheric Ozone Concentration Increase	NMVOC eq
Water Use	User Deprivation Potential (deprivation-weighted water consumption)	m^3 water eq
Particulate Matter Formation	Impact on Human Health	Disability-Adjusted Life Years (DALY) or another measure of impact (DI)
Energy Resources: Non-Renewable	Abiotic Depletion Potential (ADP): Fossil Fuels	MJ

Normalization and weighting were performed to the indicator results for applications 1 and 2. These steps allow benchmarking in a quantitative way of the indicator results across impact categories where a higher score means a higher degree of relevancy for the system under study. Normalization and weighting factors are based on the EF 3.1 approach and are made explicit in confidential Appendix B sheet 'absolute results.' It is important to mention that weighting is always performed on a normative basis and thus, subjective. Even so, it is still considered a valid approach in LCA to prioritize the relevance of the evaluated impact categories (Pizzol et al., 2017).

The robustness of the results was evaluated with a sensitivity analysis and using data quality checks. It is common for LCAs to evaluate the robustness of the study stemming from among others technical processing uncertainties, modeling decisions, and the formulation of the functional unit. Thonemann et al., (2020) state that prospective LCAs have additional dimensions of uncertainty surrounding upscaling/maturing of production systems and the future setting. A one-at-a-time approach was taken as sensitivity analysis. This entails that one parameter at a time is changed and the effect observed on the indicator results. Through a consistency and completeness check, the data quality and comparability were assessed. From all previous steps, the conclusions land recommendations follow. Traditionally, the sensitivity analysis and the quality checks are part of the interpretation phase of the LCA, but in this case, to better align with the format of a master's thesis, it was decided to group them under Impact assessment' in the 'Results' chapter and the other elements of the interpretation under the 'Discussion' and 'Conclusion and Recommendations' section.

2.2 Goal and Scope

2.2.1 Goal

The goal of this study is threefold. Firstly, it aims to compare the environmental impacts of Gal-A applications derived from SBP with existing commercial alternatives for Cosun's operations in 2030. This comparison will help in understanding if the innovative biobased Gal-A can meet its promise of reducing environmental impacts while providing comparable performance. This will become an important criterion to consider when investing in further developing and commercializing the product. In addition to identifying the environmental impact, this study also seeks to pinpoint hotspots within the production system. Identifying these hotspots will highlight areas where improvements can be most effectively implemented.

Secondly, the research seeks to contribute to the academic and practical understanding of the environmental impacts associated with novel biobased product applications. By utilizing prospective LCA, this study aims to provide robust and quantifiable evidence of the environmental benefits or drawbacks of using Gal-A in various applications. This information is relevant for among others policymakers, agricultural professionals, and industries involved in the development and deployment of biobased products.

This study is conducted by Koning as part of his master's thesis in Industrial Ecology, under the university supervision of Dr. Ir. Thonemann and Dr. Ir. Posada, from Leiden University and Delft University of Technology respectively. Royal Cosun is the commissioner of this study. Dr. Ir. Moejes and Dr. Ir. Huijgen, process engineer and scientist & project leader respectively, are the company supervisors. The collaboration with Royal Cosun does extend further, to individuals such as the inventor of the issued patent Ing. Lazeroms, and environmental technologist Ing. Raap.

Given the innovative nature of this research, it is essential to treat all data related to the processes, impacts, and proprietary information with strict confidentiality. The results are intended to be shared with the academic supervisors, Cosun, and published in the public thesis repository of TU Delft, provided that proprietary information is adequately anonymized and protected.

2.2.2 Scope

This prospective attributional LCA study is cradle-to-grave, covering all stages from the extraction of raw materials to the end-of-life of Gal-A applications and their alternatives. This boundary encompasses the entire lifecycle of Gal-A, including cultivation, production, distribution, application, and disposal or recycling stages.

While the goal of LCA is to include all elements of a product system, practical limitations mean some inputs or processes might not be covered, creating a 'cut-off.' Processes that do not emit significant emissions and are hard to quantify, such as the storage of SBP were not included. The coating application process for the zinc-plated steel for application 2 is cut-off. Packaging of the chemicals is cut off as reusable containers are assumed. But also, some more relevant processes and functional elements of the applications after careful consideration were left out of scope as made explicit in the 'Applications, Function, Functional Unit and Alternatives' section.

The temporal scope focuses on current practices and projections up to 2030 to capture potential advancements in regulations and shifts in technology. The geographical scope is primarily the Netherlands, reflecting Cosun's operational base and the primary market for Gal-A applications.

The study follows the ISO14040 and ISO14044 standards for LCA. The Ecoinvent 3.9 cut-off by allocation database and system model have been used for modeling the background data. The Activity Browser was used for LCA modeling. Foreground data was collected through collaboration with Cosun, literature reviews, and expert consultations to ensure accuracy and relevance. This has been reported in greater detail in the 'Framework' section of the 'Method and materials'.

In LCAs, a distinction is made between environmental flows and economic flows. Environmental (elementary) flows are those that enter or leave the product system without human intervention, such as emissions to air and water. Some flows, like those involving agricultural soil or water, may be challenging to categorize definitively as either economic or environmental. In this LCA, the treatment of wastewater is considered part of the product system because it is managed by human activity until its final discharge. Waste streams during the end-of-life phase are also regarded as economic processes due to human involvement in waste management.

Gal-A and its compounds are not characterized by the EF 3.1 method. Due to biodegradability and it being non-mutagenic, it is assumed that no human and ecotoxicological effects are presumed from Gal-A leached into the environment. Though, non-mutagenic does not mean non-toxic. In combination with high biodegradability, no toxicity is deemed a justified assumption.

2.2.3 Applications, Function, Functional Unit and Alternatives

Two applications have been identified in consultation with Royal Cosun's internal experts based on the likelihood of materializing by 2030 judged by perceived technical feasibility and marketability. The alternatives are based on literature research and extensive consultation with Royal Cosun and their internal commissioned tests and external user feedback from customers.

Application 1

For application 1, the assumed chelation quantity, disodium galactarate being a drop-in, is assumed to be equal as per internal expert consultation. 0.06% of the formulation is the chelating agent on a mass basis in line with Kumar et al., (2023). Additionally, yearly usage is computed the following way: twice a week 10 g. So, 1.04 kg * 0.06 = 0.0624 kg of chelation agent is assumed to be used per year. This leads to the following:

Function: Provision of chelation for shampoo usage.

Functional Unit: Provision of chelation functionality to shampoo via a chelating agent, as part of the shampoo formulation, used for hair washing over a year.

Reference flow 1: Provision of chelation functionality to shampoo via 0.0624 kg of disodium galactarate, as part of the shampoo formulation, used for hair washing over a year.

Reference flow 2: Provision of chelation functionality to shampoo via 0.0624 kg of disodium EDTA, as part of the shampoo formulation, used for hair washing over a year.

Reference flows 1 and 2 for application 1 are from this point referred to as 1a and 1b respectively throughout the paper.

Application 2
For application 2, the focus of the function is anti-corrosive performance. Increased paint adhesion and a decorative finish are other benefits of Cr(III) coatings frequently mentioned in the literature but have been left out of scope for this study. The duration for which the coatings last, especially for disodium galactarate, is hard to estimate because it is highly dependent on the environment the coatings are exposed. For disodium galactarate, little is known about the duration of the coating due to its novelty. It is decided not to make the time element explicit.

It was found that the thickness and chemical quantities of the created layers deviate quite substantially between the two alternatives. The disodium galactarate layer is assumed to completely consist of disodium galactarate, has a thickness of 10nm, and weight of 17 milligrams per m2 passivated, assuming a density of 1.7 g/cm3 for disodium galactarate. For Cr(III) the total mass per m2 passivated is 60 milligrams per m2 with a thickness of approximately 220 nm assuming no addition of cobalt and an immersion time of 60 seconds (Hesamedini et al., 2018). Chromium(III) Chloride (CrCl3) is chosen as the Cr(III) salt for this study, as it is a common compound for this application and the production route is well understood by the author. 60 milligrams of Cr(III) correspond to 182 milligrams of CrCl3 (Appendix x). This leads to the following:

Function: Improving anti-corrosive properties of zinc-plated steel via a surface coating.

Functional unit: Providing increased anti-corrosive properties to 1 m2 of zinc-plated steel through a surface coating formed via a chemical reaction by immersing the substrate at ambient temperature (approximately 20-25°C) for a duration of 1 minute.

Reference flow 1: Providing increased anti-corrosive properties to 1 m2 of zinc-plated steel through a surface coating consisting of 17 milligrams of disodium galactarate formed via a chemical reaction by immersing the substrate at ambient temperature for a duration of 1 minute.

Reference flow 2: Providing increased anti-corrosive properties to 1 m2 of zinc-plated steel through a surface coating consisting of 60 milligrams of Cr(III) formed via a chemical reaction by immersing the substrate at ambient temperature for a duration of 1 minute.

heeft verwijderd: 1

Ambient temperature refers to approximately 20-25°C. The disodium galactarate coating is assumed to wholly consist of that molecule. For Cr(III) based coating, it is important to note that other elements and compounds are also present in the formed coating.

Reference flows 1 and 2 for application 2 are from now on referred to as 2a and 2b.

2.3 Inventory analysis
This section covers the LCI inventory modeling done in the Activity Browser. It provides an overview of the product systems, the main modeling assumptions made and a visual representation of the modeled foreground systems. The uncharacterized LCI results for applications 1 and 2 and the economic and environmental flows related to the unit processes can be found in Appendix D.

2.3.1 Product system 1b
The production of EDTA is a long-established process that has some environmental concerns. The synthesis involves the reaction of ethylenediamine, formaldehyde, and sodium cyanide in an aqueous solution, followed by neutralization and crystallization to obtain the final product. The production of chemicals, like hydrogen cyanide, sodium hydroxide, propylene, and formaldehyde is energy intensive and relies heavily on fossil fuels usage. Additionally, the processes generate significant amounts of byproducts, including formaldehyde, hydrogen cyanide, nitrogen oxides ammonium, and other organic

compounds, which can be highly toxic to humans and to natural ecosystems if leached into the environment (Jaszczak et al., 2017).

EDTA is particularly problematic in the environment due to its high stability and resistance to degradation. When released into waterways, EDTA can remobilize heavy metals previously settled in sediments, thus reintroducing them into the aquatic environment where they can become bioavailable and toxic to aquatic life (Yu et al., 2023). Moreover, the presence of EDTA in waters can hinder the effectiveness of biological wastewater treatment processes by inhibiting the growth of microbes crucial for degrading organic pollutants (Yu et al., 2023).

In the Netherlands, sewage treatment plants (STPs) are largely ineffective at breaking down EDTA. This inefficiency is due to several factors inherent in the activated sludge process used by these plants. For effective biological degradation, EDTA concentrations need to be significantly higher than those typically found in municipal wastewater. Research indicates that EDTA concentrations in household wastewater generally range from 10 to 70 µg/L, whereas effective degradation requires influent concentrations of 20-30 mg/L (Fuerhacker et al., 2003; Nörtemann, 1999). This sensitivity to concentration levels is highlighted by an example from the dairy industry where removal rates increased from 89% to 96% caused by a change in the influent concentration from 33 mg/L to 67 mg/L respectively at a pH between 7.5 and 8.0 (Van Ginkel, 1999).

Additionally, the pH levels in standard STPs are not optimal for EDTA degradation as raising the pH above 8 can significantly improve removal rates. López-Vázquez et al., (2008) found that the average pH level ranged from 6.6 to 7.2 of 7 Dutch STPs using the activated sludge system. In a small-scale experiment done by Van Ginkel et al., (1997) at a pH of 7.5, only 34% of EDTA was removed, whereas at a pH of 8, the removal rate increased to 59%, and at pH 8.5, it reached 82% at EDTA concentrations of 10 mg/L (Van Ginkel et al., 1997).

Despite the potential of advanced technologies like electrically driven membrane filtration, which can degrade EDTA and its complexes up to 99% within a few hours (Li et al., 2020), these methods are not widely adopted in Dutch STPs. Although three STPs in the Netherlands did install membrane technology in the first decade of the 21st century, these facilities were eventually closed due to the high costs of membrane cleaning and energy requirements for the pumps (Redactie Waterforum, 2022).

The data, although somewhat dated, remains relevant because the fundamental processes and challenges associated with EDTA removal have not significantly changed. The primary mechanism used in Dutch STPs is still the activated sludge method, which is inherently limited in its ability to degrade EDTA effectively. Consequently, EDTA passes through the treatment process unchanged and enters the environment.

Uncertainty exists about exactly what amount of EDTA from shampoo chelation would leach to the environment. Fuerhacker, M., et al. (2003) established that an average of 85% of EDTA influents leach from STPs to the environment through effluents. However, this number is an overestimation for EDTA from residential wastewater, because 60% of the wastewater came from industrial sources, with relatively high concentrations of up to 15 mg/L of EDTA compared to 0.01 to 0.07 mg/L. Based on the aforementioned factors and findings, it is probably a negligible amount.

Despite clear environmental concerns, for 1b the EDTA production process is likely to remain unchanged in the near future. The alkaline cyanomethylation of ethylenediamine to produce EDTA has been the main commercial production route for decades (Hart, 2000). None of the chemicals involved in the process of producing EDTA are on the REACH SVHC (candidate) list, so regulatory restrictions are unlikely. No, literature on new production routes of EDTA could be found. Instead, Ryczkowski (2020) concludes that EDTA as a chelating agent will likely be replaced in the future by biodegradable alternatives.

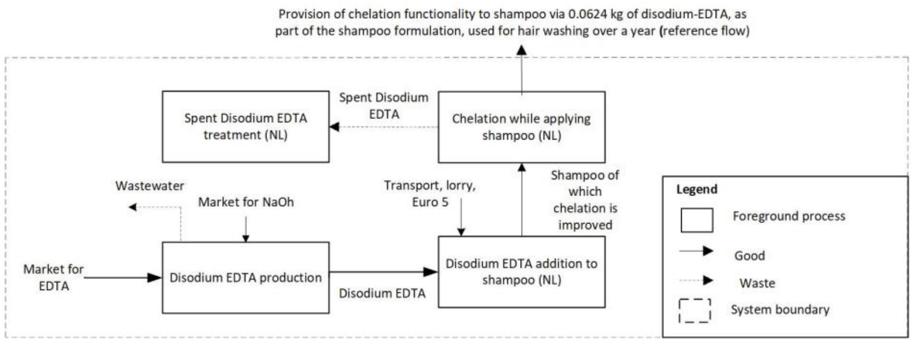
For the assumptions related to 1b, to produce EDTA, the market activity for EDTA production from Ecoinvent is taken for which the origin of the production is Germany. To create disodium EDTA, stochiometric calculations have been used as shown in Appendix A. Water is its byproduct and is assumed to be treated via an average wastewater treatment process linked to Ecoinvent. No transport is assumed as both are market activities.

The addition itself is assumed to be a simple mixing process as outlined by Rakesh et al., (2010) for which no emissions are assumed. Transport to the mixing facility is assumed to be 50 km. For the chelation while applying shampoo no transport step is assumed here either to the transport to the point of sale and to the consumer, because the transport is not allocatable to the function of chelation, but rather to the function of washing hair. The reason this process is carried out is because someone's hair needs to be washed, not because chelation needs to be improved. Packaging is also excluded using that same logic. Spent Disodium EDTA treatment It is assumed that all Disodium EDTA bypasses the activated sludge wastewater treatment system and ends up in freshwater systems.

From these assumptions the visual representation as Figure 6 follows. The flow charts depicted in Figure 6, Figure 7, Figure 8 and Figure 9 show the life cycle stages of Gal-A applications and their conventional alternatives and follow form the modeling decisions. These charts provide a visual representation of the foreground processes and their economic flows included in the prospective LCA. The CML convention for the creation of the flow chart has been followed.

Figure 6

Product system 1b flow diagram



2.3.2 product system 1a

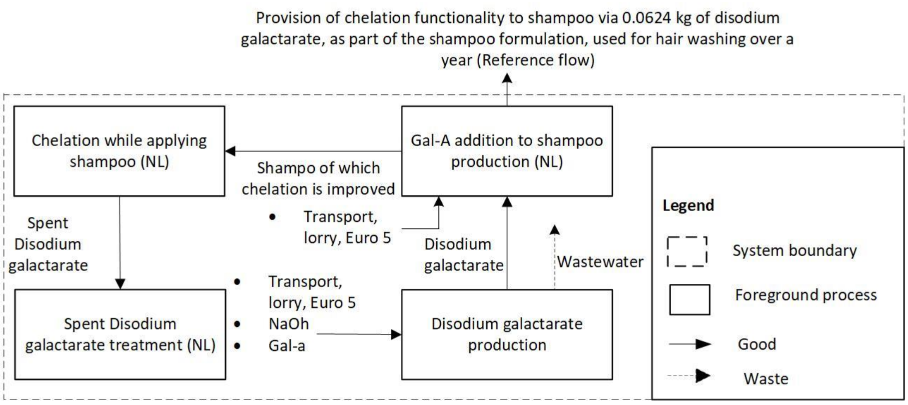
The coverage of Gal-A production, related assumptions and flow chart have been moved to Appendix E, because it is proprietary information that is covered in that section. Assumptions related to the application phase and EoL have been left in the main text and are described in the subsequent paragraph. Figure 7 visually represents the product system. For the flow charts of 1a (Figure 7) and 2a

(Figure 9), Gal-a has been modeled as a background input to a foreground process. This is done because the production process of Gal-a is proprietary information.

Disodium Galactarate production, and Disodium Galactarate addition to shampoo and chelation while applying shampoo follow the same logic and procedure as their EDTA-based chelating counterpart. Stochiometric calculations for disodium galactarate production can also be found in Appendix A. Spent Disodium galactarate, which ends up in the sewage system after showering is expected to fully biodegrade through the activated sludge process. It is expected to biodegrade and emit CO2. Because the emissions are biogenic, and sequestration is not accounted for during crop cultivation it is also not accounted for during its release. Water and sodium are accounted for and are assumed to be released in freshwater systems as environmental flows for which the quantities are stoichiometrically calculated as per Appendix A.

Figure 7

Product system 1a flow diagram



2.3.3 product system 2b

Chromium coatings, especially hexavalent chromium (Cr(VI)), have been the industry's preferred choice as surface coatings due to their excellent corrosion resistance and self-healing properties. However, Cr(VI) is highly toxic and carcinogenic, posing significant health and environmental risks during production, application, and use phases for conversion coatings (Prasad et al., 2021). Alvarez et al. (2021) state that several health detriments have been linked to it, such as dermatitis, nasosinusal, kidney and liver problems, as well as hematological and chromosomic aberrations.

Adverse health effects from Cr(VI) are caused through various routes. Inhalation and dermic contact represent the main routes of occupational exposition. For non-occupational health-related problems, it is caused by contamination of food and water that is being consumed. Consequently, the use of Cr(VI) compounds is banned for an increasing number of applications in the EU through the REACH regulation (Altfort, 2017).

Chromium trivalent (Cr(III)) coatings have gained popularity as a safer alternative, but are also not without potential environmental hazards. Cr(III) coatings offer generally slightly worse, but still very good corrosion, resistance without the severe health risks associated with Cr(VI). However, a study by Rochester and Kennedy (2007) shows that Cr(III) coatings can oxidize to Cr(VI) over time, potentially reintroducing some environmental hazards when released into the environment. Chromate coatings maintain their thickness in corrosive environments according to Kendig et al. (1993), indicating minimal leaching of chromium. Zangh et al., (2004) found however, significant pits when exposing a Cr(III) coating to NaCl for a prolonged period, indicating corrosion/breakdown of the coating that could leach into the environment causing contamination. Transverse cracking and delamination can occur when exposed to tensile stress, leading to localized chromium release (Guillon et al., 2023; Qi et al., 2023). During the production of Cr(III) as a Chromium (III) trioxide (Cr2O3) compound, environmental contamination occurs such as the leaching of Cr(VI), particularly during the manufacturing of sodium dichromate and its reaction with sulfur dioxide to produce Chromium(VI) trioxide (CrO3) which in turn gets converted to Cr2O3 (Alifieris et al., 2021).

Applying trivalent chromium conversion (TCC) coatings involves several key steps. Hesamedini et al. (2018) outline the procedure in their research on TCC formation. The steel panels are first cleaned and then plated with a zinc layer either through an electroplating process or by means of hot dip galvanization. The surface is then activated using a NHO3 solution. Finally, the panels undergo a controlled immersion in a chromium (III) bath. The Cr(III) is converted to a more soluble state to a Cr(III) salt, either Cr(III)Chloride, sulfate, or nitrate. The bath also contains complexing agents and optionally cobalt. The panels are immersed for 40 to 80 seconds at an ambient temperature. The coating itself is made up of metal hydroxides and a metal oxide outer layer.

Pollution of passivation baths is becoming less of a concern due to technological developments. Passivation baths in electroplating often become contaminated with tramp ions such as zinc and iron, decreasing the bath's purity and reaction quality. Typically, this necessitates replacing the bath every six weeks to maintain efficacy which is costly and resource-intensive to neutralize, with some leaching being inherent to nature. However, the introduction of Emulsion Pertraction Technology (EPT), which is already implemented in industrial settings allows for the selective removal of these contaminants while retaining essential chromium, significantly extending the bath's operational life (Diban et al., 2011; García-Antón et al., 2014). With EPT, the replacement interval can be increased dramatically reducing waste and the frequency of chemical replenishment. Diban et al., even describe it as a material recovery and waste minimization strategy that chases a “zero discharge” goal, in the surface finishing industry.

In Europe, most steel gets recycled in arc furnaces. For the Cr(III) coating, the recycling process involves the oxidation of Cr(III) during the melting phase in most commonly an electric arc furnace. The high temperatures facilitate the conversion of Cr(III) to Cr2O3, which then becomes part of the slag(Kittaka et al., 1985). The slag is treated in an electric arc furnace slag material landfill which attempts to prevent environmental contamination.

For 2b, some uncertainty surrounds the future production of Cr2O3 due to the use of sodium dichromate and CrO3, which contain chromium in its 6th oxidation state. These substances are on the EU’s candidate list for substances of very high concern (SVHC), requiring authorization for use. While usage restrictions are expected to increase, the timeline and extent remain unclear. CrO3, listed since 2010, is authorized for electroplating until at least December 31, 2028, due to its deemed benefits outweighing risks (European Commission, 2023). Restrictions apply only to manufacturing, selling, or using these chemicals (European Parliament and Council, 2006), but Cr2O3 production likely remains unaffected as if restricted, Cr2O3 could be imported from outside the EU preventing the need to use CrO3 and sodium dichromate.

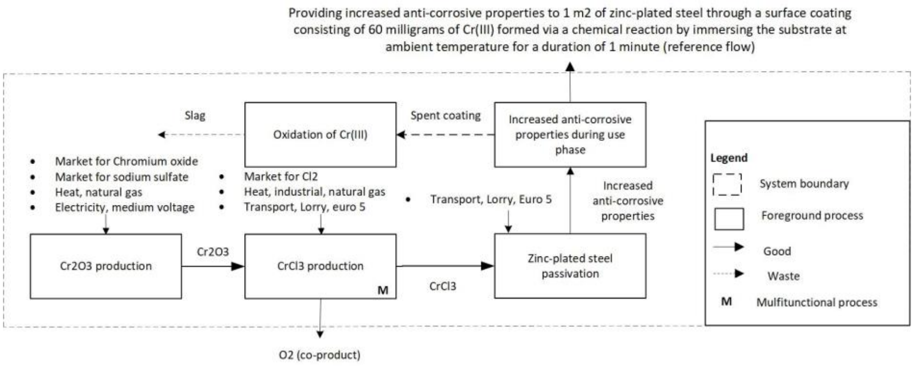
Cr3O2 production is based on LCI data from Olympios et al., (2021). The production of CrCl3 is stoichiometrically calculated with consideration of the heat demand to make the reaction happen (Gaballah et al., 1998). The calculation can be found in Appendix A. It is assumed to be at the same facility as where the Cr2O3 has been produced. The co-product O2, is economically allocated. 98% is allocated to the CrCl3 based on market value and quantity produced.

The production of zinc-plated steel is left out of scope, as the function relates to the protection provided by the Gal-A and Cr(III) based coating. Due to the circular potential of EPT technology for passivation baths and the lack of data, a unique approach is taken for the passivation process where the economic flow equals the content of the coating. The rest is classed as recyclable. For example, the left-over chlorine is extracted free of burden. This is a simplified approach, but given the resources of the study, it was hard to approach this another way. The production location is assumed to be in the same industrial cluster, so a transport distance of 10 km is assumed.

Increased anti-corrosive properties during the use phaseIt is assumed that no Cr(III) is leached to the environment for the base case. It is assumed that at the EoL, the steel is recycled in an electric arc furnace. The steel is melted and repurposed. Therefore, it is fully allocated to the steel and not the coating leaving that out of scope. The Cr(III) oxidizes and becomes Cr2O3 and is part of the slag. The oxidation increases the weight of the Cr compound, which is computed in Appendix A. The slag gets treated through the 'treatment of electric arc furnace slag, residual material landfill' from Ecoinvent. In this process, concentrations of Cr are included, making it a suitable treatment approach. Figure 8 visually represents the LCI modeling done following from the assumptions.

Figure 8

Product system 2b flow diagram



2.3.4 product system 2a

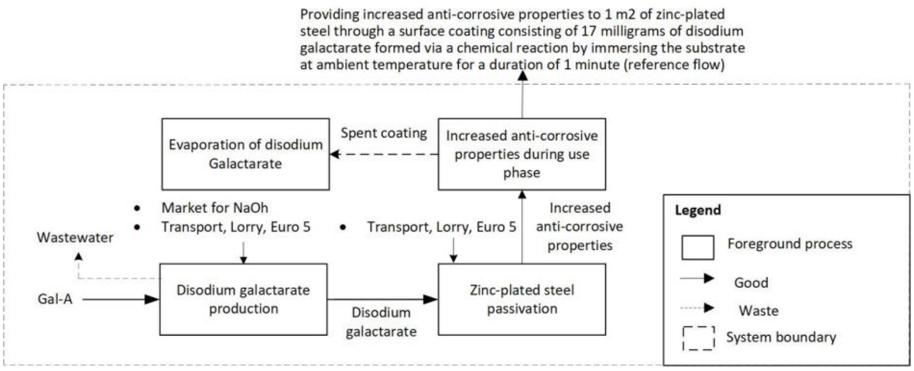
Disodium galactarate as a surface coating for steel and aluminum, forming an oxidative layer that acts as a barrier to corrosion, has a simple application procedure. The application process involves immersing steel in a galactarate salt solution, forming a thin film (10nm) on the substrate consisting fully of disodium galactarate. Experiments have shown that Gal-A provides excellent corrosion resistance (Coöperatie Koninklijke Cosun U.A., 2018). Feedback from suppliers to Royal Cosun has reported results on par with Cr(III) coatings applied to zinc-plated steel. They highlighted the benefit of having a much tinner Gal-A-based coating layer, reducing the quantity required.

Disodium galactarate production follows the same approach as for the chelation application. 'Zinc plated steel passivation' and 'Increased anti-corrosive properties during use phase' follow the same line of reasoning as 2b, with the economic flows determined by the formed coating and no leaching to the environment during the use phase assumed. When the steel gets recycled, it is assumed that the disodium galactarate evaporates at temperatures exceeding 1600 degrees Celsius in the furnace. So, slag treatment is irrelevant for this product system.

For zinc-plated steel with disodium galactarate coatings, the organic component of the coating will combust in the high-temperature environment of an electric arc furnace. This combustion process converts the Gal-a into carbon dioxide (CO2) and water (H2O). The CO2 and water vapor are released into the atmosphere as part of the flue gases. The residual salts remain in the furnace and integrate into the slag. These assumptions are visually represented as Figure 9.

Figure 9

Product system 2a flow diagram



3 Results

This section constitutes the impact assessment. It follows from the LCI results. It gives the characterized indicator results, normalization and weighting, contribution analysis, sensitivity analysis and completeness & consistency check.

3.1 Characterized indicator results

The characterized indicator results allow to compare the environmental footprint of the applications across impact categories. Figure 10 and

Figure *11* show the comparative indicator results per impact category for application 1 and 2. Figure 10 compares the cradle-to-grave impact categories of application 1 on a logarithmic scale, where 1a scores significantly better than 1b for climate change, Ecoxicity, freshwater, human toxicity cancer & non-carcer and resource use, fossils. 1b scores significantly better on eutrophication, terrestrial, land use, and acidification, particulate matter, and water use. For the remaining impact categories, the comparative results are closer, but better scoring for 1a. The absolute results can be accessed in Appendix B application 2 'results' for a more precise comparison of those impact categories.

Figure *11* compares the cradle-to-grave impact categories of application 2 on a logarithmic scale, where 2a scores better on each impact category.

Figure 10

Application 1 indicator results

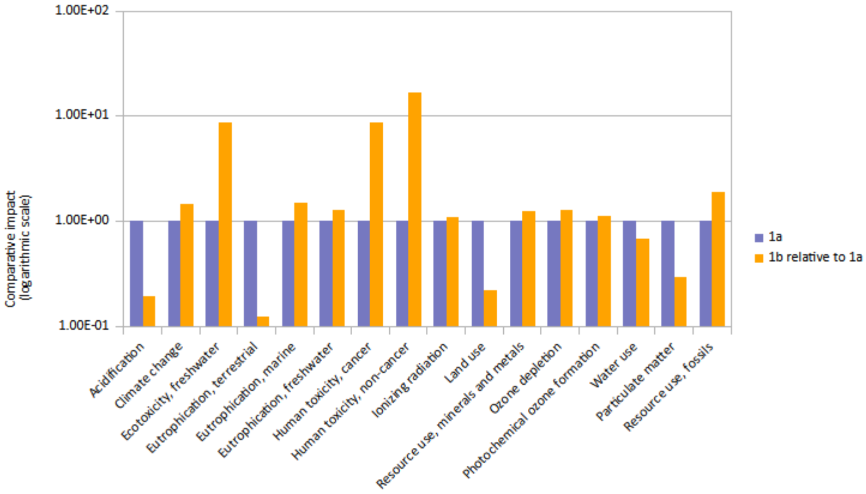
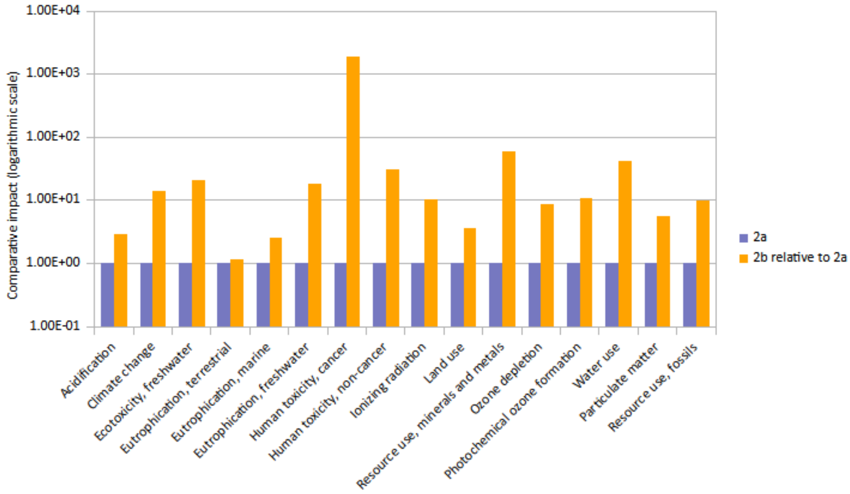


Figure 11

Application 2 indicator results



3.2 Normalization and weighting

Normalization and weighting provide a structured quantitative approach to prioritize across impact categories and decide on their relevnace. Figure 12 shows the normalized and weighted comparative impact for 1a and 1b. For 1a, acidification, climate change, eutrophication, terrestrial, resource use, minerals and metals, particulate matter and resource use fossils stand out as particularly relevant. For 1b, Climate change, Ecotoxicity, freshwater, human toxicity, non-cancer resource use, minerals and metals and resource use, fossils are prominent impact categories. The results for application 2 are provided in Figure 13 on a logarithmic scale. For 2a, the same impact categories are relevant as for 1a. Interesting to note, 10 impact categories for 2b exist that score higher than the highest for 2a (acidification). For 2b, human toxicity, cancer, resource use, minerals and metals are very dominant. But also, ecotoxicity, freshwater, and water use are very relevant.

Figure 12

Normalized and weighted comparative impact of Application 1

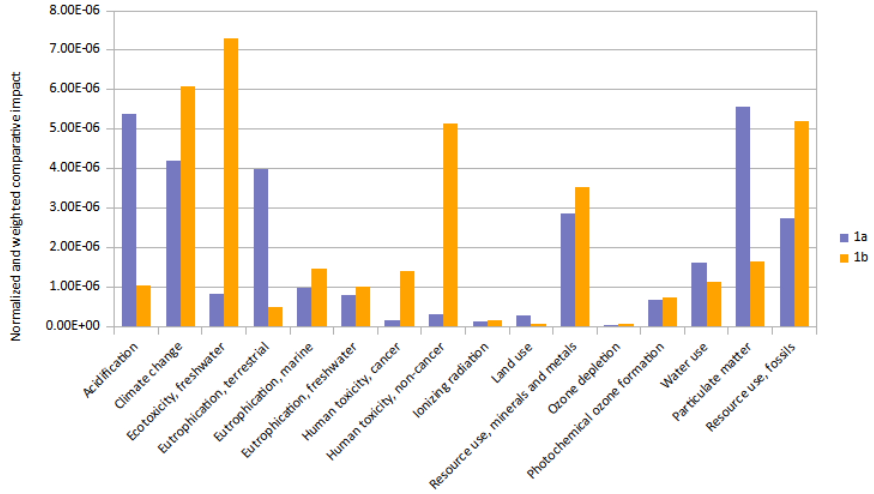
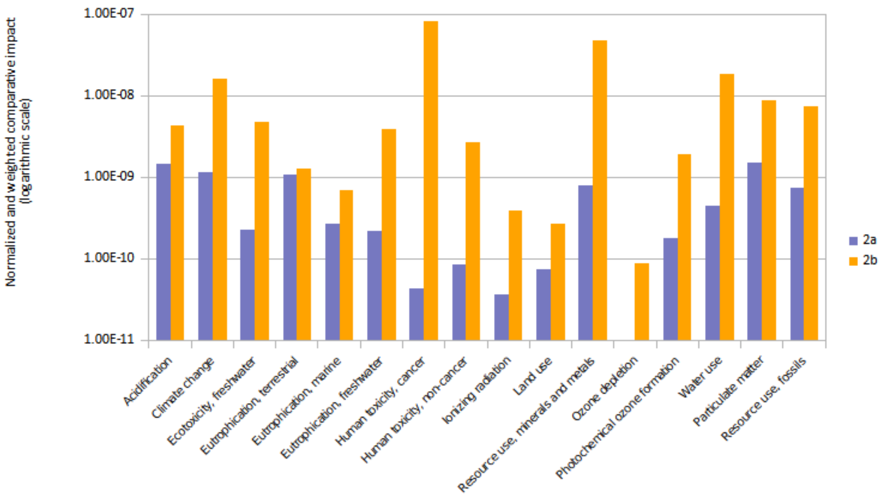


Figure 13

Normalized and weighted comparative impact of Application 2



3.3 Contribution analysis

Figure 14 shows the relative contribution of each process to the production of Disodium galactarate and by proxy of 1a and 2a. Disodium galactarate production is responsible for at least 99% of the impacts for 1a and 2a as shown in Appendix E. This implies that by evaluating the relative process contributions of disodium galactarate production, 1a and 2a also get evaluated by extension as their lifecycle impacts all most exclusively pertain to it.

The impacts are well traceable to a few products. 9 products capture for each impact category at least 90% of the indicator results. Sugar beet cultivation is most dominant for acidification, ecotoxicity, particle matter formation, and the 3 eutrophication impact categories. Human toxicity, non-carcinogen has a negative indicator results for sugar beet production as it has a positive impact on human health. The beet cultivation process involves sequestration of lead, mercury and cadmium which are responsible for the negative indicator result. The exact environmental flow contributions can be found in Appendix B 'sb human toxicity'.

Cellulase and pectinase production exclusively used during the enzymatic hydrolysis step have similar contribution patterns across the different impact categories and contribute strongly to climate change, ecotoxicity, freshwater, eutrophication, freshwater & marine, human toxicity carcinogen & non-carcinogen, ionizing radiation, and water use.

NaOH production is very dominant for ozone depletion, ionizing radiation, eutrophication, freshwater and human toxicity cancer & non-cancer and resource use, minerals and metals. It also contributes a noteworthy amount to climate change, resource use, fossils and water use, photochemical oxidant formation, resource use, minerals and metals, water use, and human toxicity impacts. NaOH is mainly used to create disodium galactarate by reacting it with Gal-A. This step is responsible for 62% of the NaOh usage. The other 38% is used to produce Gal-a.

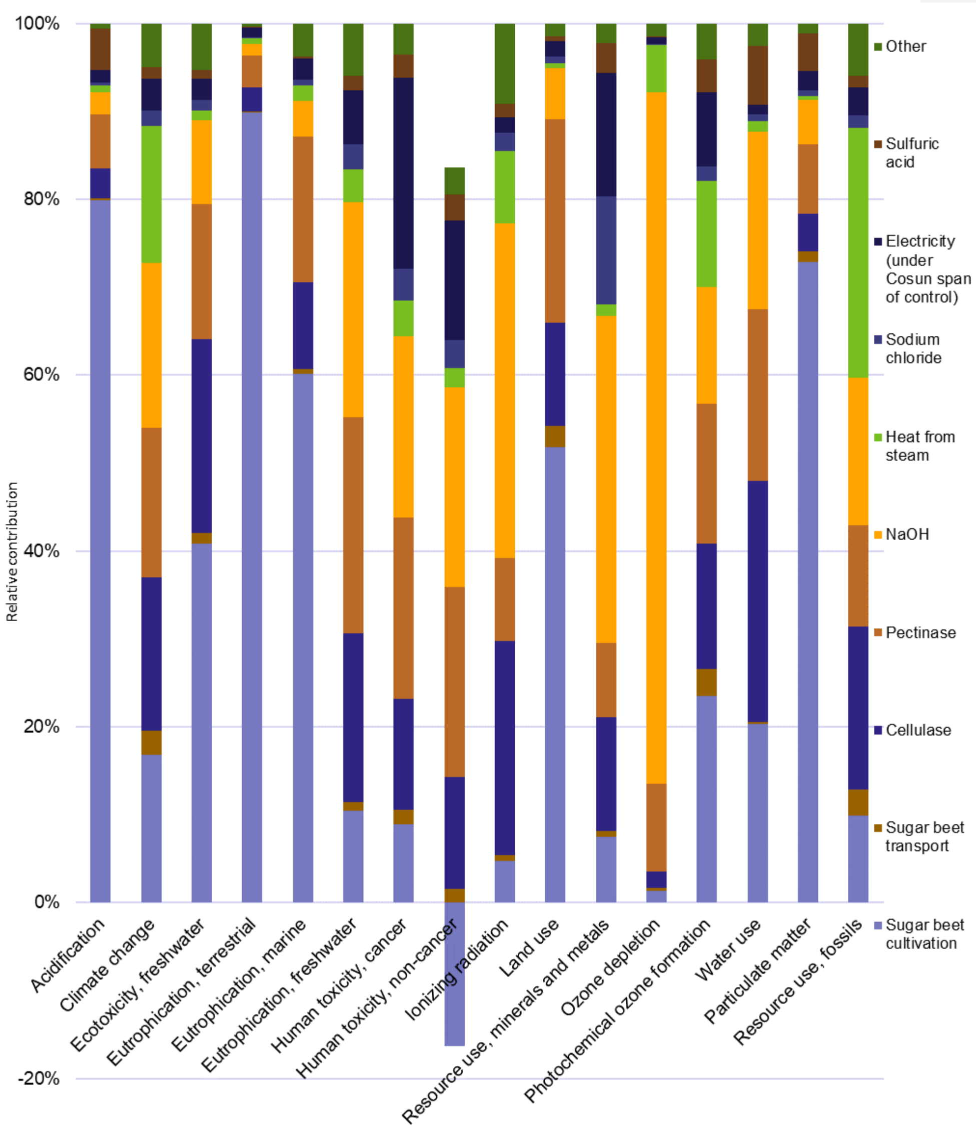
Heat to produce steam is contributing significantly to resource use, fossils, climate change, ionizing radiaton and photochemical ozone formation. Heat from steam pertains to the two concentration steps during the conversion of SBP to Gal-A and during the production of SBP as a co-product from the conversion of sugar beets to sugar. Heat from steam is used during other processes such as to produce electricity, but this is excluded here to avoid double accounting. SBP production is responsible for 31% of the impacts related to heat from steam. Concentration 1 & 2 are responsible for 51% and 17% respectively showcased in Appendix B application 2 'results'.

Electricity production strongly contributes to human toxicity, cancer & non-cancer, resource use, minerals and metals and photochemical formation. Electricity refers here to electricity used under the span of control of Cosun. This relates to the production of SBP all the way to the production of Gal-A. External inflows, such as electricity used to produce cellulase are excluded to avoid double accounting.

Sulfuric acid production, sugar beet transport, sodium chloride production, contribute to a less dominant degree to the various impact categories. None of them have an individual contribution of 4% or more for any of the indicator results. Absolute contributions can be found Appendix B application 2 'results.'

Figure 14

Process contributions of disodium galactarate



Note. The individual contributions are process contributions. Cellulase refers to the production of cellulase.

When exploring the contributions for 1b, it becomes clear that the impact categories that performed comparatively poorly and were shown to be very relevant are in part explained by the disodium EDTA that leaches to the environment. 31% and 91% of the impacts related to ecotoxicity and human toxicity, non-carcinogen respectively are caused by spent disodium EDTA leaching into the environment as can be seen in Appendix B application 1 'Leached EDTA'.

Application 2b scored worse on each impact category, but to a very extreme degree on the toxicity-related impact categories. 99% of the human toxicity, carcinogen, is caused by Cr(VI) as can be seen in Appendix B application 2 'toxicity'. This is explained by the leaching of Cr(VI) into the environment at the production of disodium dichromate (54% of total impacts for human toxicity, carcinogen as per the same appendix), which is a product used for the production of the eventual CrCl3. Another culprit is the EoL treatment of the Cr2O3 slag leaving the electric arc furnace (45% of total impacts for human toxicity, carcinogen).

For ecotoxicity, freshwater, we see similar results. Treatment of the slag from electric arc furnace (26%), treatment of waste during disodium dichromate production (32%) collectively account for 58% of the impacts which were all caused by Cr(VI). The graphical representation of this can be found in Appendix E.

3.4 Sensitivity analysis

Various sensitivities have been developed to test the robustness of the results for the proxy for 1a and 1b, the production of Disodium galactarate using a one-parameter alteration at a time approach. The following parameters are altered: electricity production under the span of control of Cosun, the heating source to produce steam for SBP production, concentration 1 & 2, the valorization of sugar during Gal-A production, sugar beet production, the carbon source to produce cellulase, the yield of Gal-A per unit of input. The results of the alterations are shown in Table 2. In this section, the most significant results are explicitly covered. In Appendix B, the full data is available.

Royal Cosun procures its electricity from renewable sources. This is justified but can potentially dilute the outcome of the comparative results. For 1B and 2B, the general electricity mix is assumed each time. The difference in electricity source can influence energy-related impact categories such as climate change and might skew them in favor of 1a and 1b. Thus, a scenario has been modeled where to produce Gal-A the regular electricity mix is used. The results show significant comparative changes for eutrophication freshwater (94% increase), ionizing radiation (293% increase), and photochemical ozone formation (14% increase) in favor of 1b. A significant comparative change is defined int this context as a situation where before 1a > 1b or 1b > 1a and that is reversed after parameter alteration. It shows an increase in climate change impacts and resource use fossils by 34% and 61% respectively, which are not comparatively significant.

The heat source to produce steam has shown to be a major contributor to various impact categories, such as climate change, resource use, fossils, photochemical ozone formation. In the base case, steam is produced relying on natural gas, it is interesting to explore the gains and trade-offs of a biobased source which constitutes another modeled scenario. The results show no trade-offs and reduction on each impact category or at least no increase. Noteworthy reductions for climate change impacts, photochemical ozone formation, resources use, fossils, with 15%, 11% and 27% respectively.

During Gal-A production, a co-product is produced, neutral sugar, specifically, arabinose. It is assumed that it can be valorized. If this economic flow turns out to be not fit for sale, it might influence the results as it would have to be treated as a waste instead of co-product making (economic) allocation invalid. No economic allocation as a lack of valorization led to an increase in results for each impact category ranging from 5% to 13%.

Sugar beet is a very dominant product when it comes to its contribution to most impact categories. Sugar beet production is based on Ecoinvent data for Germany. Different cultivation practices soil types lead to vastly different indicator results. Given the relative importance of sugar beet cultivation to the indicator results and given the potential variability, it was decided to explore alternative data sources to produce sugar beet cultivation. For this scenario, LCI data from a study published by Blonk is used for which the LCI data is available in Appendix C 'Sugar beet production Blonk'. The results are quite strongly impacted by this alteration. Significant comparative changes are observed for climate change, eutrophication, marine & freshwater, ionizing radiation, resource use, minerals and metals, ozone depletion, which are now higher for 1a. Ecotoxity, freshwater, human toxicity, cancer & non-cancer, land use and resource use fossils, are all impact categories of which the results increased, though not to a degree where they induced a significant comparative change, however to a noteworthy degree by 89%, 48%, 121%, 64%, and 43% respectively.

Cellulase production is also a significant contributor to the environmental footprint of disodium galactarate production. Various carbon sources can be used to produce it and it is not known which will be used. For the baseline production, maize starch is assumed, which is altered to wood chips and is based on LCI data by Gilpin and Andrae (2017). Only ionizing radiation had a significant comparative change. The results for Land use increased by 138%, water use decreased by 22%.

Uncertainty related to the production yield of Gal-A is explored and its effect of disodium galactarate and by proxy the functional units of 1a and 2a. In consultation with process technologists, it was decided that a 10% interval higher or lower is a plausible range for the yield compared to what is assumed in the base case. The main uncertainty is related to the crystallization processing step. That is why it is decided, that a 10% +- Gal-A crystals yield parameter alteration. The results showed no significant comparative change, and a lower yield led to increases in the results for each impact category ranging from 4% and 11%. A higher yield leads a leads to a decrease in the results for each impact category ranging from 4% and 9%.

For 2a the percentages are identical as can be seen in Appendix E. However, only one combination of a parameter alteration and impact category result led to a significant comparative change. For alternative sugar beet and eutrophication marine, a significant comparative change was observed where 2a > 2b after alteration.

Table 2

Results sensitivity analysis application 1 (disodium galactarate production)

	Acidification	Climate change	Ecotoxicity, freshwater	Eutrophication, terrestrial	Eutrophication, marine	Eutrophication, freshwater	Human toxicity, cancer	Human toxicity, non-cancer	Ionizing radiation	Land use	Resource use, minerals and metals	Ozone depletion	Photochemical ozone formation	Water use	Particulate matter	Resource use, fossils
regular electricity mix	3%	34%	3%	1%	4%	94%	-2%	8%	293%	6%	-4%	4%	14%	10%	0%	61%
steam (biowaste)	-1%	-15%	-1%	-1%	-2%	-1%	-4%	-2%	-1%	0%	-1%	-5%	-11%	-1%	0%	-27%
No sugar valorization	13%	9%	11%	14%	12%	8%	8%	5%	8%	10%	9%	5%	10%	9%	12%	10%
alternative sugar beet	-3%	88%	89%	-7%	621%	159%	48%	121%	15%	64%	29%	30%	75%	-7%	-2%	43%
cellulase (softwood)	-1%	0%	-11%	-2%	-7%	13%	0%	-3%	55%	138%	-4%	1%	0%	-22%	-2%	8%
lower yield	10%	8%	9%	11%	9%	7%	7%	-4%	8%	8%	8%	5%	8%	8%	10%	9%
higher yield	-8%	-6%	-7%	-9%	-7%	-6%	-6%	-4%	-6%	-7%	-6%	-4%	-7%	-6%	-8%	-7%

Legend

(green) No significant comparative change

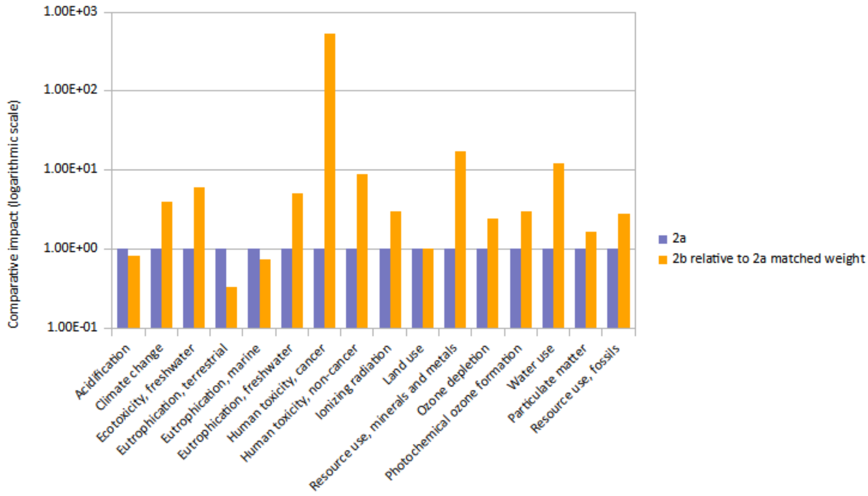
(orange) Significant comparative change -> Gal-a chelating agent > EDTA chelating agent

Note. The percentages denote by what percentage the absolute results of 1a change following from the alteration of the parameter indicated in the row. A green cell means that there is no significant comparative change for the altered parameter impact category combination. A significant comparative change is defined for the purpose of this study as a change where before 1a > 1b or 1b > 1a and that is reversed after parameter alteration. Orange means that there is a significant directional comparative change, where now 1a > 1b, for which the opposite held true prior to parameter alteration.

As highlighted previously, the reduced weight of the Disodium galactarate required is a comparative advantage of 2a. By equalizing the weight of the compounds in the coating for Cr(III) and disodium galactarate, it becomes possible to see the effect of this advantage. The factor applied 0.311 to reduce the Cr(III) content in the coating per m2. Figure 15 shows that 2a still scored better on each impact category except for the ones related to eutrophication, land use, and acidification.

Figure 15

Contribution analysis of weight application 2: Active component weight equalized by adaptation of coating thickness



While it is valid to scale the background to 2030, it is also valuable to look at a further moment in the future, because the product is not intended to be only used in the year 2030. A factory will have to be built, which is an investment for decades, therefore it is interesting to research whether the background time setting is sensitive to the overall results. The background is scaled to 2050 for application 1 which results in a significant comparative shift only for the impact category for ionizing radiation, where scaled for 2050, this was observed to be lower for 1a than 1b ceteris paribus contrasting with the results of 2030. This is shown in appendix E among more detailed results related to scaling the background. For application 2, the results are robust, and no change was observed.

As stated before, it is plausible that a small share of the Cr(III) based coating ends up in nature during its use phase. In this scenario, the potential effect of this is explored. It is assumed that 5% of the Cr(III) mass ends up in nature, specifically the industrial soil compartment. Additionally, it is also likely that a part of the Cr(III) present as a coating oxidizes to Cr(VI). So, an additional scenario has been created where 5% of the leached Cr(III) converts into Cr(VI). The impact categories affected by this phenomenon are ecotoxicity, human toxicity carcinogen, and human toxicity, non-carcinogen. The leaching of Cr(III) has a noteworthy effect on the results for ecotoxicity, freshwater and on human toxicity, cancer by over 131% and 227% respectively as can be seen in a table in Appendix B application 2 'results'. Whether part of the Cr(III) oxidized to Cr(VI) did not influence the results.

3.5 Completeness and consistency check

The thesis is checked by Prof. Dr. Ir. N. Thonemann and Prof. Dr. Ir. J. Posada. Additionally, it is checked by Dr. Ir. S. Moejes and Dr. Ir. W. Huijgen for data accuracy and confidentiality. Their supervision has been aimed to prevent the incompleteness of this study.

▪ **Differences in data sources**: The production of Gal-a is based on a bill of materials. The production of Chromium trioxide is based on LCI data from a published LCA article and the production of EDTA is taken from Ecoinvent. Though the sources are different, they all exhibit a high level of detail and scientific standard. The further processing of these compounds is based on stochiometric data found in published articles. For application 2, both alternatives exclude the bath formulation as a whole and account only for the coating created. The use phase and EoL are based on the literature review performed and are linked to Ecoinvent where appropriate. To produce Gal-A renewable electricity is assumed, contrasting with the alternatives which make use of the average electricity grid. The effect of this decision is discussed to avoid misplaced conclusions.

▪ **Differences in data accuracy**: Differences in data accuracy are an inherent concern of comparing emerging product systems with commercial product systems as outlined by Thonemann et al. (2020). Because the foreground is modeled ex-ante for Gal-a production and its applications. There is uncertainty related to the eventual production and its performance. Specifically, the yield of Gal-A per unit of input and the performance as a coating. For the former, the implications of this are analyzed in the sensitivity analysis. For the latter, this is managed by working with a theoretic thickness change, where coating concentrations per m2 have been set to an equal level. Rationale behind the latter is that a thicker coating leads to a better performance.

▪ **Temporal differences and differences in data age:** All alternatives are scaled to 2030. A section in the prospective foreground details possible anticipated changes in the product system, which was deemed inapplicable due to the short time horizon. The background is scaled consistently using the PREMISE approach as outlined in the Methods and materials section. Data sources related to the treatment of Disodium EDTA in STPs are something two decades or even older. It has been thoroughly validated that, though old, the conclusions are still relevant. sugar beet cultivation is from 2009-2012.

▪ **Differences in geographical representativeness:** The foreground processes and the technologies are all relevant for Europe, mostly Western Europe making it representative. The primary production processes related to Gal-a pertain to the Netherlands. Exceptions to this are market activities, such as sulfuric acid inflows and the production of sugar beets and enzymes, of which the unit process data is relevant for Germany and France respectively. EDTA production is a market activity based on German factories. Cr_2O_3 production is originally modeled for Greece, but all the economic flows are connected to either the Netherlands or to Europe in general.

▪ **Differences in the function performed**: For application 1, the same functioning is assumed, as Disodium galactarate is assumed to be a drop-in for Disodium EDTA. For application 2, the scope is kept narrow, strictly to anti-corrosive performance. This ensures consistency between the functions performed.

4 Discussion

Having presented the results in Chapter 3, the following sections reflect on the key findings, and discuss some of the main limitations of this work.

4.1 Key findings

This study has provided a comprehensive analysis of the environmental impacts associated with the production and application of Gal-A and its alternatives.

For 1a and 2a, acidification, climate change, eutrophication, terrestrial, resource use, minerals and metals, particulate matter and resource use fossils stand out as particularly relevant. For 1b, Climate change, Ecotoxicity, freshwater, human toxicity, non-cancer resource use, minerals and metals and resource use, fossils are relevant impact categories. 1a outperforms 1b for the relevant impact categories, climate change, resource use, fossils, and ecotoxicity, freshwater, human toxicity carcinogen & non-carcinogen. Of the relevant impact categories, 1b scores significantly better on eutrophication, terrestrial, acidification and particulate matter. 2a outperforms 2b on each impact category. For 2b, human toxicity, cancer, resource use, minerals and metals are the most critical impact categories. But also, ecotoxicity, freshwater, and water use are very relevant.

The contribution analysis highlighted that for 1a and 2a, via the proxy of Disodium galactarate production, 9 processes contribute to at least 90% of the results for the impact categories identified as relevant for 1a and 2a. Notably, sugar beet cultivation's contribution is very dominant for 3 of the 4 most relevant impact categories, acidification, eutrophication, terrestrial, particulate matter, individually contributing to at least 75% of the indicator results. Cellulase and pectinase used during the enzymatic hydrolysis step contribute strongly to climate change, resource use, minerals and metals & fossils. NaOH, mainly used to react with Gal-A to create disodium galactarate and during the production of Gal-A. This process is very dominant for climate change, resource use, minerals and metals resource use fossils. Heat from steam mainly used for the SBP production and concentration 1 step and to a lesser degree for the concentration 2 step is contributing a significant amount to the results for climate change and resource use, fossils. Sodium chloride and electricity production under the span of control of Royal Cosun contribute strongly to resource use, minerals and metals by 12% and 14% respectively.

For 1b, the impact categories that performed comparatively poorly, human toxicity, non-cancer and ecotoxicity, freshwater, and were shown to be very relevant are in part explained by the disodium EDTA that leaches to the environment. 2b performed worse to a very extreme degree on the toxicity-related impact categories. Even though the coating is Cr(III) based, 99% of the indicator results for human toxicity, cancer and 56% for ecotoxicity, freshwater were caused by Cr(VI). This is explained by the leaching of Cr(VI) into the environment at the production of sodium dichromate and the EoL treatment of the Cr2O3 slag leaving the electric arc furnace.

The sensitivity analysis showcased the importance of renewable energy usage two of the relevant impact categories. A regular electricity mix resulted in steep increases for climate change and resource use, fossils of 34% and 61% respectively. Though eutrophication, freshwater almost doubled and ionizing radiation leading to a significant comparative change as a result of a regular electricity grid, the relevance of the impact categories remained low. While biogas to produce steam reduced the impacts of climate change and resource use, fossils by 15% and 27% respectively.

Sugar beet cultivation proved to be very sensitive to the alteration for relevant impact categories. Indicator results for climate change, resource use, minerals and materials resource use increased by 88%, 29% and 43%. Other impact categories initially of secondary interest increased by a lot reevaluating their relevance. Eutrophication marine, freshwater lead to a significant comparative change by increasing with 621% and 159% and while considered of secondary interest initially, these impact categories have gained relevance.

The other sensitivities related to disodium galactarate production yielded fewer sensitive results. Cellulase from softwood increased the indicator results or ionizing radiation and land use by 55% and 138% respectively. However, these impact categories have been deemed of secondary interest, even when considering these large relative increases. No sugar valorization, a high and low Gal-A yield did result only in incremental changes on the different indicator results never increasing them by more than 14% or reducing them by less than 9%.

2 sensitivities were explored for application 2b. Reducing the Cr(III) content in the coating per m2 led to significant comparable changes for relevant impact categories, acidification and eutrophication, terrestrial, where 2b outperformed to 2a. Cr(III) leaching into the environment during the use phase of 2b is a serious concern, even for a relatively small share of the coating (5%), more than doubling and tripling the results of ecotoxicity, freshwater and human toxicity, cancer each.

The results proved to be robust when scaling the background further into the future for the impact categories of interest. Scaling the sectors in the background covered by PREMISE to 2050, led only to one significant comparative change to an impact category of secondary interest, namely ionizing radiation for 1a became smaller than 1b.

4.2 Limitations

Overall, the results have shown no problematic sensitivities except for sugar beet cultivation. Significantly different results are acceptable for parameters which are related to strategic production decision, where the LCI data is well understood such as to opt for renewable electricity or biogas instead of natural gas. For processes which are very sensitive and relevant, and the primary data is not available or up to date, it becomes problematic. This is the case for sugar beet cultivation, a critical process from a contribution analysis perspective, compromising the quality of the study.

Pectinase is used as a black box process decreasing the transparency of the study. It is unclear what LCI data was used to compute the results, making it impossible to assess the comprehensiveness. Additionally, it was not possible to scale the background of this process to the future.

The coating application process for application 2 is cut off reducing comprehensiveness. Parameters such as complexing agents, bath pollution progression, and subsequential cleaning thereof are not yet conceptualized fully beyond a patent. These are excluded for applications 2a and 2b. This ensures comparative consistency between 2a and 2b, but might result in omitting impactful processes for the absolute and comparative results. For example, if application 2a requires more chemicals that pollute the bath faster, then this is a relevant factor that has not been accounted for in this study.

The performance of the coating for 2a is not well understood in an absolute and comparative sense. Coatings are meant to last for a long time, but as disodium galactarate as a coating is novel, the long-term performance in a real-world setting is not well validated yet. The coating function was also reduced to only anti-corrosive properties, which might be a bit to reductionist, as other factors, such as color, paint adhesion are typically considered as integral part of a surface coating performance.

5 Conclusion and recommendations

5.1 Conclusion

This thesis aims to contribute to the understanding of the performance of SBP-derived Gal-A applications, specifically as a chelating agent and as a surface coating in a future comparative context. This was done by considering the following research question:

What will be the cradle-to-grave environmental impacts of SBP-derived Gal-A as a conversion coating and chelating agent compared to that of Cr(III) and EDTA respectively in the Netherlands in 2030?

The environmental performance of the alternatives for application 1 exhibits notable trade-offs related to the relevant impact categories. 1a outperforms 1b on climate change, resource use, fossils, and Ecoxicity, freshwater, human toxicity, non-carcer. 1b scores better on the relevant impact categories, eutrophication, terrestrial, acidification and particulate matter. Sugar beet cultivation is largely responsible for the results of 1a on the impact categories 1b scores better in contributing at least 75% to each of them individually. Royal Cosun's strategic decision to procure renewable electricity is for a large part responsible, but not fully, for the superior performance of 1a on 1b for climate change and resource use, fossils. EoL leaching of Disodium EDTA is for a significant part responsible for the results of ecotoxicity, freshwater and human toxicity, non-cancer, which are 2 of the 4 most prominent impact categories for 1b. This highlights the advantage of the biodegradability of Gal-A where EoL is not contributing to these impact categories.

2a outperforms 2b on each (relevant) impact category. For acidification and eutrophication terrestrial, this in part was due to the thinner coating for 2a requiring less disodium gal-a per m2 passivated. 2a outperformed 2b, to an extreme degree for the toxicity-related impact categories. For human toxicity, cancer, the most relevant impact category, and for ecotoxicity, freshwater, 2b scores more than 1800 and 20 times higher than 2a. The results for 2b for these impact categories could be multiplied many times when considering that part of the coating leaches into the environment during the use phase. Cr(VI), released during the production of Cr(III) and at EoL, is largely responsible for these high impacts, which is interesting, because, Cr(III) coatings are seen as a non-carcinogenic safer alternative by the chemical industry.

5.2 Recommendations for Royal Cosun

Whether it makes sense for Royal Cosun to pursue 1a depends on its prioritization of environmental impact categories. The results for application 1 are in line with the expectations outlined during the introduction. 1a can deliver on its promise to reduce CO2 eq. emissions and a reliance on fossil resources compared to 1b. It is also less toxic to humans and ecosystems. Trade-offs exist for acidification and eutrophication, terrestrial and particulate matter, mostly caused by sugar beet cultivation.

The comparative environmental results for application 2 are very clear in favor of 2a. 2a outperforms 2b on each impact category and in most cases by multiples. 2a is especially advantageous when prioritizing toxicity reduction and when accounted for bits of the coating leaching into the environment during its use phase. The positive toxicity results for 2a can in part be attributed to its environmentally benign EoL treatment and its production processes. Though coating thickness is an advantage for 2a, it does only to a very small degree impact the overall results. For example, human toxicity, cancer, which is the most relevant impact category, is still more than 600 times higher after equalizing the coating weight. While the coating application process has been left out of scope, and some uncertainty exists surrounding the performance equivalence between 2a and 2b, the results still are deemed robust due to the convincing comparative results.

Royal Cosun can play an important role in reducing the environmental footprint of 1a and 2a. All the impacts almost exclusively pertain to disodium galactarate production, which up until the production of Gal-A lies under their span of control. Renewable energy usage, a high Gal-A yield, and the valorization of sugar co-products are low hanging fruit to improve the environmental footprint of the applications with no noteworthy drawbacks. Sugar beet cultivation has proven to be the most dominant individually contributing process to most relevant impact categories for 1a and 2a. This makes more sustainable agriculture practices the most promising process step to reduce environmental impacts. Lastly, reducing enzyme usage during enzymatic hydrolysis could also be an important leaver to explore.

5.3 Recommendations for future research

Future research can focus on improving the robustness of the results with better data quality and more transparency for some of the parameters. Given sugar beet cultivation's dominance on the results, up-to-date primary data will significantly improve the accuracy and representativeness of the results of the study. Pectinase is modeled as a 'black box' process and for cellulase the carbon source, which is a critical aspect of its environmental footprint, is uncertain. Primary and up-to-date LCI data for pectinase and cellulase production will improve the transparency and accuracy of the study results.

Extending the scope of this study can also be done in future research. For application, some elements were left out of scope. Specifically, including the application process of the coating will improve the overall results. A relatively narrow functional unit has been used for application 2, only considering the anti-corrosive properties, the use phase has been left unspecified, lacking details on the nature of the steel substrate that is coated, its lifetime, and its corrosive context during the use phase.

For each application, only 2 alternatives were researched. Future research could include more alternatives, it would specifically be interesting to include more biobased alternatives for application 1 from biobased sources other than the sugar beet. This study was useful, particularly for application 1, to expose typical environmental trade-offs between biobased applications and petrochemical applications. To get a better understanding of the performance of 1a and 2a as biobased applications, benchmarking them against other biobased alternatives could be an interesting next step. This would allow the narrative to move from: Do we see the trade-offs we expected between biobased and petrochemical, to which biobased source is preferred? The environmental footprint of Gal-A from orange peels could be compared to that of SBP or Gal-A to another biobased molecule with similar properties. More experimentation can be done with various technical parameters simultaneously to give more detailed advice to Royal Cosun on Gal-A on optimizing the Gal-A production process. By exploring the interplay between enzyme quantities, electricity usage, and the yield during the enzymatic hydrolysis step a preferred configuration could be discovered from an environmental perspective.

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Appendices

Appendix A

Table A1

Stochiometric calculations Disodium EDTA production

Components	Moles (mol)	Molecular Mass (g/mol)	**Role**
EDTA (C10H16N2O8)	1	292.28	Reactant
Sodium Hydroxide (NaOH)	2	40	Reactant
Disodium EDTA (C10H14N2Na2O8)	1	336.24	Product
Water (H2O)	2	18.02	Product

Note. EDTA per kg disodium EDTA produced is 0.86926 and Na is 0.13074

Table A2

Stochiometric calculations Disodium Galactarate production

Components	Moles (mol)	Molecular Mass (g/mol)	**Role**
Galactaric Acid (C6H10O8)	1	210.14	Reactant
Sodium Hydroxide (NaOH)	2	40	Reactant
Disodium Galactarate (C6H9Na2O8)	1	254.1	Product
Water (H2O)	2	18.02	Product

Note. H20 and Na per kg disodium Galactarate released during evaporation/biodegrading are assumed to be 0.637544 and 0.180952. Based on the number of H and Na atoms present in 1 kg Disodium galactarate

Table A3

Stochiometric calculations of CrCl3 production

Components	moles	Molecular Mass (g/mol)	**Role**
Cr2O3	0.5	151.99	Reactant
Cl2	1.5	70.9	Reactant
CrCl3	1	158.36	Product
O2	0.75	32	Product

Note. The energy (heat) required to produce 1 kg CrCl3 is 761 KJ. Stochiometric data and heat requirement is derived from Gaballah et al., (1998).

Table A4

Stochiometric calculations of oxidation of Cr(III)

molar mass Cr2O3	molar mass Cr	multiplication factor oxidation
151.9904	51.9961	2.923111541

Note. This relates to the factor of mass increase of Cr(III) from the coating produced in the electric arc furnace that ends up being slag

Appendix B

Appendix B is externally provided as Excel sheets. These Excel sheets are mainly pertaining to the raw data for the results section.

Appendix C

Appendix C is externally provided as an Excel sheet. This pertains to data used to model the product systems, such as the mass balance sheet for Gal-A production.

Appendix D

This appendix consists of a link to uncharacterized LCI inventory results for applications 1 and 2. It also includes the export of the databases developed in AB to model the results. Two databases have been developed to declutter them and improve the workflow during modeling. Database 'Gal-A foreground' is used to model the production of Gal-a. Database 'Applications' has been used to model the rest. This appendix is