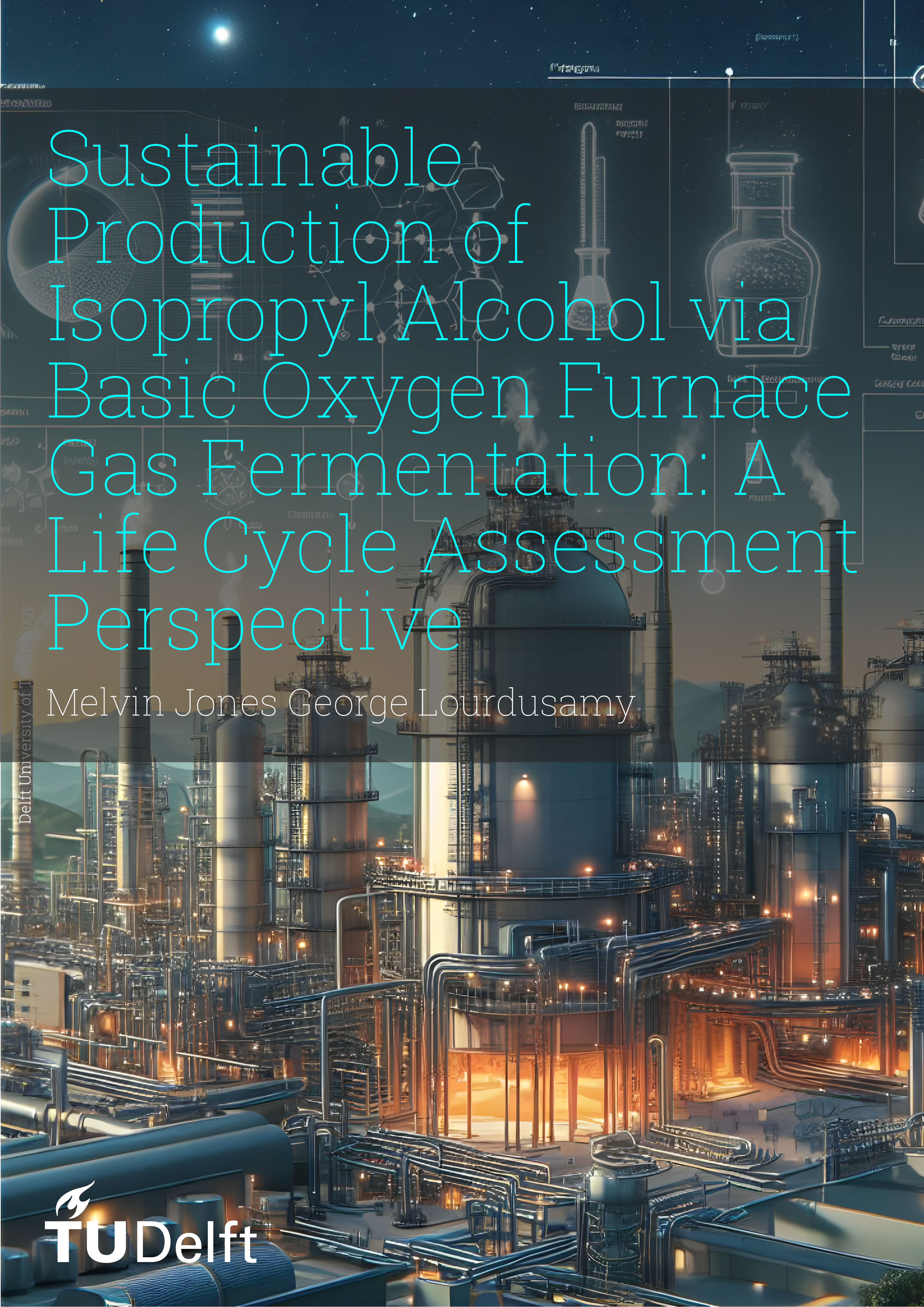

Sustainable Production of Isopropyl Alcohol via Basic Oxygen Furnace Gas Fermentation: A Life Cycle Assessment Perspective

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Preface

All glory to the almighty God.
Dear Ladies, Gentlemen, and my beloved friends, Revealing this research highlights the collaborative efforts and steadfast guidance of my supporters. Dr. John Posada Duque, you have been the greatest mentor, and your guidance has been a compass pointing me toward scholarly shores, guiding me through the turbulent waves of research with unwavering resolve. Professor Frank Hollmann, you are more than a supervisor; your faith in my abilities and your guidance as a green list supervisor, without any recompense, leave me indebted in gratitude. Mr. Gijs Brouwer, you have been more than a supervisor; your patient tutelage was akin to a skilled craftsman shaping raw talent into refined expertise. Your trust in my journey paved the way for growth and mastery. A heartfelt thank you to the Biotechnology & Society research group for bestowing upon me this incredible thesis opportunity and a great workspace. I have relished every moment of it.

To my friends, you have been the lifeline in this academic journey. Your humor has been my relief, your encouragement my strength, and your unwavering presence, my true north. Your spirited antics kept me grounded. Mr. George and Mrs. Victoria, special thanks for believing in me and being there for me in my lowest moments and my successes. I have flourished through your words of care and support; your blessings propel me forward in life. A special gratitude to my grandparents for your constant care and support.

As I prepare for my thesis defense, I do so not in solitude but as a mosaic of influences and a harmony of support. Each of you has enriched my journey, turning what began as an academic pursuit into a dynamic and fulfilling adventure.

I would like to express my sincere gratitude to the mentors, friends, and family who have supported me throughout this thesis defense journey, enabling me to navigate challenges with resilience and achieve success. Your unwavering support has transformed this experience into a testament to collective effort and shared victories. May all continue to prosper and flourish.

Melvin Jones George Lourdusamy
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Abstract

The CO_2 emissions started to peak during the start of this century and the steel manufacturing sector accounts for 25% of the global CO_2 emissions. The majority of steel production is based on the route of the basic oxygen furnace (BOF) route, which is energy efficient. This production route results in the emission of BOF gas. So a new method to produce Isopropyl alcohol via BOF gas fermentation was developed for the pilot scale plant and the LCA was performed by Liew et al., (2022). The carbon-negative emissions were calculated and estimated in the pilot scale study. A few inconsistencies were identified in the calculation method, in which the components utilized for the production process contributed less than 5% to the Global Warming Potential value, and the replacements provided to the steel mill for the BOF gas redirection were cut off. The LCA value for the pilot-scale plant was incomplete and inconsistent, and only the GWP was chosen as the prominent midpoint indicator. Based on this pilot-scale plant, an industrial-scale (46 kton/ yr) base case process model was developed for the gas-fermentation process to produce IPA. The fermentation is the major step involved in the production of IPA, which involves the acetogenic bacteria *Clostridium Autoethanogenum*. The initial process involves the capture of the emission of BOF gas for compression and cooling performed because the temperature of BOF gas is around 1100°C. This compressed gas is fermented using of microbes and filtered out to obtain the filtered broth. Then the IPA is separated from the filtered broth using extractive distillation, using glycerol (Brouwer, 2023). The major product of IPA is processed out of the system. This research aims to analyze and estimate the environmental impacts of this process model of BOF gas fermentation to produce Isopropyl alcohol. The assessments were performed for the base case and the 11 process parameters of CO conversion, Volumetric mass transfer rate of CO, Product selectivity, Dilution rate, Extractive distillation glycerol mole fraction, Temperature offgas condenser, Anaerobic waste conversion, Extractive distillation molar reflux ratio, Biomass liq-liq mole fraction and the broth and glycerol purges. The impact assessment results help to identify the potential contributors in the process that affect the environment, so the process model can be optimized to yield lower impact values concerning the environmental perspectives.

The 7 midpoint indicators namely Global Warming Potential (GWP), Stratospheric Ozone Depletion (SOD), Fine Particulate Matter Formation (FPMF), Freshwater Eutrophication (FE), Marine Eutrophication (ME), Human Carcinogenic Toxicity (HCT), and Land Use (LU) were chosen to obtain a detailed view on the ecosystem, human health, and the environmental effects. The replacement calculations estimated for 1 kg of IPA production is 4.324 MJ of heat, and 0.877 kWh of electricity, has to be replaced for the steel mill. The impact assessment for the base case model was performed and compared with the conventional IPA production method (GWP: 2.026 kg CO_2 eq.), the global warming potential for the BOF gas fermentation method (GWP: 27.656 kg CO_2 eq.) estimated to be a 1265% increase compared with the conventional IPA method. Similarly, all seven impact categories are estimated to have a huge increase in values. An elaborate study compared and identified the most influential process parameters. The process parameter of dilution rate in which the dilution rate is lowered by 30% from the base case value appears to be the process parameter with a lower impact value of 20.464 kg CO_2 eq. for the Global Warming Potential (26% lower than base case), 1.72E-05 kg CFC11 eq. for the Stratospheric Ozone Depletion (31% lower than base case), 9.618E-03 kg $PM_{2.5}$ eq. for the Fine Particulate Matter Formation (38% lower than base case), for the Freshwater Eutrophication the value is 9.853E-04 kg P eq. (53% lower than base case), 5.531E-03 kg N eq. for Marine Eutrophication (33% lower than base case), 1.733E-01 kg 1,4-DCB for the Human Carcinogenic Toxicity (53% lower than base case), and the 3.265 m^2a crop eq. (32% lower than base case) for the Land use impact categories. The major contributors are the high-pressure and low-pressure steam utility contributing greater than 56% for the impact category values of the GWP, FPMF, FE, and HCT particularly. The glycerol used for the extractive distillation process contributed greater than 92% for the impact categories of SOD, ME, and LU. The impact assessments across different indicators were interpreted and the major process parameters that are more influential in reducing the impact values are identified. The results indicate that the major contribution to the impact value is reduced by the emission credit $\approx$ 40% for preventing the BOF gas from flaring. The carbon dioxide emission from the process, glycerol component, and steam utility collectively contribute majorly which account for more than 90% of the total impact values in the impact categories. Lowering the dilution rate, glycerol purge fraction, and glycerol mole fraction by -30%, and increasing the volumetric mass transfer rate by +30% of the process model could result in lower impact values. The CO_2 emitted from the process is estimated to be 9.34 kg CO_2 eq. This emission is higher than the feedstock (BOF gas) used for the gas-fermentation process. The entertainer glycerol is anaerobically digested and combusted leading to the 10% of the total CO_2 emission of the process model. The process model should be updated with the process parameters listed above and a similar life cycle impact assessment has to be performed to compare the impact values. This updated process model might have comparatively better results. The sensitivity study has been performed to estimate the percentage effects of the combined glycerol and steam components on the midpoint indicator impact value. Cutting off the components of glycerol and steam from the process model still yields the GWP value of 6.16 kg CO_2 eq. for industrial scale process which is a 204 % increase than the conventional IPA process. This implies that the updated process model with similar process steps cannot obtain impact values lower than the conventional IPA method. To lower the impact value of GWP, the CO_2 emission from the process should be sequestrated (carbon capture) to lower the GWP value by 42% from the base case.

Keywords

Life cycle Assessment; Isopropyl alcohol; Basic Oxygen Furnace gas; gas fermentation; glycerol; dilution rate; steam utility; *C. Autoethanogenum*

Contents

Nomenclature

Abbreviations

Abbreviation	Definition
BOF Gas	Basic Oxygen Furnace Gas
CAGR	Compound Annual Growth Rate
CFC	Chloro Fluoro Carbon
CH_4	Methane
CO	Carbon monoxide
CO_2	Carbon dioxide
DCB	Di-Chloro Benzene
DHOP	Direct Hydration of Propylene
EAF	Electric Arc Furnace
EIA	Environmental Impact Assessment
EU	European Union
FE	Freshwater Eutrophication
FPMF	Fine Particulate Matter Formation
FU	Functional Unit
GHG	Green House Gas emissions
GMO	Genetically Modified Organisms
GWP	Global Warming Potential
H_2	Hydrogen
HCT	Human Carcinogenic Toxicity
IHOP	Indirect Hydration of Propylene
IPA	Iso-Propyl Alcohol
ISO	International Standards Organization
KPI	Key Performace Indicator
LCA	Life Cycle Assessment
LCI	Life Cycle Inventory
LCIA	Life Cycle Impact Assessment
LDG	Linz- Donawitz gas
LU	Land Use
ME	Marine Eutrophication
N eq.	Nitrogen equivalent
N_2	Nitrogen
NASA	National Aeronautics and Space Administration
O_2	Oxygen
OHF	Open Hearth Furnace
P	Phosphorous
PM	Particulate Matter
ROI	Return of Investment
SOD	Stratospheric Ozone Depletion

1

Introduction

The major peak in environmental emissions around the world started to peak during the Industrial Revolution in the 18th century and further continued even during the first, and second oil crises and Economic collapse in the world (Bersalli, Tröndle, & Lilliestam, 2023). The major polluter in terms of emission is Carbon monoxide (CO) which is twice as strong as carbon dioxide due to its Global Warming Potential (GWP) value (20 years) of 2.8 kg CO_2 eq. Carbon monoxide (CO) is a colorless, odorless gas that is emitted when a carbon-based material is incinerated or burnt incompletely. As cited by NASA the CO gas is not consistently emitted from particular parts of the world, whereas it is emitted seasonally like agricultural burning based on the harvesting seasons alternating on the northern and southern hemispheres (NASA, n.d.). On a contrasting note, a considerable amount of CO and H_2 are emitted constantly over the period, and the sector that accounts for this emission is the Industrial and manufacturing sector. There is a steep growth in the emissions by this sector. In particular, the Steel production industry has a significant share in this nearly 7.2%. However, due to the recent advancements in the technological world, the emission per tonne of steel produced is lowered. From 1.54 ton CO_2/ ton steel in 2015 to 1.32 ton CO_2/ ton steel (IEA, 2023). The steel mill emissions does not have a similar composition all the time. 20% nitrogen, 50% carbon monoxide, 20% carbon dioxide, and 10% hydrogen is the composition of steel mill emission (BOF gas) as cited by (Liew et al., 2022), of which the Carbon monoxide and hydrogen are utilized for the newest IPA production technique.

Isopropyl alcohol commonly known as Isopropanol or IPA, is an essential compound used widely in the medical, cosmetics, chemical, and construction sectors. In addition to this, it is utilized in quick-drying inks and oils, IPA is also a solvent for gums, shellac, and essential oils. Moreover, it is present in hand lotions, after-shave lotions, and body rubs (Xu, Chuang, & Sanger, 2002). It is a colorless, flammable compound compatible with water, alcohol, and hydrocarbons (Xu et al., 2002). Conventionally there are three different methods for the production of Isopropyl alcohol. When considering the impacts on the environment during this production method, the impact values are considerably lower when the values are compared with the compounds of similar properties (Dai et al., 2019). On an interesting note, the IPA has no major environmental issues or effects during its conventional synthesis. However, when considering its previous form from where it is derived it might lead to major effects on the environment as well as humans. IPA is the derivative of propylene, which is the second-largest petrochemical produced after ethylene (Phung, 2021). Based on the continuous demand, IPA is expected to be huge by 2030 (Lin & Jingwen, 2021). Some disadvantages in the traditional petroleum-based synthesis of IPA include high temperature and pressure requirements, low propylene yield, and major use of fossil (petroleum) based raw materials (Phung, 2021). When the life cycle analysis is performed, not just the production process for IPA is considered but also the raw materials (petroleum-based) utilized will also be accounted for. Three ways are known to date for the production of IPA from propylene: Direct hydration of propylene (Diala, 1987), Indirect Hydration of propylene (Diala, 1987), Catalytic hydration of propylene (IARC, 1970). A full comparative study of the different IPA production methods will be elaborated in the later parts of this report. The demand for isopropyl alcohol was 3100 thousand tonnes in 2022. Of this, nearly 42% was consumed only by the pharmaceutical industries (Chemanalyst, n.d.). The expected demand for IPA is to be nearly 4700 thousand tonnes with a compound annual growth rate (CAGR) of 3.25%. The conventional way of producing isopropyl alcohol involves the usage of propylene or acetone as the raw material. These conventional methods don't evolve the hazardous emission compounds during their production processes. The environmental effects can be accounted for by tracing back the raw materials sourced for the conventional IPA production processes.

The demand for chemical compounds in the modern world is humongous, and the ways to synthesize them involve the usage of non-renewable resources. Using these non-renewable raw materials could have adverse environmental impacts like global warming and environmental depletion. So, technologists were interested in looking forward to alternative green and carbon-negative approaches. The IPA via BOF gas fermentation is one such process that involves altering the conventional unit process methodology which is energy-intensive, by using the microbes for the syngas fermentation, which could be the carbon-negative effective method (Sun Xiao, 2019). The major raw material for this process is syngas (BOF gas), which is emitted from the basic oxygen furnace of the steel mill. This syngas has a major composition of carbon monoxide (CO) and hydrogen (H_2) are the feedstock requirements for the microbes to undergo gas fermentation. Liew et al., (2022) published that the pilot scale plant has carbon-negative emission for the gas fermentation process.

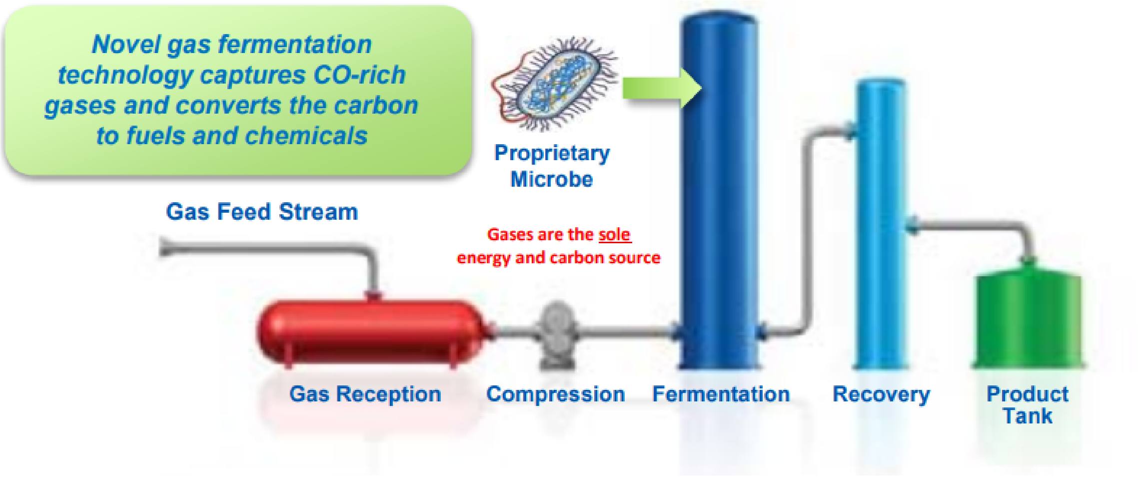

Figure 1.1: Lanzatech's process (Lanzatech, (2016))

The model for pilot scale plant by Lanzatech, was represented in figure 1.1 (Lanzatech, 2016). This figure represents the production method for the ethanol from the syngas utilizing the microbes for syngas fermentation. Both the ethanol and IPA process have similar production steps. However, these microbes are genetically modified to achieve the desired product output (F. Liew et al., 2017). This process starts by feeding in the BOF gas and by compressing it. Then the compressed gas is fermented with the help of microbe *Clostridium Autoethanogenum*, and the synthesized Isopropyl alcohol is recovered and directed into the product tank. The base case model was modeled by Gijs Brouwer in his master thesis project, representing the pilot scale plant's results and modeling the industrial scale process based on it. He has identified particular Key Performance indicators. These KPIs were selected based on their indication of overall performance on the process model. The sensitivity analyses were also performed for all the process parameters to identify the effect. So, the environmental impact assessment was performed for the base case scenario along with the sensitivity analysis scenarios based on the process parameters that could have more environmental impacts differing from the base case.

1.1. Environmental impact assessment

Environmental Impact Assessment (EIA) is a method that is used to assess both the positive and negative impacts of a proposed project or work (NLgovt, n.d.). When it comes to the process industries, it must be assessed in the early stages of the project design even before execution (pilot-scale). Most countries across the globe don't mandate the need for EIA, but it is advisable to assess for the impacts (UKGovt, n.d.). Researchers across the world have a difference of opinion regarding the usage of environmental impact assessment methods. Some researchers claim the positive aspects as the contribution to sustainable development and the negative impacts have the potential to stop projects that are likely to have good economic return of investment (Nita, Fineran, & Rozylowicz, 2022). The environmental impacts of any particular process should also account for the impacts that are caused by the process, in the case of the new implementation strategy. This is considered due to the replacement that is done to replace the raw materials if it is redirected for another process. So, the actual process which depends on the actual pathway will be forced to find an alternate to adjust for the products or utilities which is now redirected from that original pathway. Let us consider a process in which the final product emits emissions into the air, along with the utilities that will be recirculated in the process. If the final product is redirected and used in such a way it has less environmental impact, the actual process should be looking for alternate resources to account for the loss of utilities. These replaced resources should also account for the impacts along with the environmental impacts of the upcoming process.

1.2. Problem Description & Research Questions

The Life cycle analysis work performed by (Liew et al., 2022), has only considered the system boundary for the BOF gas fermentation method. But the BOF gas emissions from the steel mill are not only flared and emitted as CO_2, instead heat recovery and electricity production are taking place. The replacements for steel mills were not considered by Liew et al.,(2022). So, this thesis work aims to perform an environmental impact assessment of an effective integrated process to produce Isopropyl alcohol from Basic oxygen furnace gas, which is emitted from steel mills. This impact assessment involves the whole process, in which the BOF gas emission is captured and the initial process of compression and cooling is performed because the temperature of BOF gas is to be around 1100°C (Brouwer, 2023). Next, this compressed gas is fermented with the help of microbes and filtered out to obtain the filtered broth. Then the IPA is separated from the filtered broth using extractive distillation, with the help of glycerol (Brouwer, 2023). The major product of IPA is processed out of the system. This also evaluates the impacts caused by the steel mill, when the alternative for BOF gas is considered for the heat and electricity usage. The Life cycle analysis will be performed for all the sensitivity analyses to assess the impacts caused by altering the key values.

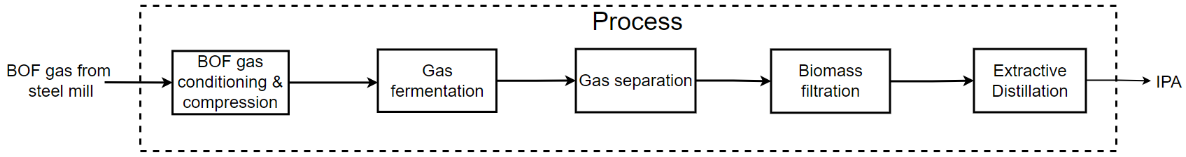

Figure 1.2: IPA production process

To obtain approval for production on an industrial scale, the process should be feasible in the aspects of economic, environmental, and process efficiency. However, the process should also have lower environmental impacts along with economic feasibility. The three criteria include well-process design, less environmental impact, and economic feasibility. One production technique that satisfies all three criteria of effective process design, lower environmental effects, and economic feasibility is suited for commercial-scale production. In this case, the comparison of environmental effects between all the sensitivity analysis case scenarios will provide information or input about the most impactful material that has been utilized throughout the process. By identifying them, the usage of that particular feed can be modified to reduce the impact. Generally, the environmental impact assessment (EIA) can be carried out with the life cycle assessment method. This LCA method has two different assessment methods, the midpoint and endpoint indicator categories. The midpoint category deals with the immediate environmental impacts like emissions and usage of resources, but the endpoint category results provide an overall view of the environmental assessment in terms of human health, the environment, and the ecosystem. In most life cycle assessments performed for different products and processes, only the midpoint indicator category of global warming potential (kg CO_2 eq.) is considered. To estimate the overall impacts on the ecosystem, human health, and environment the seven midpoint indicators were chosen. The seven midpoint indicators include global warming potential, stratospheric ozone depletion, fine particulate matter formation, freshwater eutrophication, marine eutrophication, human carcinogenic toxicity, and land use. The reason for choosing the seven midpoint indicators will be discussed in the later part of this report. This EIA will include the assessment for all the processes mentioned. The main research question that the project seeks is:

- *What are the cumulative environmental impacts of the industrial scale BOF gas-fermentation to IPA production, considering the combined effects across impact categories of global warming potential, stratospheric ozone depletion, fine particulate matter formation, freshwater eutrophication, marine eutrophication, human carcinogenic toxicity, and land use ?*

To effectively address the main research question regarding the environmental impact assessment of the IPA production process, the research question is split further into sub-research questions.

1. What are the environmental impacts associated with the industrial-scale BOF gas to IPA production method along with the impacts accounted for the replacement of the energy compensation (BOF gas) in steel mills?
2. Which components of the production process have the greatest contributional effects on the environment?
3. How are the environmental impacts varied for all the sensitivity analysis case scenarios including CO conversion, Volumetric mass transfer rate of CO, Product selectivity, Dilution rate, Extractive distillation glycerol mole fraction, Temperature offgas condenser, Anaerobic waste conversion, Extractive distillation molar reflux ratio, Biomass liq-liq mole fraction and the broth and glycerol purges?
4. How does the carbon emission profile of the industrial-scale BOF gas-fermentation to IPA production (46 kton/ year) vary from the pilot-scale IPA production plant (Liew et al., 2022)?
5. Comparing the conventional petrochemical production method of IPA and the BOF gas fermentation method of IPA production, which method possesses the lower impact values?
6. Which is the most influential process parameter when assessing environmental impacts?
7. How do the environmental impacts of the global warming potential, stratospheric ozone depletion, fine particulate matter formation, freshwater eutrophication, marine eutrophication, human carcinogenic toxicity, and land use for the industrial scale BOF gas fermentation to IPA could be improved?

2

Literature Review

2.1. Emissions from Steel-mill

Nearly 1715.1 Mt of steel has been produced over the year 2023. Of this huge volume of production, the major contributor is the Asian region (WSA, 2023). On average nearly 25% of the global CO_2 emissions are emitted particularly by the iron and steel sector (Lei et al., 2023). Three different routes for steel production are identified they are, basic oxygen furnaces (BOF), electric arc furnaces (EAF), and open hearth furnaces (OHF). Out of these three routes, the main route for production would be the basic oxygen furnace route, which accounts for nearly 63% of the world's total crude steel (Lei et al., 2023),(Wang, Jiang, Wang, & Roskilly, 2020). This is assumed to be the most efficient and cost-effective route for steel production (Leão et al., 2023).

The blast furnace of the BOF route is the least energy-intensive process in terms of usage and GHG emissions (Leão et al., 2023). The secondary energy in terms of steel production is by-products and waste heat. During the process, a large amount of gasses are emitted namely coke oven gas (COG), Basic furnace gas (BOF), and Linz-Donawitz gas (LDG) (Wang et al., 2020). This emission can account for nearly 30% of the total energy production for the total process (Leão et al., 2023). As cited by Liew et al.,(2022), the emitted BOF emission approximately consists of CO (50%), CO_2 (20%), N_2 (20%), and H_2 (10%). During the steel production process, the BOF gas produced is the feedstock for heat and electricity generation. The majority of this gas is not flared, so considering the type of flows for this waste heat is an economic flow (Keys, 2019). To reduce and account for the emissions to the environment caused by the steel manufacturing industry, a new-gen technology has been formulated by Lanzatech, which has helped to reduce the emissions by fermenting with the help of microbes for biofuel synthesis (Lanzatech, 2016).

2.2. Emission to the environment

The gases from the steel mill (basic oxygen furnace gas) are well recycled or utilized. In most cases, to generate an additional revenue stream and have a stable & profitable operation, the residual gases are flared and electricity is generated and sold for profit (de Kleijne, 2020). If the BOF gas is emitted directly to the environment could cause more direct effects on the environment. The BOF gas is mostly commonly ended up as internal use in steel mills to meet the heat demand, flaring, and combustion in a power plant for electricity generation (de Kleijne, 2020). The major steel producer of the Netherlands, Tata Steel has equipped the heat recovery and electricity generation facilities to recover the heat liberated and the BOF gas flaring for internal usage (Keys, 2019). It is identified from the calculations performed by Tata Steel, that the heat efficiency of the process is around 38% and the electricity to heat ratio is 1.37:1 (Keys, 2019).

But recently due to the investments and involvement in renewable-based electricity production, the prices for the electricity produced by the steel mill were lowered (de Kleijne, 2020). This is mainly due to the sharp cost reductions in renewable-based energy production because of the subsidies funded by the government for the sustainable transition for the fossil industries (de Vries, 2019). The investment

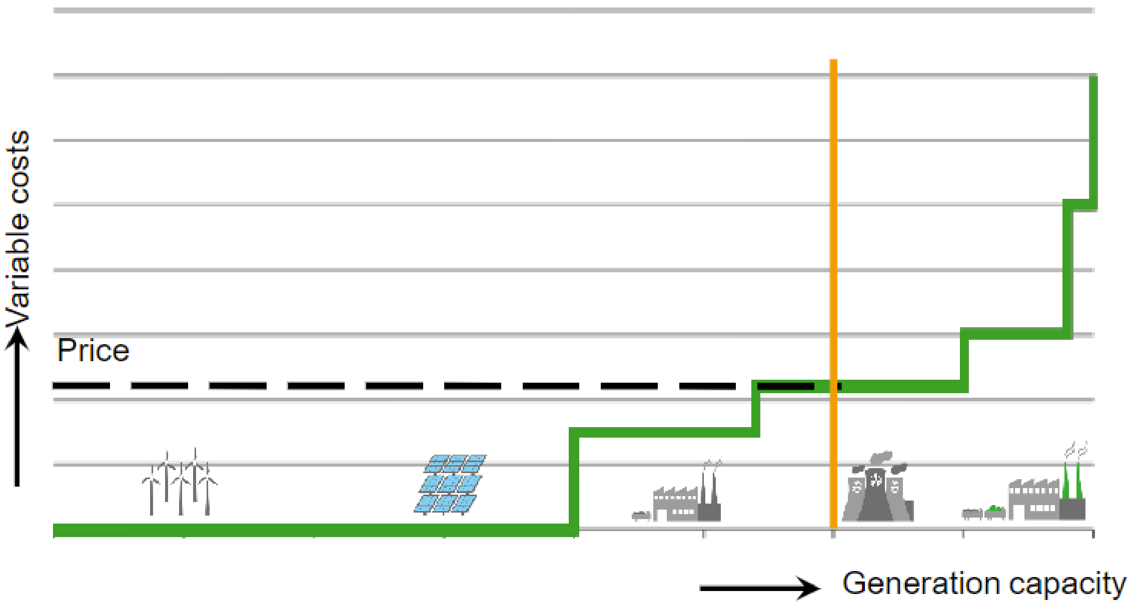

Figure 2.1: Electricity production across different technology (de Vries, 2019)

for renewable-based energy production techniques involves a one-time investment and the payback period is resilient. The major contributor to fossil-based energy is fuel cost, but renewable-based energy generation has no considerable operational cost like fuel costs for the generation. It only has maintenance and service costs (Herder, 2017). So producing electricity using non-renewable sources is much more expensive when compared to renewable sources. Especially in the Netherlands due to the day ahead market, particularly on the seasons favoring renewable energy sources, the price of electricity drops to a very minimum (Gabriella, 2016). Figure 2.1 illustrates the plot representing all the electricity production technology. Considering the consumption of electricity in the Netherlands, the renewable-based energy generators will be only able to sell, as the day ahead market works on the lowest cost for energy providers (de Vries, 2019). These might affect the stable and additional profitable operation of the steel mill. Another factor to be considered here is the increase in carbon price in the EU emission trading scheme. This relates that the cost for the steel manufacturer is shot up (de Kleijne, 2020).

2.3. Biofuels

An alternative to fossil fuels is identified as biofuels, which possess a lower carbon footprint and be synthesized in an environmentally sustainable way (Jeswani, 2020). Throughout all the ages from the past biofuel production has also evolved along with humans, First-generation fuels are derived from crops like maize, and corn, Second-generation fuels are from agricultural by-products and energy plants, and also from forest residues. Third-generation biofuels include those derived from aquatic biomass such as algae. But the major innovation is the fourth-generation fuels which are derived from the syngas through genomically prepared microorganisms and genetically engineered bio-substances. These microbes possess major advantages like enormous growth rate in a short span and non-requirement of major piles of land.

Considering the European landscape, the fourth-generation biofuel production method might be the suitable choice. The fourth-generation biofuels involve the usage of genetically modified microorganisms for the generation of biofuel from syngas. The lack of cultivable lands leads to a large limitation on biofuel fuel production through second generation. Companies like Lanzatech have invested in research and identified a solution to the problem by which the syngas emission from the industries can be trapped and fermented with the microorganisms for biofuel production. The LCA study for the pilot scale BOF gas fermentation process was assessed to be a net negative carbon emissions profile (Liew et al., 2022). To synthesize a specific bioproduct requirement, the microorganism should be metabolically modified (F. Liew et al., 2017).

2.3.1. Advantages of Bioproducts

The demand for alcohol-based biofuel has rapidly increased in the industrial and health sectors over the years. Since the new way of gas fermentation was introduced, there could be a way by which a part of this demand can be satisfied. This gas fermentation could be considered as a better method due to some advantages like:

- Non-toxic, Eco-friendly (Dürre, 2017)
- Avoids food vs fuel controversy (Dürre, 2017)
- Free from climate, geographical, and seasonal restrictions (Dürre, 2017).
- Significantly reduced environmental carbon emission (Dürre, 2017), (Liew et al., 2022).
- Similar composition and calorific value when compared with the alternative petrochemical-based production (Dürre, 2017).

2.3.2. Conventional IPA Conversion Technologies

Production method	**Description**	**Advantages& Disadvantages**	**References**
Direct Hydration of Propylene (DHOP)	• Widely used commercial scale for IPA production. • Involves the reaction of propylene with water in the presence of a solid acid catalyst, typically a strong acid resin-like **Amberlyst 15**. • The reaction is carried out under controlled conditions – **Temperature**: 100-150°C – **Pressure**: 6-20 MPa – Distillation is employed to separate water and IPA	Advantages: • It is a straightforward and efficient process • No generation of hazardous waste • Makes it a relatable environmentally friendly approach considering other methods for conventional IPA production method Disadvantages: • Involves usage of fossil fuel-based raw material/feed (petroleum-based propylene) • Requires high-purity propylene feed	(Onoue, Mizutani, Akiyama, Izumi, & Ihara, 1973)

Indirect Hydration of Propylene (IHOP)	• Referred as the Sulfuric acid method, an older IPA production technique. • Once a predominant method, it declined in use due to its environmental impact. • Involves reacting propylene with concentrated sulfuric acid, resulting in the formation of isopropyl sulfate. • Isopropyl sulfate is then hydrolyzed with water to produce isopropyl alcohol.	Advantages: • Better yields • Relatively simple process Disadvantages: • Energy-intensive process • Hazardous waste generation	(IARC, 1970)
Catalytic Hydrogenation of Acetone	• Least common method for the IPA production, compared to DHOP/IHOP. • This method is used when acetone is available as a byproduct from other processes. • Involves reaction of acetone with hydrogen in presence of NiO_2/ CuO_2. – **Temperature**: 150-250°C – **Pressure**: 2-10 MPa – Distillation is involved in the separation of acetone and IPA	Advantages: • Utilizes the byproduct ideally for product formation. Disadvantages: • Can be performed only when acetone is available • Considerable high raw material cost for production purposes	(Liu et al., 2023)
BOF gas fermentation	• Involves usage of BOF gas emissions from the steel mill, and the BOF gas temperature is lowered. • Then this is fermented with the help of microbes, which produces IPA along with biomass waste • For better yield glycerol is used as an entrainer for the IPA removal. • Distillation is involved in the separation of glycerol and IPA	Advantages: • Could possibly reduce the emission of steel mill. • Considered Environmental friendly for pilot scale production. Disadvantages: • Continuous supply of BOF gas from steel mill would cause inadequacy for the IPA production if the steel production is done by alternate EAF method instead of BOF method.	(Liew et al., 2022), (Lanzatech, 2016)

Table 2.1: Production methods of IPA

In the table 2.1, the different methods for the production of isopropyl alcohol are identified. Of these, the widely used method is direct hydrogenation of propylene. This is considered the most efficient process. Considering only the usage of fossil-based propylene (Onoue et al., 1973). When considering other methods like indirect hydrogenation, this method involves the usage of sulfuric acid and major electricity consumption (IARC, 1970). There is an alternative to the usage of propylene, the method is known as catalytic hydrogenation of acetone. This involves the usage of other chemical processes byproduct acetone, to produce Isopropyl alcohol (Liu et al., 2023). But considering the process with a standalone situation, the raw material Acetone is expensive in terms of production of the IPA. This method involves propylene reaction with oxygen to form IPA and CO_2, like DHOP/IHOP this also equips the distillation process for the separation.

Upon considering all the methods for the production process, some might have environmentally friendly processes without any hazardous emissions, but they involve the usage of huge environmentally impactful raw materials that are sourced from fossil-based resources. So, these cannot be considered to be environmentally friendly. But our method of production of IPA from BOF gas uses industrial emission (constituents like CO, H_2, CO_2, and N_2), which reduces the impact of the previous process as the BOF gas is redirected for the synthesis of IPA, which technically reduces the emission. The major disadvantage of this process, it is mandated to have syngas every time for the production of IPA. If the IPA production plant is constructed as an integrated plant with the steel mill. But on a positive note, steel production is not going to be completely stopped. If the feedstock of BOF gas from the steel mill is no longer available, flexible syngas production can be done from the biomass to satisfy the necessary needs (Lv et al., 2007). However, the problem will occur shortly if the BOF gas fermentation plant is integrated into the steel mill because the blast furnace-based steel production might be potentially replaced by the electric arc furnace plants.

2.4. Syngas Fermentation

One of the options for replacing fossil fuels will be bio-based transition. Advanced conversion technologies with biomass feedstocks that are customized for the purpose will be necessary for the effective conversion of biomass to energy. Enzymatic or thermochemical conversion are the two different processes that can be used to transform lignocellulosic biomass into useful energy products (Tanger, Field, Jahn, DeFoort, & Leach, 2013). In this thermochemical conversion process, it can utilize a various range of feedstocks that are available but involve a large amount of heat and often produce syngas intermediate product (Griffin & Schultz, 2012). But for this research study, syngas fermentation would be an ideal method for utilizing the particular environmental issue which is the emission of the steel mill "BOF gas". The major constituents of BOF gas in our case are Carbon monoxide (50%), hydrogen (10%), and nitrogen (20%) each, and the rest are Carbon dioxide (20%) (Liew et al., 2022). So this syngas fermentation pathway is identified. Syngas-fermentation of synthesis gas(syngas), is a microbiological process. The anaerobic bacterium like *Clostridium Autoethanogenum* use this gas as an energy source. Syngas can be subsequently transformed into chemicals or fuels (Bengelsdorf & Dürre, 2013). The acetogenic bacteria *C.autoethanogenum*, genetically modified (selectively) is used to synthesize the desired bio-based products (Bengelsdorf & Dürre, 2013). The syngas fermentation is used for Isopropyl alcohol production by modifying the microbe to achieve the desired fuel output.

2.5. Lanzatech Solution for IPA production

LanzaTech is a startup that helps and enables the production of useful chemicals/biofuels by using genetically modified microbes (Lanzatech, 2016), (Bengelsdorf & Dürre, 2013). It is carbon capture by transforming them into something more valuable. In this process, the emitted carbon is recycled into fuels and chemicals (Lanzatech, 2016). Every year steel mill emits about 2.6 Gt of BOF gas (Collis, Strunge, Steubing, Zimmermann, & Schomäcker, 2021). This has a potential so that it can be used for the production of IPA. It is also made a consideration with the production of electricity, it is made clear that producing chemicals instead of electricity is a huge profiting business (Lanzatech, 2016). The pilot scale plant for IPA production is considered to be a net carbon-negative process. However, the major limitation is that the LCA assessment is not performed for all the materials, whereas most of it is considered cut-off to lower the impacts caused by the process (Liew et al., 2022).

2.6. Waste treatment for the biomass out

The research and model development work for a pilot scale plant done by (Liew et al., 2022) considers the biomass waste that is generated in the pilot scale plant during the process is considered as an alternative to the soybean meal, and they have performed LCA. Around the world, nearly 77% of soybean meal production is utilized only for animal husbandry, used as feed. Out of this 77%, over 5.6% is utilized in aquaculture as feed (Howlader et al., 2023). If the treated biomass waste has to be replaced with soybean meal in the fish feed. Proximate analysis has been carried out to identify the crude protein content of the feed. The maximum crude protein requirement for the fish feed is about 45%, which can be easily satisfied by the soybean meal with a protein content of 460.5g/kg, dry matter (46%) (Xue et al., 2023). If the same amount is replaced by the treated biomass waste, which has a protein content of 866.70 g/kg, dry matter (86.67%) (Xue et al., 2023) could lead to several problems in the metabolism of fish. So the study has been performed to analyze the replacement percentage in the fish feed.

However, the acetogenic microbes (*C.Autoethanogenum*) are involved in the process is genetically modified organisms, which is altered according to the specific needs of our process. In the case of considering them as an alternative, a treatment method should be carried out to make the product less impact on the environment and cause no harm to the living species that consume them. The two regions, Europe and the USA were considered as the geographical locations. The European Union Commission has banned the usage of GMOs to protect human and animal health and the environment (EFSA, n.d.). To initiate the usage of this alternative, the European Food Safety Authority (EFSA, n.d.) has to approve this treated biomass waste as a no-impact product. The testing and approval will be followed based on the transparency regulation (EFSA, n.d.). Similar to the EU region, The United States of America, also has some regulations that will be performed by the Food & Drug Administration (FDA) authority (FDA, n.d.). These steps involve the producer approaching the FDA with an elaborate explanation of the composition and usage of the GMOs. Then they submit food safety assessments and information to the FDA, and the evaluation procedure happens and resolves any issue with the owner. If the FDA approves the product, the consultations will be made public (FDA, n.d.).

2.7. Clostridium Autoethanogenum Protein

The China Agricultural University performed a research study to analyze the alternative to replace soybean meal with *Clostridium Autoethanogenum* Protein (CAP) (Wu et al., 2022). This protein source was provided by Beijing Shoulang Biotechnology Co., Ltd., with a protein content of 84.69% crude protein. This protein source was developed and also considered treated with the waste treatment procedure. The fish feed consisted of about ±45% protein content along with essential carbohydrates, ash, water, and a trace of vitamins and minerals. In 100 g of fish feed, over 40 g of the composition is soybean meal. This test was performed on *Ctenopharyngodon idllus* a local fish variety in mainland China. Three different groups of tests were performed to obtain accurate results, the first batch of fish was fed with 0% replacement of soybean meal in the fish feed. The second set of the fish group was fed with 5% replacement of soybean with CAP, and the third set with 10% replacement. The major advantage of the replacement is that the CAP has all the essential amino acids composition and other compounds with ±1% change in values, the only drawback is the protein content which is twice the required and allowed level. So the complete replacement is not possible but there is a change with percentage substitution.

2.8. Life Cycle Analysis

The major products that are synthesized in the manufacturing units or plants involve a wide range of products at major levels right from production to the disposal of those products (Amelio, Genduso, Vreysen, Luis, & Van der Bruggen, 2014). The majority of the materials used after once can't be utilized again. Such materials could viably cause a lot of impacts on the earth we live on (Amelio et al., 2014). For this case, a quantitative assessment of impacts caused by material usage can be estimated through the life cycle analysis and environmental impact assessment. Many types of LCA can be performed like cradle to gate, gate to gate, cradle to grave, and so on (Farjana, Huda, & Mahmud, 2018). To perform the Life Cycle Analysis, there are four major steps to focus on (Amelio et al., 2014).

- Goal definition & Scope

- Inventory analysis
- Life cycle impact assessment
- Life cycle interpretation

In our LCA study, the cradle-to-gate LCA is performed. The main motive of this LCA study is to assess and compare the different process parameters of the same process. And to identify which process parameters have higher impacts on the environment and to further lower their impacts by distributing the burdens evenly across the life cycle stages (Ibrahim Menouf, 2011). The four steps listed above does not represent a linear progression path. It is a kind of iterative process, even after the third step of impact assessment, the change in raw materials can be done which further lowers the environmental impacts of the process.

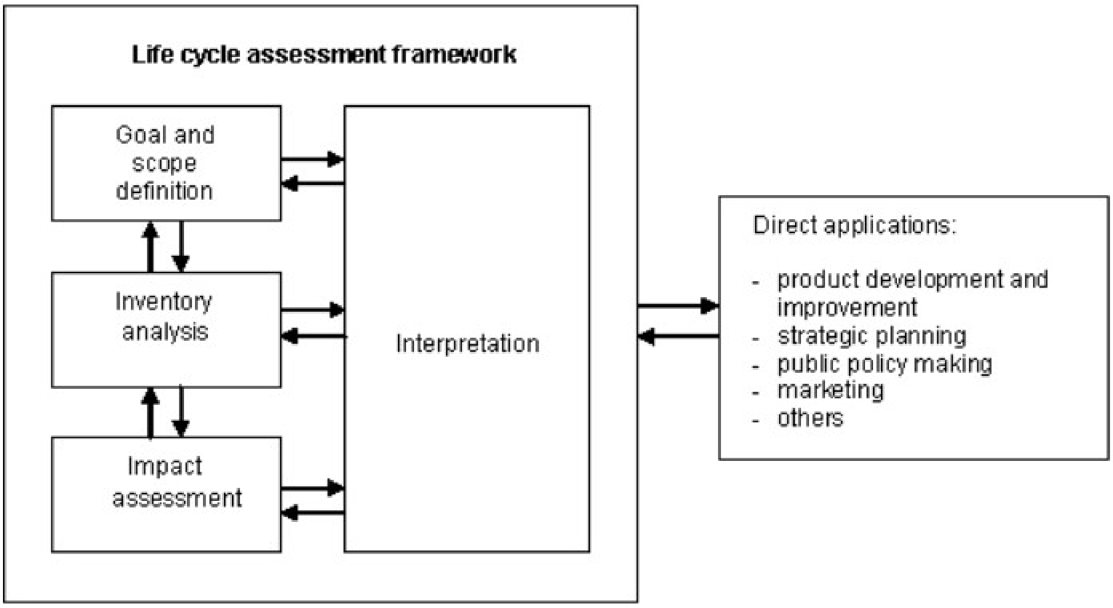

Figure 2.2: Framework of LCA based on ISO:14040 (Menouf,2011)

2.8.1. Goal & Scope Definition

The Goal and Scope definition is the first and iterative stage, in which the materials or components that are about to be assessed should be defined along with its system boundaries, assumptions that are considered for the LCA and even methodologies (Hauschild & Rosenbaum, 2018). This scope and goal is the base step in guiding the LCA to obtain more reliable results.

Functional Unit

A functional unit (FU) is a unit that associates the references to which all the inputs and outputs are related. Also employed to assess and measure the functional outputs and inputs of the product system's performance. To obtain a quantitative analysis of the different ways in scope definition, this FU is used (Hauschild & Rosenbaum, 2018). For example, when different utilities like electricity, steam, and raw material in kg are used, this FU helps in normalizing the factors to the level per kg of the product. So that the impact assessment can be equally, evenly, and easily estimated. Even considering the way how LCA is performed, is based on the Functional unit. It influences the results, and interpretation(Hauschild & Rosenbaum, 2018). This FU stands as a point of reference to know how the unit process might affect the calculation procedure we might take upon (Dijk, 2012).

Reference flows

The product flows are also called reference flows in which the outputs and inputs of the system boundary process are quantitatively related. Also in other terms, the quantity of material/ energy needed to attain the functional flow is referred to as reference flow (Hauschild & Rosenbaum, 2018).

2.8.2. Life Cycle Inventory Analysis

Inventory analysis is the second stage in the LCA, also known as the iterative stage in the LCA. It is usually referred to as the data collection stage. In this stage, the materials, energy consumed, atmospheric & waterborne emission, and emission to land (Muthu, 2020) through all the stages of the product life cycle stages are quantified thoroughly (Hauschild & Rosenbaum, 2018). One of the major advantages of this inventory in LCA is the quantification and technology vary from region to region as such the products do too. The inputs of the inventory are purely dependent on the type, quantity, natural resources, materials, methods for transportation if included, and even disposal of a product.

2.8.3. Life Cycle Impact Assessment

The impact assessment is the third step of the LCA in which the interpretation is done, by accessing the list of materials and energy consumption and quantifying them (Ibrahim Menouf, 2011). Then later it is interpreted and transformed to the impact indicator category. It is an ISO standard that aims at the potential environmental impact evaluation of the product system for the whole life cycle (Muthu, 2020). Every material/energy that is used has a certain set of impact categories associated with it. Likely, Global Warming Potential (GWP) is a measure to trap heat in the atmosphere layer for a specified amount of time. For example, the Global Warming Potential(GWP) of methane is 25 and of carbon dioxide is 1, which means that per kg of methane released in the atmosphere has the same effects on global warming as like 25 kg of carbon dioxide in the atmosphere (IPCC, n.d.). The major feedstock for our process is carbon monoxide and hydrogen the GWP values are 100-year GWP for CO would be 1 to 3 kg CO_2 eq. (IPCC, n.d.) and for the 20-year GWP would be 2.8 to 10 kg CO_2 eq. (IPCC, n.d.). This time horizon depends on the long-term and short-term effects on the environment. Usually, the short-time horizon GWP values would be larger, because, over the 100-year long-term horizon, this is not staying in the atmosphere, whereas the indirect effects on the climate by the forming methane and troposphere ozone slowly when compared with the GWP of short-term horizons. Just like GWP, there are other 18 midpoint category indicators, and each midpoint indicator is related by damage pathways which finally results in 3 different Endpoint indicators namely (damage to human health, ecosystems, and resource availability) (NIPHE, 2018). The characterized results of the interpretation are referred to as midpoints and the reflection of issues of concern and ultimate damages are done by Endpoints (Dijk, 2012).

As described by Muthu et al.,(2020), there are some steps involved in the impact assessment that should be carried out to conduct a Life cycle assessment. The steps are listed below,

1. **Selection & Definition of impact category** - The major step is to identify the relevant impact category to the specific impact that is related to the process (Muthu, 2020).
2. **Classification** - Assigning the impact categories to the obtained LCI (Life Cycle Inventory) results (Muthu, 2020).
3. **Characterization** - This step is to model the impact categories by quantitatively modeling the life cycle impacts associated with emission/ resources along with it (Muthu, 2020).
4. **Normalization** - In this step, the characterized impact is modified or altered based on the reference, which could enable the factor of comparison between them (Muthu, 2020).
5. **Grouping** -Based on the region and locality of the process/ raw materials, the impact categories can be related (Muthu, 2020).
6. **Weighing** - All the impact categories are identified and the cumulative expression of the LCI results as an environmental indicator will be done (Muthu, 2020).

2.8.4. Impact category

A category of impact integrates various emissions into a single environmental consequence. Since the emissions from gathering raw materials vary considerably from generating electricity, these emissions take on a variety of forms. Impact categories are used in this particular instance. Our goal in a Life Cycle Impact Assessment (LCIA) is to combine these disparate emissions into useful figures. Many emissions with similar effects are combined into a single impact unit, which corresponds to a single impact category.

The impact category "climate change," for instance, is expressed in kg CO_2 eq. Methane (CH_4), sometimes known as laughing gas (N_2O), is one greenhouse gas emission that contributes to climate change in addition to carbon emissions (CO_2). By estimating these additional greenhouse gas emissions in kg CO_2 eq. using various measurement units. It is feasible to arrive at a single climate change indicator by using an impact category.

Considering the impact category, there are two different categories for the impact category. The two categories include the midpoint indicator and the endpoint indicator

Midpoint category

The Life Cycle Impact Assessment (LCIA) midpoint category is an analytical method for calculating a product or process's environmental impact. The impact assessment process has intermediary steps called "midpoint categories," which concentrate on particular environmental consequences that happen in between the initial emissions and the final endpoints of adverse environmental effects. This also has key characteristics which include assessing specific environmental impacts that are caused by the emission from the product or process (Weidema, n.d.), (Ismaeel, 2018). And also has quantifiable indicators that help in quantifying the magnitude of impact values (Heijungs, n.d.). This midpoint category has 18 different indicators (Weidema, n.d.). Out of 18 different indicators, the seven major indicators were considered which include Climate change (GWP), Ozone depletion, Eutrophication potential, Land use, and Human toxicity. These mainly focus on the impact of emissions on global warming, stratospheric ozone concentrations, nutrient-rich emissions on water bodies, and the impact of toxins on human health (Weidema, n.d.), (Ismaeel, 2018). The significant advantage is that the targeted mitigation measures can be performed based on the midpoint categories. This is also quantifiable, which enables comparing the impact values between the processes or products (Ismaeel, 2018).

Endpoint category

A method used in Life Cycle Impact Assessment (LCIA) to measure the final environmental effects or damages brought about by emissions or resource usage from a process or product is called an endpoint category (Heijungs, n.d.). Compared to midpoint categories, endpoint categories are more thorough and integrated because they fully account for the effects of environmental changes on ecosystem services or human well-being. Endpoint categories, such as consequences on human health, ecosystem quality, and resource depletion, represent the ultimate environmental effects or damages brought about by emissions or resource use (Heijungs, n.d.). Endpoint categories offer a broader view of the final effects on the environment, which may be more pertinent for making decisions.

Advantages of using midpoint category over endpoint category

Despite all the advantages, the Midpoint categories are often chosen in Life Cycle Impact Assessments (LCIAs) over endpoint categories due to

1. **Modeling**: Compared to endpoint categories, midpoint categories are typically easier to model and require less information and presumptions. They are clearer and simpler to understand because of their simplicity.
2. **Direct link with inventory**: Midpoint categories are more directly applicable to the particular product or process under evaluation since they have a closer relationship with inventory data and the sources of environmental consequences.
3. **Easy verification**: Midpoint indicators are closer to the impact source, they are frequently simpler to calculate and verify. However, endpoint indicators are associated with more complexity and uncertainty.
4. **More comparable**: Midpoint categories are more commonly used and standardized in the LCIA community, which improves their comparability and consistency between different assessments and analyses.

Therefore, the midpoint category has been used for the LCA of the BOF gas fermentation process. This ReCiPe 2016 midpoint H indicator category has 18 total midpoint indicators, and the overall review of the effects caused by the BOF gas fermentation process was identified. The global warming potential could potentially assess the greenhouse gas emissions emitted from the process and quantify the prevention of the BOF gas from flaring which ends up in the environment. The stratospheric ozone depletion could assess any potential component affecting the ozone layer and causing depletion. The next impact category of ionizing radiation evaluates the impacts caused by the utilization of radioactive materials for the process, ozone formation (human health) deals with the human health caused by the emission of ground-level smog and fine particulate matter formation deals with the emission of fine particulate matter which affects the environment. Next, the ozone formation (terrestrial ecosystem) can be applied to assess the effects due to the emission of ozone-contributing components on the environment. This ozone formation (human health and terrestrial ecosystem) deals with the direct utilization of ozone-depleting substances. If the process has this type of component usage, this impact category plays a major role.

Terrestrial acidification measures the effects on the ecosystem for the release of potential acidic substances. Eutrophication deals with the effects of nutrient emissions in the marine and freshwater bodies. Then the terrestrial, marine, and freshwater ecotoxicity evaluate the effect on the release of toxic substances in the soil, marine, and freshwater bodies. Based on the direct human health effects two impact categories namely, human carcinogenic and human non-carcinogenic toxicity can be utilized to evaluate the emission that could potentially contribute to cancer and the non-cancer effects on humans. The land use quantifies the usage of land for the production of the components that are used in the process. The impact category of mineral resources and fossil resource scarcity could be used to evaluate the depletion of the fossil and mineral resources for the production process. Finally, the water consumption is used to evaluate the quantity of water utilized for the process and their potential impacts on the environment considering the scarcity of water. Out of these 18 categories, the most important category which deals with the direct effects on the environment, human health, and ecosystem could be chosen to perform the life cycle study of the process.

2.8.5. Multi-functionality approaches

Multi-functionality is an approach to an activity by which several outputs or services can be dealt with. Multi-functionality can have both favorable and unfavorable effects on the environment, the economy, and society. There are two different approaches when considering multifunctionality, the first approach views multifunctionality as an economic activity characteristic, and the second approach considers it as a policy objective, by which the goal of the system is maintained (OECD, n.d.). There are a few methods introduced to deal with the multi-functionality,

- **Substitution**: Substitution is a method for dealing with multifunctionality. It involves switching out a product or method for another that serves the same purpose but has a different environmental impact. Substitution can be used to find areas for improvement and to compare the environmental effects of various products or processes.
- **System Expansion**: It involves broadening the multi-functional system's boundaries to encompass all of its constituent products and operations. This method can assist in capturing the entire spectrum of the system's environmental effects and discovering areas for improvement.
- **Economic Allocation**: Allocate a multi-functional system's environmental effects among its various services and goods. It involves evaluating each product or service's environmental impact according to its economic worth or other pertinent factors.
- **Subdivision**: The objective of this method is to improve the modeling resolution by breaking the multi-functional unit process down into smaller components. It involves breaking down a multi-functional unit process into smaller units.

2.8.6. Life Cycle Interpretation

This systematic technique obtains the results by identifying, quantifying, checking, and even evaluating the information of the process (Cao, 2017). The results from the life cycle inventory and life cycle impact assessment are interpreted and summarized in this phase. Also ISO (ISO, 2006) has set some standards for the interpretation step, the rules are to identify the issues from LCI and LCIA, evaluation of study, completeness, sensitivity analysis, and consistency checks, and even limitations, recommendations (Cao, 2017).

3

Methodology

Life cycle assessment is a systematic tool to analyze, assess, and calculate the environmental effects, which could be possibly caused by the process, product, or even an activity. This assessment is based on the product's complete life cycle from cradle to cradle, cradle to grave, cradle to gate, or even gate to gate, or anything it could be (Farjana et al., 2018).

3.1. Goal and scope

In our case, the Cradle-to-Gate LCA is performed. The term cradle refers to the BOF emission from the steel mill and the term gate refers to the production of the main product Isopropyl alcohol. The goal and the scope of the LCA were to assess the environmental impacts of industrial-scale BOF gas fermentation-based Isopropyl alcohol production (46 kton/year). Along with the effects, causes the steel mill to replace the BOF gas. On the whole, the main perspective of this goal is to calculate the impacts per mid-point category to interpret the environmental impacts caused by the compounds of the particular process. The end of life of the isopropyl alcohol is out of the scope of the LCA work.

The impact category for this process was based on climate change, human health, and land usage. The foreground process data for the CO_2 emissions and the background process data for the system can be obtained from the specific impacts of the impact categories. The carbon dioxide is emitted out of the system.

The functional unit (FU) of the impact assessment process is **1 kg of IPA**.

To identify the impacts of the improved case scenario, the different iterated and technically improved cases will be assessed and the impact calculation will be performed.

3.2. Assumptions

In this section, the steps taken for the BOF gas-to-IPA process LCA modeling in SimaPro are described. For the industrial-scale model of the BOF gas to IPA fermentation process, the following assumptions were made

- Based on the technical and process modeling carried out (Brouwer, 2023), the 11 key performance indicators were assumed to be process parameters for this impact assessment study.
- The BOF gas used as the feedstock for the process has the composition of 50% CO, 20% CO_2, 20% N_2, and 10% H_2.
- The BOF gas coming out of the steel mill is assumed to be 100% BOF gas without any impurities or other compositions.
- The biomass waste co-produced in the process is assumed to be incinerated concerning the fact of the ban by the European Union on GMOs in the EU region.
- The environmental impacts of the acetogenic bacterium C. *Autoethanogenum* used for the fermentation procedure is considered neutral and the impacts are neglected.

- The approach has been identified to deal with biomass waste by treating and replacing the soybean meal in the fishmeal.
- The traces of acetic acid, NH_3, and $NaOH$ in the waste liquid (residual wastewater) and biomass waste are not accounted for.
- The biomass waste is considered treated in one of the comparison studies. This treated biomass formation is the byproduct that replaces the fishmeal.
- The N_2 emission from the production process and the biomass incineration is inert and does not have any effects on the environment.
- For the heat and electricity replacement calculations, the temperature of the BOF gas was assumed to be reduced from $1100^{\circ}C$ to $169^{\circ}C$.
- During the flaring process, the BOF gas is reacted, and water and carbon dioxide are liberated. As the BOF gas already has 20% of CO_2, this CO_2 is added with the liberated CO_2 and accounted for.
- The impact assessments were performed, considering the landscape of the European region for the data collection from the Ecoinvent database.
- The steam utility data from the Ecoinvent database has no difference between the HP and LP steam and assumed that these are both averaged to these data.

3.3. CO_2 emission from the process

Usually the steel mill production process involves the usage of fossil fuels like coal, and natural gas for heating (ING, 2023) and ores. So the carbon dioxide emitted during the process (from the system) is considered as fossil CO_2 emissions. However, the IPA production process through the BOF gas fermentation technique uses acetogenic bacteria (C.Autoethanogenum), which consume carbon sources for metabolism and growth and convert them into organic compounds. This method is referred to as carbon fixation procedure (Garritano, 2022). Although the CO_2 emitted could be termed as biogenic, tracing them back to the previous form from which it is derived has long carbon cycles that might be due to the geological time scales, so the CO_2 emission is an addition to the atmosphere along with the net CO_2 concentration in the environment. However, this BOF gas fermentation process considers the CO_2 emission not as biogenic and it contributes to the global warming potential because the initial carbon is sourced from the ores.

3.4. Midpoint indicators

In our case, seven different midpoint indicators/ impact categories were considered. Global Warming Potential, Stratospheric Ozone Depletion, Fine Particulate Matter Formation, Freshwater Eutrophication, Marine Eutrophication, Human Carcinogenic Toxicity, and Land Use were those seven indicators.

1. **Global Warming Potential** - Carbon-containing gases, such as CO and CO_2, syngas are fermented to produce IPA. Determining the process's environmental impact requires an understanding of any potential function that greenhouse gas emissions (such as CO_2) may have in global warming. So this category is considered.
2. **Stratospheric Ozone Depletion** - The syngas fermentation in our case doesn't have any direct emission of ozone, which might impact the stratospheric ozone. But considering the feedstock or process emission which might be a viable hazard for the ozone-depleting substances. This is the major reason why the impact category is taken into account.
3. **Human Carcinogenic Toxicity** - This category can relate to account for the substances that could have the potential to cause cancer in human beings. Since other categories deal with human health like human non-carcinogenic toxicity, the carcinogenic toxicity category is chosen because it has a direct fatal effect on human health, rather than being able to be treated with relatively easy health measures compared to cancer.
4. **Fine Particulate Matter Formation** - Based on the specific conditions and emission of the BOF fermentation process, this fine particulate matter formation impact category is considered. Not only does the syngas fermentation methodology cause this impact, but all the raw materials involved in the process can also account for this particular impact. So to source back all the impacts, particularly this impact category is taken into consideration.

5. **Freshwater Eutrophication** - Most of the process around the world involves the discharge of nutrients like N and P in the environment. This impact category is considered to evaluate and verify whether this process has considerable low emission/ discharge of nitrogen and phosporous in the environment (water bodies). More emission of this nutrient causes the growth of algae and other algal blooms which causes depletion of the oxygen content of water resources and causes damage to the aquatic species.
6. **Marine Eutrophication** - Similarly, the same case of nutrient discharge like N and P could end in the marine environment, which also accounts for the eutrophication like in the previous case.
7. **Land Use** - The syngas fermentation process involves the usage of raw materials and feedstock, considering them could involve the usage of land to produce them or even infrastructure to consider waste management. So, this particular impact category is assessed.

3.5. Multi functionality

3.5.1. Steel mill replacement

The BOF gas in our case is a technosphere flow. It was never an environmental flow, because the emission (BOF gas) is directly taken from the steel mill. This BOF gas is also multi-functionality, due to its considerable usage as two different goods function. One such is feedstock for the production of IPA via fermentation. The other function is the energy feedstock for the electricity, heat generation, and flaring process (Keys, 2019). For this scenario, both functions have economic value and cannot be considered as waste flows. As per the rules of ISO 14044 certain rules have to be followed when considering the multi-functionality. The multifunctionality approaches to deal with the problem are discussed below.

1. **Subdivision**: Subdivision is not possible, because of its insufficient data to characterize the individual BOF gas emission processes.
2. **System expansion**: As described by Müller et al.,(2020) the system expansion, might alter the functional unit to include the energy generation of the multi-functionality of the process. This would not be ideal in our case if we're considering comparing the different scenarios of the process.
3. **Allocation**: To use the rule of allocation, two methods can be used, one of such is to answer the question following the hierarchy of the allocation, and the next one is if the substitution is not possible (no process to apply substitution) use allocation (Müller et al., 2020). In our case, there is some process to which substitution can be applied, so allocation is neglected (Müller et al., 2020).
4. **Substitution**: In this rule for dealing with the multi-functionality, an emission credit was awarded for the emission that could be avoided by neglecting the BOF gas for generation of energy (electricity/heat) (Müller et al., 2020). The energy that has to be accounted for, should be substituted with the energy source of the main process (Müller et al., 2020). This could become part of the IPA production via the fermentation process. So, this multifunctionality criterion is chosen to be the ideal way to deal with the replacement consideration in the steel mill.

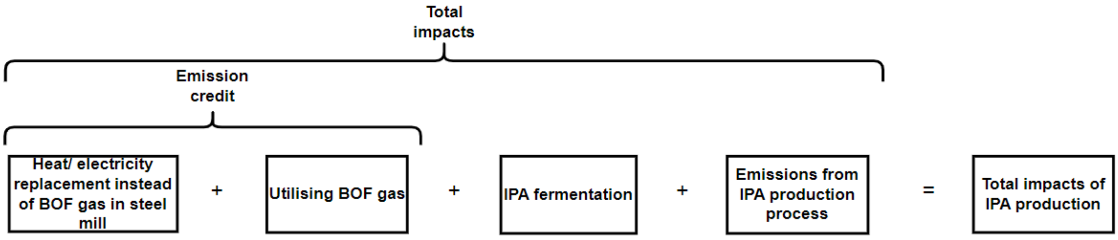

Figure 3.1: Substitution: Emission credit for the final climate change impact

The steel mill's replacement energy supply generated an emission credit based on the difference between the retained emissions from the energy generation from BOF gas and the impacts associated with the provision of alternative energy. Formally, there is no change in the emissions of the steel system because this credit was entirely allocated to the system and the energy supply replacement for the steel mill. The total impact for the IPA production is the summation of both the impacts of the process of fermentation to produce IPA along with the impacts due to the replacement energy for the BOF gas in the steel mill, due to its purpose of fermentation (Müller et al., 2020). By considering the substitution method, the total climate change environmental impact of utilizing the Basic Oxygen Furnace gas can be assessed without changing the Functional Unit of the steel mill system (Müller et al., 2020).

Let us assume the CO_2 emission of the total process, the CO_2 that is emitted from the steel mill enters the IPA production plant in the form of BOF gas, and during the IPA production process. It is transformed into the Isopropyl alcohol. So, it is taken into consideration that the CO_2 from the steel mill ended up as IPA in our process. We are not considering how the CO_2 might end up thinking the end of life of the produced IPA. Since our process is a cradle-to-gate LCA process. The basic ideology of this process is to consider the BOF gas emission from the steel mill, replacements for diverting the emission to the IPA process instead of satisfying the heat and electricity demand, and the production of IPA through the gas fermentation technique. The end-of-life of IPA product is out of scope consideration.

3.5.2. Biomass waste / co-product

Considering the biomass waste out of the system, there are two methods by which the biomass waste can be handled. The first method is to incinerate the biomass and the second method is to consider the biomass waste undergoes a treatment process and can be utilized as an alternative to soybean protein in the fish meal. Initially, anaerobic digestion is performed followed by the incineration of biomass waste, this biomass emits water, nitrogen, and carbon dioxide as an emission. When the second method is considered for the environmental impact assessment, the biomass waste is treated and can be utilized for another process, so the treated biomass waste is no longer considered to be a waste flow but instead assumed as a co-product. In terms of dealing with the multifunctionality of the process, there are a few approaches,

1. **Economic Allocation:**In this economic allocation method, the environmental impacts are divided based on the economic value of the products. So the main product Isopropyl alcohol and the co-product biomass have to be determined and the market prices for the IPA and the biomass have to be identified. This is the most utilized method for the multifunctionality problem, but in our case, it can't be performed because the biomass out prices cannot be determined as there is no market availability for this co-product, and this utilization of biomass waste is still in the idea phase and the experiments are still carried on. So, economic allocation is not suitable for the impact assessment.
2. **System Expansion:**In this method, the system boundary should include the avoided products. Biomass out was replaced by soybean in the aquaculture feed, so the environmental impact of the soybean meal has to be determined and our total production of biomass waste has to be estimated. Which could replace the soybean. The impacts of the soybean (could be replaced) have to be subtracted from the total impacts of the process. This could provide the solution to the multifunctionality problem of the biomass w in the system. So, this method is used to substitute the effects of soybean meal as prevented emissions.

$$\text{Impact value} = \text{Impact values of system} - \text{Impact value of co-product}$$

3.6. Life cycle inventory

3.6.1. Plant level diagram of Steel mill plant

In this plant level diagram (Figure 3.2) of the steel mill, the steel is being produced along with the emission of BOF gas and other industrial gasses. This process begins by utilizing coal for the coke plant, iron fine, natural gas, limestone for the sinter plant, and pellet plant. then the coal is preheated and burned to generate the necessary heat for the process. Then the iron fine is sent to the blast furnace where the iron is heated and this process proceeds further with the pig iron sent to the basic oxygen furnace to produce crude steel. The Pig iron is the major output of this blast furnace and industrial gasses like Blast furnace gas are emitted which is fed back again into the coke plant due to its high

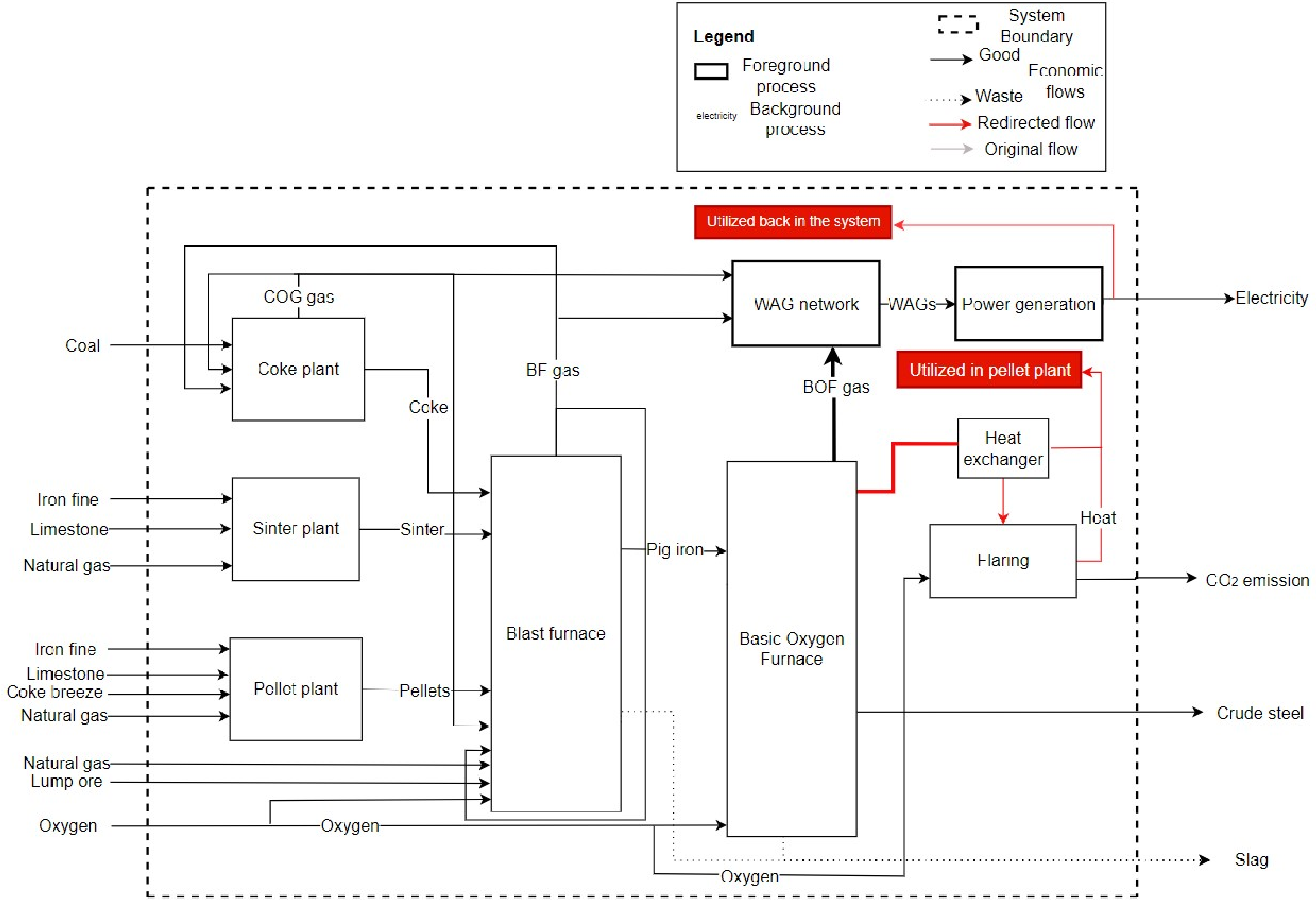

Figure 3.2: Plant level diagram for the steel mill BOF gas production (Keys, 2019)

calorific value. Then the major output of pig iron is fed back into the basic oxygen furnace. From which crude steel is the major output. From this Basic oxygen furnace, the desired input of BOF gas is emitted, which is fed to the WAG network for electricity and heat generation. The BOF gas is sent to the heat exchange unit process, which liberates the heat and is utilized within the system. Then the BOF gas is fed in along with oxygen for the flaring process. This emits CO_2 and some heat, of which the heat is utilized back to the system. The electricity produced in this process is sent back and used again in the process, and the excess is transmitted to the power grid. This is the major consideration for our LCA work, as we have already discussed that the BOF gas from the steel mill has more uses in terms of heat recovery and electricity generation. Since we are redirecting the BOF gas to the IPA production process, it is evident how the steel mill has been affected by the redirection of BOF gas. This information cited by Keys et al.,(2019) provides in and out information for assessing the impacts caused by the production of BOF gas.

3.6.2. Plant level diagram of BOF gas fermentation plant

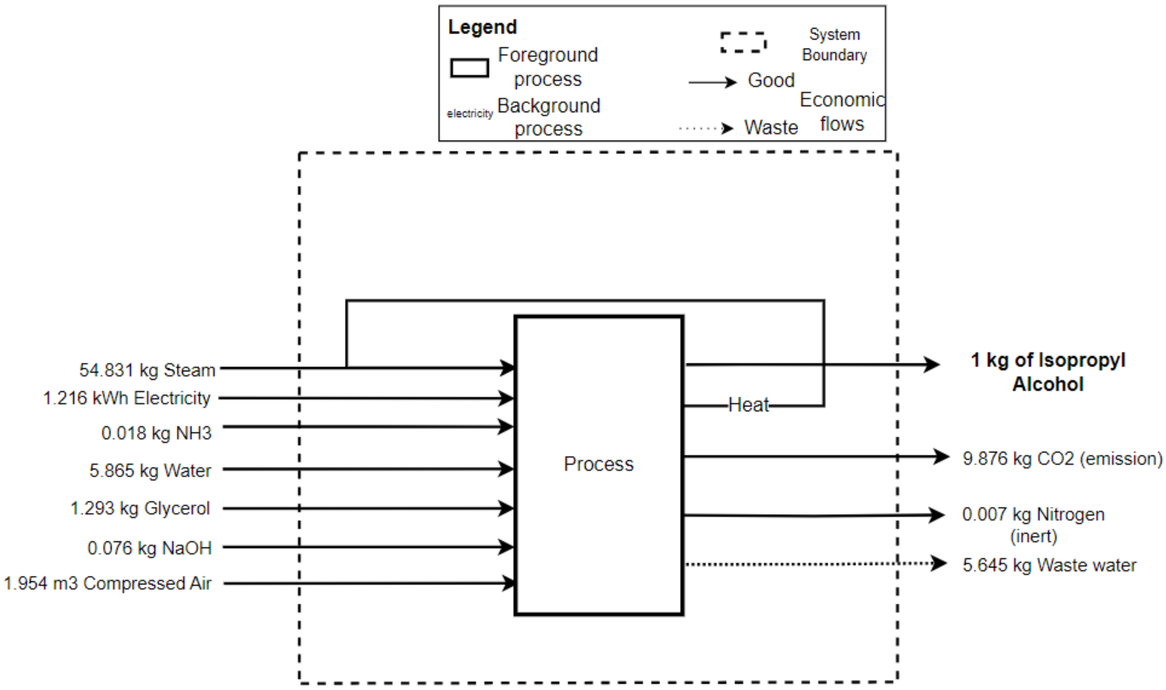

Figure 3.3: Plant level diagram for Isopropyl alcohol production via BOF gas fermentation

The plant level diagram (Figure 3.3) of the IPA production is described as a single-step process, irrespective of its multi-level steps. In this, the BOF gas is fed in along with the utilities like electricity, $NaOH$, water, compressed air, and NH_3. Considering the entrainer, the glycerol is recovered using the glycerol recovery distillation part. But the 10% of the glycerol is purged and combusted. So, a small amount of glycerol is continuously fed into the system. These are processed and the Isopropyl alcohol is produced as the major product, with N_2, CO_2, and wastewater as emissions to the environment. Apart from the N_2 and CO_2 other components like acetic acid and others are produced. The other by-products are neglected because they are produced in negligible amounts (so avoided). This process also emits carbon dioxide, with residual wastewater and the residual gas (nitrogen) as emissions.

3.6.3. Plant level diagram of combined steel mill and IPA production plant

This plant level diagram (Figure 3.4) is the process diagram of how the IPA production plant functions. In this, the pellet, sinter, and coke are fed in the blast furnace, and the major output is the pig iron. The recovered Blast furnace gas is recirculated to the coke plant for heating purposes. Then the pig iron is further fed in the Basic oxygen furnace, from which the crude steel is made along with the emission of

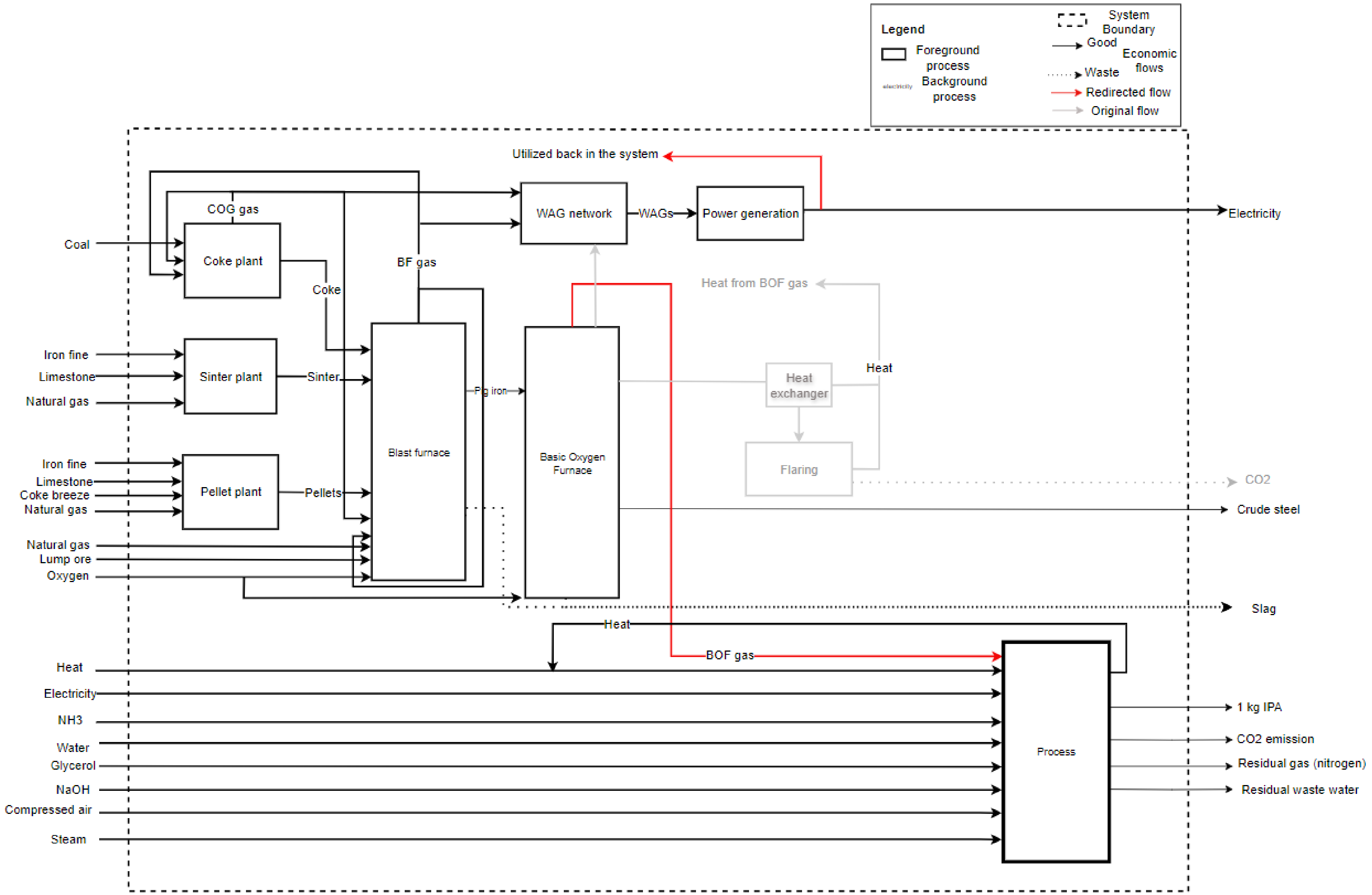

Figure 3.4: Combined Plant level diagram of redirected BOF gas to Isopropyl alcohol production

BOF gas. During these processes, blast furnace gas, COG gas, and the important Basic oxygen furnace gas are produced in the furnace. Usually, the COG gas from the coke plant is recirculated for the preheating purposes of the coal. The blast furnace gas is also sent to the coke plant for preheating and the basic oxygen furnace gas is used for preheating, this involves preheating pellets in the pellet plant. along with the purpose of preheating, the gasses also help to generate power which could be utilized by the system. But in this integrated system figure 3.4 illustrates that only the BOF gas is redirected to the BOF gas fermentation process, the rest gasses like BF gas and COG gas are utilized in the same steel mill system. Instead of using it for reheating purposes, generating electricity, or flaring, the BOF gas is redirected to the syngas fermentation process. As the BOF gas has higher CO content, it is well suitable for the gas fermentation technique. This process involves the usage of utilities like NH_3, $NaOH$, water, glycerol, electricity, and heat for the gas-fermentation process. After the process of gas fermentation, the desired output of Isopropyl alcohol is synthesized along with the co-product of biomass waste. This biomass waste is considered incinerated. During the incineration process CO_2, N_2, and water is emitted into the environment. This also adds up with the emission to the air as residual gas majorly consisting of carbon dioxide and nitrogen and emission to the land by residual wastewater.

3.6.4. LCA system model for the BOF gas fermentation process

This figure 3.5 relates to the LCA system model for an integrated system of Isopropyl alcohol production using gas fermentation with a steel mill. The inputs like heat, electricity, NH_3, water, glycerol, $NaOH$, and compressed air are being fed into the processing system, and the main product IPA along with emissions of residual gas (nitrogen, carbon dioxide), and residual waste water is emitted.

This redirection of BOF gas might be a good way to reduce the environmental impacts, but redirecting them from the steel mill could also have some impacts related to the steel mill. The BOF gas plays a huge role in heating the pellet plant, the heat is recovered from the high temperature of the BOF gas at nearly 1100° C, and electricity generation from the high temperature as well. This usage of BOF gas in the steel mill has to be replaced. This can be done by additional heat/ electricity supplied to the steel mill in the place of BOF gas. The life cycle assessment of this process should account for the impacts of the replacement in the steel mill (BOF gas redirect) and for the BOF gas prevented from flaring. It might be a contrasting thing to note that in the system boundary, the BOF gas as input is not considered. This is because the LCA method accounts for the impacts caused by the products and the cradle-to-gate analysis is performed, the BOF gas is going to end up as CO_2 in the steel mill process and additional generation of heat. So, this CO_2 and heat are to be considered rather than considering the composition of the BOF gas like CO, H_2, CO_2, and N_2. The calculation for the emission credit of BOF gas replacement in the steel mill is performed in Appendix A.

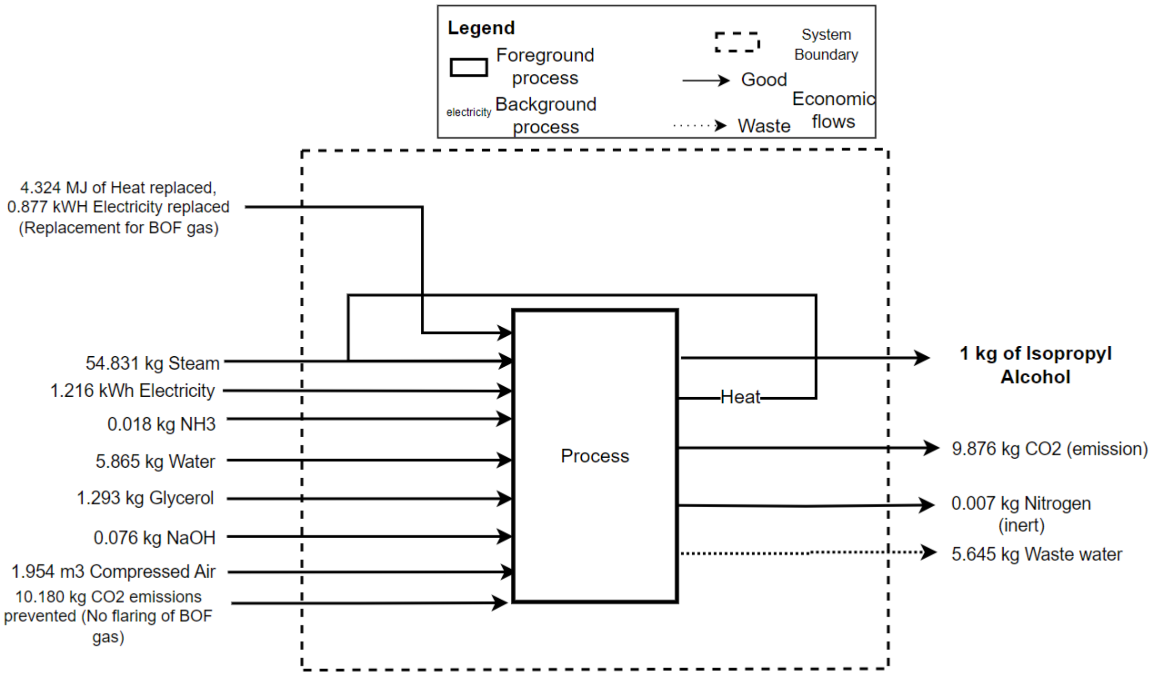

Figure 3.5: LCA system boundary for the BOF gas fermentation to produce IPA (components usage per kg IPA produced)

The system boundary of this diagram is represented by the process and has some good and waste economic flows that are the inputs and outputs for the process. Isopropyl alcohol of 1 kg is produced by this process which is the good economic flow (main product) going out of the system boundary along with the emissions like wastewater, CO_2, and N_2. To produce 1 kg of the desired IPA, the good flows like heat, NH_3, water, glycerol, and $NaOH$ are fed into the process together with the heat and electricity replacement (BOF gas replacement in the steel mill). These inputs are accompanied by the credits for preventing the BOF gas from flaring in the steel mill.

3.7. LCA using SimaPro software

The Life cycle analysis was performed using SimaPro software. The "Ecoinvent 3.6 - allocation, cut-off by classification - system" is the database used for this LCA work. The major reason for choosing the Ecoinvent 3.6 database in the assessment tool is to easily perform the cut-off approach for the allocation to deal with the emission credits of flaring prevention of CO_2 and the co-product of biomass alternate process in one of the comparison studies. The new project is created with the title Basecase. The step-by-step process explaining how to model the impact assessment is depicted in Appendix B. The table below represents the inventory, which shows the amount of compounds like ammonia, water, and other materials used to produce 1 kg of IPA. For the impact assessment, the ReCiPe 2016 midpoint H method is chosen to have a vision of the wide range of midpoint environmental impact indicators. The ReCiPe 2016 is the life cycle impact assessment method which has both the midpoint and endpoint categories. However the midpoint H (hierarchist) model is chosen over all the other midpoint models. This H model is based on the policy relating to the wide time frame which provides the effective effects on the long-term environmental impacts (ReCiPe, 2016). But the other midpoint I (individualist) and E (egalitarian) models are applied for the short-term approach and the prediction of effects on the environment (ReCiPe, 2016). The electricity and heat in the input to the technosphere table are the replacement energy needed for the steel mill if the BOF gas is redirected to the gas fermentation process instead of using it for internal purposes.

Process: 1 kg Isopropyl alcohol production	**Amount, unit**
Inputs for the process	
Ammonia, anhydrous,liquid {RER}| market for ammonia, anhydrous, liquid | Cut-off, S	0.017 kg
Water, completely softened {RER}| water production, completely softened | Cut-off, S	5.865 kg
Glycerine {RER}| market for glycerine |Cut-off, S	1.293 kg
Neutralising agent, sodium hydroxide-equivalent {GLO}| market for neutralising agent, sodium hydroxide-equivalent | Cut-off, S	0.076 kg
Compressed air, 1000 kPa gauge {RER}|compressed air production, 1000 kPa gauge, &lt;30kW, average generation |Cut-off, S	1.954 m3
Inputs for the process: Electricity, Steam, and Heat	
Electricity, high voltage {RER}| market group for electricity, high voltage | Cut-off, S	1.217 kWh
Steam, in chemical industry {RER}| market for steam, in chemical industry | Cut-off, S	54.831 kg
Heat, air-water heat pump 10kW {Europe without Switzerland}| heat production, air-water heat pump 10kW | Cut-off, S	4.324 kg
Electricity, high voltage {BA}| treatment of blast furnace gas, in power plant | Cut-off, S	0.877 kWh
Heat, district or industrial, natural gas{RER}| market group for heat, district or industrial, natural gas | Cut-off,S	52.748 MJ
Avoided product	
Carbon dioxide, liquid {RER}| market for carbon dioxide, liquid | Cut-off, S	-10.180 kg
Emissions: Air and Water	
Carbon dioxide	9.340 kg
Waste Water	5.603 kg
Nitrogen	0.007 kg

Table 3.1: Components table

The {RER} refers to the Rest of Europe Region, {BA} refers to the Bosnia and Herzegovina region, and {GLO} refers to the Global region.

A detailed impact assessment using SimaPro was performed and the figures of these procedures can be found in the Appendix B section. When the components that are referred to in 3.1 are inputted in the SimaPro software, the data has to be inputted based on the process. In this case, the functional unit is 1 kg IPA, which is the desired product of this process. So, this process is modeled accordingly. Then inputs like ammonia, water, glycerol, NaOH, compressed air, and CO_2 have to be inputted in the fields of Inputs to technosphere. The electricity, steam, heat during the combustion, and electricity, and heat replacement are entered into the inputs to the technosphere: electricity/ heat fields. The calculations to estimate the electricity and heat that has to be replaced by the steel mill in case of alternating the usage of BOF calculations were included in the Appendix A.1 section. The two inputs namely electricity high voltage [BA] and heat, air-water heat pump in the table 3.1 represent the heat and electricity replacement for the BOF gas in steel mill. The heat, district or industrial is the consideration for the chemical heat that is produced during the conversion of BOF gas. In this process, no co-product is produced in the BOF fermentation process, but the BOF gas is prevented from flaring in the steel mill has to be accounted for in our process. So this CO_2 that is prevented from flaring is accounted for by inputting them in the Output to technosphere: avoided product field. During this process, CO_2, N_2, and water is emitted from the system. These are entered in the emissions column. Usually, the biomass waste is modeled in the actual system, and as it is banned in the EU region, the biomass cannot be utilized in any form. So it is considered incinerated during the process of incineration. Biomass waste emits CO_2, water, and N_2 out of the system. This is how the N_2 emission can be seen in the system. Whereas the N_2 composition in the BOF gas is not utilized in the system as it stays inert. The N_2 composition in the BOF gas is not considered and the N_2 from the incineration process is included. This is because the nitrogen is produced during the process and it has to be accounted for in the impact calculation. The calculations for the biomass waste incineration are included in the Appendix A.3 section.

3.8. Treatment process for the Biomass out

The biomass waste produced during the IPA production process can be identified and used in two approaches. The first way is to incinerate biomass waste. The calculations are inputted in the Appendix A.3 section. The second way for the biomass waste is to treat the biomass with a waste treatment procedure and utilize it as fish feed. In this LCA work, it is assumed that the treatment for the biomass waste is carried out and there is no change in the quantity of the treated biomass. The major problem that could be considered for this treatment process is the usage of Genetically Modified Organisms (GMO) waste. The *C. Autoethanogenum* is an acetogenic bacteria modified and is specified to meet our need to produce IPA, whereas the original version usually produces acetic acid and ethanol. The European Union has banned the use of GMOs unless the committee approves it (EFSA, n.d.). The biotechnology industry in China has published a paper on "C.Autoethanogenum waste as fish feed" in the Chinese Journal of Animal Nutrition (Hongcheng, Huanhuan, & Xiaoming, 2018).

In this paper the acetogenic bacteria's waste after a certain process is treated with waste treatment steps and the nutritional values are identified and those values are compared with the conventional fish feed. This fish feed mainly consisted of soybean meal as the protein source (Hongcheng et al., 2018). Around the world, nearly 77% of soybean meal production is utilized only for animal husbandry, used as feed. Out of this 77%, over 5.6% is utilized in aquaculture as feed. If the treated biomass waste has to be replaced with soybean meal in the fish feed. Proximate analysis has been carried out to identify the crude protein content of the feed. The maximum crude protein requirement for the fish feed is about 45%, which can be easily satisfied by the soybean meal with a protein content of 460.5g/kg, dry matter (46%) (Xue et al., 2023). If the same amount is replaced by the treated biomass waste, which has a protein content of 866.70 g/kg, dry matter (86.67%) (Xue et al., 2023) could lead to several problems in the metabolism of fish. So the study has been performed to analyze the replacement percentage in the fish feed. Usually, the fish feed consisted of 24% of its composition as soybean meal, in this, nearly 5% is replaced with the treated biomass waste for better results. Replacing the 5% of soybean meal with treated biomass waste doesn't alter much in the essential amino acid requirement for the species. The change in values is nearly ±6% If the percentage is increased to 10%, this leads to liver cell damage, impaired liver function, and reduced survival rate. So the 5% in fish feed is identified as an appropriate proportion replacement rate (Hongcheng et al., 2018). The major drawback of the study is the proportion rate is not analyzed for 6-9% to obtain the appropriate ratio. This replacement of soybean meal with treated biomass waste could lower the huge demand for soybean meal in the animal feed sector and therefore prevent emissions from soybean meal cultivation. This is how the application of 5% C. autoethanogenum biomass in fish feed as a protein-rich supplement replacing a part of the soybean meal was accounted for in the LCA.

When performing the impact assessment for the case scenario of considering biomass waste as fishmeal protein (alternative to soybean meal). All the inputs to the SimaPro software remain similar, but when considering the emissions the nitrogen will not be emitted as the biomass is not incinerated, and it is leaving the process as a co-product. So it has to be entered in the Outputs to technosphere: Avoided products field. During the calculations, the impacts of this particular component will deducted from the total impacts considering the multifunctionality criteria: system expansion. The value for the components varies from the base case scenario. No longer N_2 is emitted, as the biomass waste is not incinerated.

3.9. Verification methodology

Verification methodology is an approach framed to deal with SimaPro software usage. In this method, the initial base case scenarios were performed with the help of software considering the functional unit. This acts as a prediction method in which all the inputs and outputs for the process are scaled based on the functional unit. Then the percentage change in the material consumption is estimated for the lower-bound and upper-bound values respective to the base case values. The percentage change in values is identified between the cases and these percentage change numbers are applied to the impact category values of the base case scenario. The impact category value for the sensitivity case scenarios is predicted. The verify the authenticity of this method, the impact assessment done via SimaPro is compared with the prediction method. It can be acclaimed that this might be an efficient method to reduce the reliability of the software when dealing with sensitivity cases that use the same methods and components for all processes. The calculations are performed for this methodology in the section 4.5 of the report.

3.10. Comparative analysis of sensitivity cases across midpoint indicators

Whenever the Life Cycle Impact Assessment (LCIA) study is performed for the process that produces a product, most of the time only the Global warming potential midpoint indicator is considered. Even the LCA for pilot scale production of IPA from BOF gas (Liew et al., 2022) also considered the GWP for the assessment procedure. This consideration of GWP for the LCIA is due to some reasons. Most of the national and international environmental agencies are obliged to present the environmental impacts targeting the GHG reductions. Even the Kyoto Protocol and Paris Agreement focus on the GWP rates across the world.

Considering only the GWP for the impact assessment is a trade-off to the process, in which the components responsible for the GWP might also have a potential impact value on the other midpoint indicators. Not all the 18 different midpoint indicators are necessarily to be chosen, but this selection of midpoint indicators should be based on the scope of overall effects on the environment by climate change, human health, and the ecosystem. The seven midpoint indicators namely global warming potential, stratospheric ozone depletion, fine particulate, matter formation, freshwater and marine eutrophication, human carcinogenic toxicity, and land use were chosen for the impact study. These impact categories deal with all the above-mentioned areas directly.

The base case and sensitivity cases were performed for the seven midpoint indicators. The high-impacting and low-impacting case scenarios were identified by comparing the midpoint indicators. The comparison studies were performed in the section 4.6.

4

Results

4.1. LCA method by Liew et al.,(2022) for Pilot Scale plant vs Industrial scale model

Inputs	**Usage**	**Units**	**Emission Factor**	**Value**	**Unit**	**GHG Emissions ($kgCO_2e$/kg IPA)**
Steel Mill Off-Gas	N/A	MJ off-gas/kg IPA	Off-Gas	0.00	gCO_2e/MJ off-gas	0.00
Electricity	5.35	MJ electricity/kg IPA	Electricity a,b	118.75	gCO_2e/MJ electricity	0.64
Steam	6.28	MJ steam/kg IPA	Steama,c	86.28	gCO_2e/MJ steam	0.54
LanzaTech Microbial Protein Co-Product	0.08	kg nutritional feed/kg IPA	Soybean Meal a,d	-943.45	g CO_2e/kg soybean meal	-0.08
Biogas Co-Product	1.01	MJ biogas/kg IPA	Natural Gas a	-69.02	g CO_2e/MJ natural gas	-0.07
Carbon Sequestration	1		IPA Carbon Content	-2.20	kgCO_2e/kg IPA	-2.20
Total IPA Emissions					kg CO_2 eq	-1.17
Fossil IPA e					**kg CO_2 eq**	**1.85**
Emission Savings						**-163%**

Table 4.1: Liew et al., (2022) method for LCA calculation of 120 L pilot-scale fermentation

The table 4.1 represents the LCA method performed for the pilot scale plant (Liew et al., 2022). In this, the inputs to the technosphere were considered for the electricity, steam, microbial protein co-product, bio-gas, and IPA. The technosphere refers to the system in which all the processes and products can be analyzed within the LCA study. This involves the input and output flows of materials and energy between various processes. The impact categories of soybean meal were chosen as a reference for the microbial protein because the microbial co-product is assumed to have undergone the treatment process which has the potential to replace the soybean meal. Natural gas was chosen as a reference in the impact category instead of the bio-gas co-product because system expansion is considered by providing credits for replacing natural gas. Performing the non-elaborate LCA calculations as the equivalent value is sequestrated from the environment through the inputs of the process and subtracting the equivalent value of materials evolved during the process, the total impact values of the process can be calculated. However, the LCA was inconsistent about the system boundary consideration. The article by Liew et al.,(2022) does not provide a clear reference material study. They have considered the soybean meal impact values for the microbial protein produced. Since microbial protein production involves numerous treatment methods they might have a significant difference in the impact category values. These two have a considerable difference in the production methods even the impact values. The majority of the essential raw materials like water and compressed air usage have been considered cut off from the system. The impact category of global warming potential is only considered in the LCA, and it was performed by neglecting all the inputs (GWP contribution less than ±5%) to lower the CO_2 emission values (Liew et al., 2022).

To learn more about the specific LCA method, two scenarios of industrial scale IPA production method for the production capacity of 46 kton/yr were performed using Liew et al., (2022) method.

1. Considering biomass waste as soybean replacement for fish feed application
2. Microbial biomass as a waste, thus being incinerated

Inputs	**Usage**	**Units**	**Emission Factor**	**Value**	**Unit**	**GHG Emissions (kgCO_2e/kg IPA)**
Steel Mill Off-Gas	N/A	Kg off-gas/kg IPA	Off-Gas	0.00	kgCO_2e/MJ off-gas	0.00
Compressed air	1.954	m3 compressed air /kg IPA	Compressed air	0.016	kgCO_2e/m3 compressed air	0.033
Electricity	4.379	MJ electricity/kg IPA	Electricity	0.1158	kgCO_2e/MJ electricity	0.564
Steam	54.831	kg steam/kg IPA	Steam a,c	0.287	kgCO_2e/kg steam	15.753
Water	5.865	Kg water/ kg IPA	Water	0.001	KgCO_2e/kg water	0.003
LanzaTech Microbial Protein Co-Product	0.080	kg nutritional feed/kg IPA	Soybean Meal a,d	-0.9434	kgCO_2e/kg soybean meal	-0.076
CO_2 Co-Product	9.322	MJ biogas/kg IPA	CO_2	-0.812	kgCO_2e/kg CO_2 gas	-7.566
IPA Carbon Sequestration	1		IPA Carbon Content	-2.026	kgCO_2e/kg IPA	-2.026
Total IPA Emissions					**kg CO_2 eq**	**6.688**
Fossil IPA e					kg CO_2 eq	**1.85**
Emission Savings						**+261.531%**

Table 4.2: LCA calculation for industrial-scale process by Liew et al., (2022) method (biomass as soybean meal)

The table 4.2 represents the LCA calculation for the industrial scale BOF gas fermentation method based on the Liew et al.,(2022) method. This also has the same procedures, which involve compressed air in terms of m^3/kg IPA, steam (kg/kg IPA) as additional modified inputs, microbial biomass is referenced as soybean meal alternate along with CO_2 as the output. Then the calculations were performed and the total IPA emission value was 6.688 kg CO_2 eq. comparing it with the Fossil IPA emission value, the percentage of emission has a huge increase in value of about 261.531% increase.

Inputs	**Usage**	**Units**	**Emission Factor**	**Value**	**Unit**	**GHG Emissions (kgCO_2e/kg IPA)**
Steel Mill Off-Gas	N/A	Kg off-gas/kg IPA	Off-Gas	0.00	kgCO_2e/MJ off-gas	0.00
Compressed air	1.954	m3 compressed air /kg IPA	Compressed air	0.017	kgCO_2e/m3 compressed air	0.033
Electricity	4.380	MJ electricity/kg IPA	Electricity	0.116	KgCO_2e/MJ electricity	0.564
Steam	54.831	Kg steam/kg IPA	Steam a,c	0.2879	kgCO_2e/MJ steam	15.753
Water	5.865	Kg water/ kg IPA	Water	0.001	KgCO_2e/kg water	0.003
Microbial waste Co-Product combustion	0.080	kg nutritional feed/kg IPA	Microbial waste combustion	-0.003	kgCO_2e/kg waste combustion	-0.001
CO_2 Co-Product	1.01	Kg CO_2 eq/kg IPA	Natural Gas a	-0.082	kgCO_2e/ kg CO_2	-7.566
IPA Carbon Sequestration	1		IPA Carbon Content	-2.026	kgCO_2e/kg IPA	-2.026
Total IPA Emissions					**kg CO_2 eq**	**6.763**
Fossil IPA e					kg CO_2 eq	**1.85**
Emission Savings						**+265.573%**

Table 4.3: LCA calculation for industrial scale process by Liew et al., (2022) method (biomass incineration)

The table 4.3 above represents the LCA calculation for the industrial scale BOF gas fermentation method based on the Liew et al.,(2022) method. This also has the same procedures, which involve compressed air in terms of m^3/kg IPA, steam (kg/kg IPA) as additional modified inputs, the microbial biomass is incinerated and the emission factor is referenced with the microbial waste combustion along with CO_2 as the output. Then the calculations were performed and the total IPA emission value was 6.763 kg CO_2 eq. comparing it with the Fossil IPA emission value, the percentage of emission has a surge in the value of about 265.573% increase.

The calculations for the carbon emission profile analysis were performed in the article Liew et al.,(2022) for the pilot scale. So the industrial scale plant's carbon emission profile was also performed replicating the same method as the article. This method replication is performed to show that the LCA results are not coherent because they lack inputs and the multi-functionality of the process. Contributions less than 5% were also excluded to reduce the GWP of the process significantly. In this industrial scale process, the raw materials inputs like compressed air and water were included along with the same inputs as the previous method. The LCA was performed and the value was calculated as 6.688 kg CO_2 eq./ kg IPA produced, which is considered to be ±261.5% increase in the table 4.1, and when considering the biomass waste coming out of the system was incinerated, the impact value is ±265.5% increased in the table 4.3 when comparing these values with the kg CO_2 eq. value for the conventional IPA production method of 1.85 kg CO_2 eq. The kg CO_2 eq. value for the conventional method varies when compared with the Ecoinvent data of 2.026 kg CO_2 eq. The Liew et al.,(2022) article has published the percentage decrease to be 163%, which might be calculated after cutting off the production process GHG contributors (LCA). The major contributors include water, compressed air, and CO_2. So, the LCA contribute process has to be performed to account for the substitution and the impacts caused by all the materials involved.

4.2. Impact assessment

The usual method for the impact assessment is performed. In this impact assessment, a complete environmental impact assessment including all the major contributors and emissions in the process will be assessed along with the emission credits (for the previous process of the steel mill) will be accounted. The modeling will be performed. Seven midpoint indicators were chosen for the impact assessment of the process.

4.2.1. Impact assessment: Base case scenario (biomass waste incinerated)

Impact category	Global warming	Stratospheric ozone depletion	Fine particulate matter formation	Freshwater eutrophication	Marine eutrophication	Human carcinogenic toxicity	Land use
Unit	kg CO_2 eq	kg CFC11 eq	kg PM2.5 eq	kg P eq	kg N eq	kg 1,4-DCB	m^2a crop eq
Total	**27.656**	**2.517E-05**	**1.554E-02**	**2.099E-03**	**8.261E-03**	**3.709E-01**	**4.802**
Ammonia	0.051	4.714E-09	1.000E-03	2.782E-06	1.932E-07	1.227E-03	0.000
Water	0.002	2.098E-09	1.000E-03	1.499E-06	1.144E-07	2.113E-04	0.000
Glycerol	3.594	2.336E-05	6.565E-03	1.123E-03	8.466E-03	1.745E-01	4.719
Sodium hydroxide	0.093	8.747E-08	1.939E-04	4.350E-05	3.851E-06	6.363E-03	0.003
Compressed air	0.520	2.260E-07	1.720E-03	6.569E-04	2.932E-05	1.986E-01	0.020
CO_2 from the process	9.340	0	0	0	0	0	0
Electricity consumption	0.428	1.986E-07	5.739E-04	3.839E-04	2.877E-05	2.739E-02	0.013
Steam (LP, HP)	16.968	1.985E-06	1.089E-02	1.897E-03	2.271E-04	3.131E-01	0.172
Heat replacement	0.193	9.521E-08	2.597E-04	1.527E-04	1.071E-05	1.254E-02	0.005
Electricity replacement	1.713	9.472E-08	1.322E-04	2.340E-06	3798E-07	7.090E-04	0.000
Chemical heat during conversion	2.976	3.924E-07	5.157E-04	5.757E-05	5.335E-06	4.433E-02	0.009
BOF prevented from flaring	-8.222	-1.277E-06	-5.327E-03	-2.222E-03	-5.107E-04	-4.081E-01	-0.140

Table 4.4: Impact Assessment for the basecase scenario

$$\text{Impact value} = \sum \text{Impact values of components}$$

Table 4.4 represents the impact assessment performed for the base case scenario. In this, the components are fed into the system. This base case scenario is based on biomass waste incineration, in which the biomass is incinerated and the emissions are emitted during the process. The main product is the IPA and there are no co-products produced during this process. The biomass waste produced during the process could also act as the co-product, but due to the ban on GMOs in the EU region, the scenario of biomass incineration was considered to be the main LCA aspect. The N_2, and water emitted during the process do not contribute more to the selected impact category of GWP, but the CO_2 emitted is considered fossil considering the source of the carbon from where it is derived. The steel mill uses ores which have a long carbon cycle and have a direct effect on the environment causing global warming potential. Inputs like heat replacement and electricity replacement are included. The negative sign represents the emission credit (avoided from the total impacts). The abbreviation represented in the figure 4.1 refers to the midpoint categories of Global warming potential, Stratospheric Ozone Depletion, Fine Particulate Matter Formation, Freshwater Eutrophication, Marine Eutrophication, Human Carcinogenic Toxicity, and Land Use. A detailed interpretation and the % contribution of components on the impact categories will be discussed in the later part of this chapter. The calculations for the amount of heat and electricity replacement and the BOF prevention from flaring in the steel mill are performed in the Appendix A.1.

4.2.2. Impact assessment: Biomass as fishfeed

Impact category	Global warming	Stratospheric ozone depletion	Fine particulate matter formation	Freshwater eutrophication	Marine eutrophication	Human carcinogenic toxicity	Land use
Unit	kg CO_2 eq	kg CFC11 eq	kg PM2.5 eq	kg P eq	kg N eq	kg 1,4-DCB	m^2a crop eq
Total	**27.586**	**2.516E-05**	**1.540E-02**	**2.092E-03**	**8.258E-03**	**3.676E-01**	**4.801**
Ammonia	0.051	4.714E-09	1.577E-05	2.782E-06	1.932E-07	1.227E-03	0.000
Water	0.002	2.098E-09	2.917E-06	1.499E-06	1.144E-07	2.113E-04	0.000
Glycerol	3.594	2.336E-05	6.565E-03	1.123E-03	8.466E-03	1.745E-01	4.719
NaOH	0.093	8.747E-08	1.939E-04	4.350E-05	3.851E-06	6.363E-03	0.003
Compressed air	0.520	2.260E-07	1.720E-03	6.569E-04	2.932E-05	1.986E-01	0.020
CO_2 from the process	9.321	0	0	0	0	0	0
Electricity	0.428	1.986E-07	5.739E-04	3.839E-04	2.877E-05	2.739E-02	0.013
Steam (LP,HP)	16.968	1.985E-06	1.089E-02	1.897E-03	2.271E-04	3.131E-01	0.172
Heat replacement	0.193	9.521E-08	2.597E-04	1.527E-04	1.071E-05	1.254E-02	0.005
Electricity replacement	1.713	9.472E-08	1.322E-04	2.340E-06	3.798E-07	7.090E-04	0.000
Chemical heat during conversion	2.976	3.924E-07	5.157E-04	5.757E-05	5.335E-06	4.433E-02	0.009
Fishmeal protein	-0.050	-1.235E-08	-1.391E-04	-7.369E-06	-2.319E-06	-3.259E-03	-0.001
BOF prevented from flaring	-8.222	-1.277E-06	-5.327E-03	-2.222E-03	-5.107E-04	-4.081E-01	-0.140

Table 4.5: Impact Assessment for Biomass waste as fishfeed

Then two different methods were considered for the treatment of biomass waste. First, biomass waste was incinerated. The second method is to be considered as a fishmeal protein replacement. Since the EU landscape has a ban on the use of GMO waste, the impact assessment for biomass as fishmeal protein was also carried out to estimate the impact category values. This is because if it has the potential to replace the prominent soybean in the fish meal, this impact assessment would help to consider the usage GMO's by making them undergo a treatment process and utilize them. This treated biomass is considered as a co-product When performing the impact assessment this case has less emission of CO_2 and water because the biomass is not incinerated. Considering the system expansion, the impacts that are caused by biomass waste (considered as fishmeal protein) are deducted from the total impact of this scenario. The BOF gas is also prevented from flaring is also an emission credit, so it can be deducted from the total impact. Table 4.5 represents the impact assessment for the gas fermentation considering that the biomass waste ends up as fish feed alternate. And the interpretation for these studies is performed. The comparison studies for the two cases of biomass waste as fish feed and biomass incineration are done.

4.2.3. Impact assessment for sensitivity cases

The thesis draft by Brouwer et al., (2023) indicates some of the key performance indicators (KPIs) in the process modeling. They were used to identify the relative effect on the whole process when the process parameters were altered. These 11 KPIs were considered to be the sensitivity analysis case scenarios for the base case. The impact assessment was performed and the interpretation for these scenarios is represented in the section 4.4.

4.3. Life cycle interpretation

4.3.1. Life cycle interpretation of Base case scenario

Midpoint indicator	**Unit**	Conventional IPA production method	IPA production via BOF gas fermentation (biomass incineration)	**Factor Difference**
Global warming potential	kg CO_2 eq.	2.026	27.656	13.65
Stratospheric ozone depletion	kg CFC11 eq.	1.45E-07	2.52E-05	173.79
Fine particulate matter formation	kg PM2.5 eq.	0.002	0.015	7.50
Freshwater eutrophication	kg P eq.	0.001	0.002	2.00
Marine eutrophication	kg N eq.	1.8E-05	0.008	444.44
Human carcinogenic toxicity	kg 1,4-DCB	0.057	0.371	6.51
Land use	m^2a crop eq.	0.015	4.802	320.13

Table 4.6: Comparison of Midpoint Indicators for IPA Production Methods

Component	**Global warming potential (%)**	**Stratospheric ozone depletion (%)**	**Fine particulate matter formation (%)**	**Freshwater eutrophication (%)**	**Marine eutrophication (%)**	**Human carcinogenic toxicity (%)**	**Land use (%)**
Ammonia	0.184	0.019	6.436	0.133	0.002	0.331	0.000
Water	0.007	0.008	6.436	0.071	0.001	0.057	0.000
Glycerol	12.990	92.820	42.234	53.502	102.481	47.049	98.271
NaOH	0.336	0.348	1.248	2.073	0.047	1.716	0.062
Compressed air	1.879	0.898	11.070	31.301	0.355	53.551	0.416
CO_2 from the process	33.767	0.000	0.000	0.000	0.000	0.000	0.000
Electricity consumption	1.547	0.789	3.692	18.295	0.348	7.387	0.271
Steam (LP, HP)	61.345	7.888	70.080	90.339	2.749	84.397	3.581
Heat replacement	0.698	0.378	1.671	7.277	0.130	3.381	0.104
Electricity replacement	6.190	0.376	0.851	0.111	0.005	0.191	0.000
Chemical heat during conversion	10.760	1.558	3.318	2.743	0.065	11.955	0.188
BOF prevented from flaring	-29.731	-5.072	-34.278	-105.818	-6.180	-110.052	-2.914

Table 4.7: Percentage of component contribution to the total impact of basecase scenario (biomass incineration)

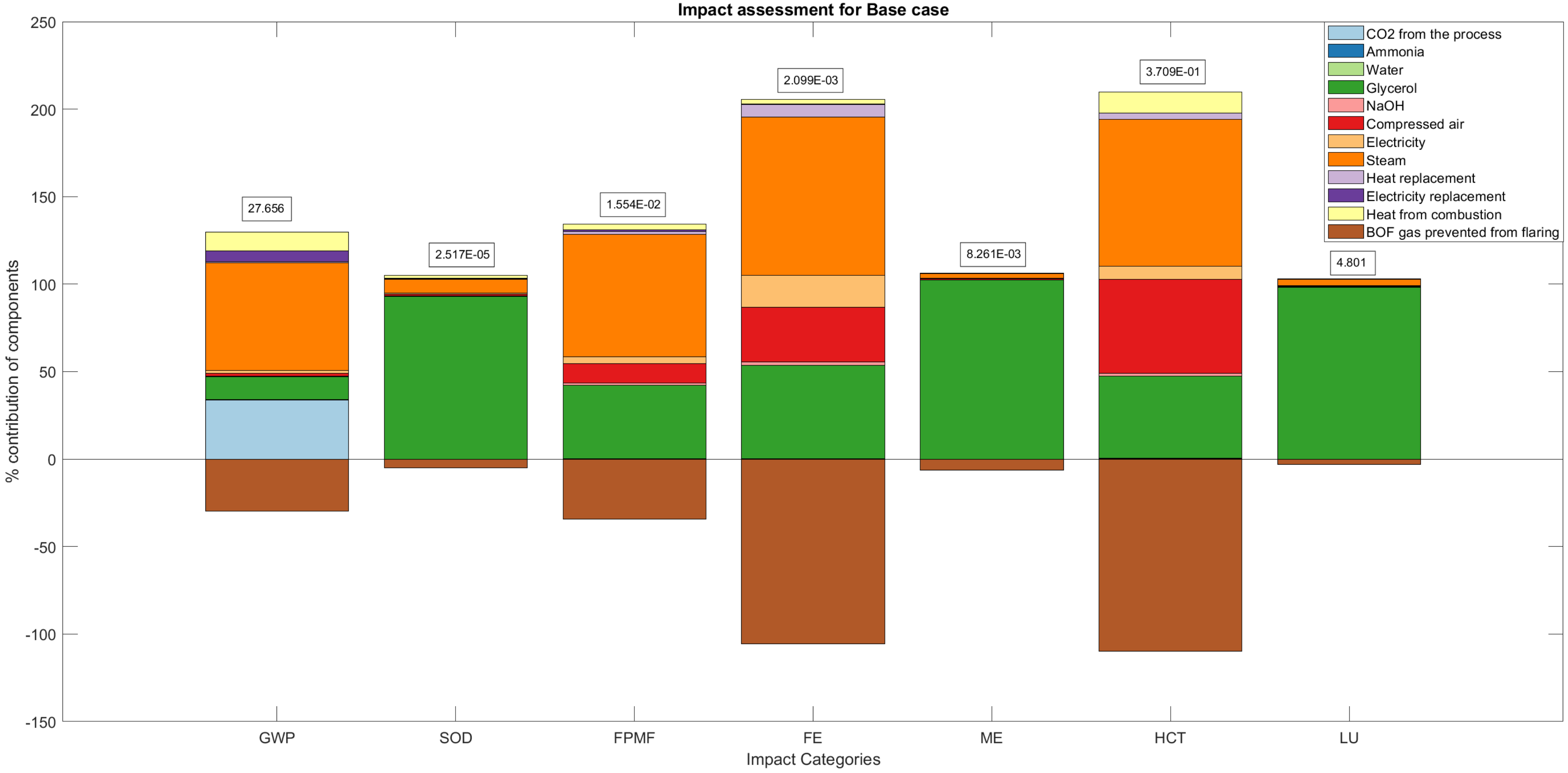

Figure 4.1: Impact assessment for the Base case scenario (biomass waste incinerated) GWP: Global Warming Potential (kg CO_2eq.), SOD: Stratospheric Ozone Depletion (kg CFC11 eq.), FPMF: Fine Particulate Matter Formation (kg PM2.5 eq.), FE: Freshwater Eutrophication (kg Peq.), ME: Marine Eutrophication (kg N eq.), HCT: Human Carcinogenic Toxicity (kg 1,4-DCB), LU: Land Use (m^2 a crop eq.)

The impact assessment for the base case scenario is performed and the midpoint indicator results are obtained. The indicator values are compared with the benchmark value to interpret the environmental burdens (midpoint point indicators). This comparison study is performed to assess the feasibility of the process. The benchmark traditional IPA production process data (fossil fuel-sourced IPA) is obtained from the Ecoinvent database. This production is based on the mix of Direct hydration and Indirect hydration of propylene (50%+ 50% mix).In general traditional IPA method midpoint indicator values are considerably overly low when comparing the values of our BOF gas fermentation method. The factor difference when comparing the conventional IPA method and the BOF gas fermentation method can be observed in the table 4.6. The impact categories of GWP, FPMF, FE, and HCT have minimal factor difference values. But the other indicators of SOD, ME, and LU have huge differences in factor values.

$$\text{Impact category} = \sum \text{Impact category value of all components}$$

The impact category values are the summation of all the component's impact values. In this base case scenario of IPA production, seven different environmental impact categories like global warming potential, stratospheric ozone depletion, fine particulate matter formation, freshwater eutrophication, human carcinogenic toxicity, and land use were considered. These impact category values have different units, but these different units are calculated per kg of Isopropyl alcohol produced. The GWP of this particular base case is 27.656 kg CO_2 eq./kg of IPA produced. This can be observed in the figure 4.6. The increase in average global temperatures caused by greenhouse gas (GHG) emissions is indicated by this impact category (*Impact category*, n.d.). The major contributor to the GWP is steam which is approximately 16.968 kg CO_2 eq./kg IPA, which is a utility consumed during the conditioning of BOF gas and utilized in the extractive distillation. The utility steam contributes to about 62% of the total Global warming potential value. If the steam consumption and the CO_2 emission from the process are not taken into total account, the GWP value would be 1.348 kg CO_2 eq. lower than the traditional IPA value of 2.026 kg CO_2 eq. Since most of the Life cycle assessments for the processes around the world are performed only based on the GWP, lowering the utility contribution by optimizing the process could be an effective way to produce Isopropyl alcohol rather than the traditional fossil IPA production method. It can be noticed from the figure 4.1, that the CO_2 emitted from the process has more percentage contribution considering the BOF gas prevented from flaring. The major reason for this increase in CO_2 from the process value is that the gas fermentation process does not have any other carbon-based components usage, however, the process has the anaerobic digestion chamber where the biogas is generated and combusted involves the additional emission of CO_2.

Similarly, the stratospheric ozone depletion has an impact value of 2.517E-05 kg CFC11 eq. per kg of IPA produced. Stratospheric ozone depletion is an indicator of air pollution that depletes the stratospheric ozone layer (*Impact category*, n.d.). In this midpoint category, glycerol (2.336E-05 kg CFC11 eq.) has a huge contribution to the value. Approximately 93% of the total SOD impacts are caused only by the glycerol. The impact values are Initially, both glycerol and ionic liquids were considered for entrainer, but glycerol was opted for due to its significantly lower environmental impact than ionic liquid. Since the glycerol is utilized in the extractive distillation process, a low-impact similar entrainer can be substituted alternating the glycerol usage in the process. Likewise, fine particulate matter formulation is an indicator of the possible prevalence of diseases brought on by emissions of particulate matter (*Impact category*, n.d.). The impact category value of this Fine particulate matter formation is around 0.016 kg PM2.5 eq. per kg of IPA produced. The major contributor would be the steam used during extractive distillation, nearly 68% of the total impact value. Considering the steam, this utility generation has some impurities leading to the high value of FPMF. In our case, biomass incineration is also carried out, but the heat produced will be low-quality heat. Since biomass waste incineration is an assumption, exact process modeling data (Brouwer, 2023) about this incineration process is not available. So the clear information regarding the FPMF cannot be explained considering the term of biomass incineration.

Next, the eutrophication of freshwater is taken into account. This indicator refers to potential toxic impacts on an ecosystem, which may damage individual species as well as the functioning of the ecosystem. The impact category value is averaged to be 0.002 kg P eq. per kg of IPA produced. And still steam is the major contributor in this impact category with a contribution of about 90% flowed by the glycerol of about 53%. The major change in impact category value is due to the emission credit preventing the BOF from flaring process. This contribution alone accounts for nearly -105% in the value which is depicted in the figure 4.1. But the total impact value is contributed to 100% by other inputs to the process like compressed air consumption, and the heat replacement for the steel mill. Similarly, marine eutrophication is taken for consideration, this is an indicator that represents excessive amounts of nutrients, especially nitrogen and phosphorus, are introduced into marine ecosystems (Ecochain, 2024). Algal blooms, a phenomenon caused by an overabundance of algae and other aquatic plants, can result from this enrichment. Marine ecosystems experience oxygen depletion as a result of these, algae use of oxygen in the water causes oxygen depletion and affects the marine environment. The total value of this impact category is 0.008 kg N eq./kg of IPA produced. This impact value looks concerning when compared with the marine eutrophication value of the conventional IPA production method. Glycerol is the major contributor to this impact category accounting for 102.481% of the total impacts. Rest inputs are accounted only for about 4%. Preventing the BOF gas flaring reduces the total impact by 6.5%. As explained previously the major contributor glycerol which is used as an entrainer in the distillation column should considered to be replaced. It can be claimed that the nitrogen coming out of the system behaves inert, and doesn't take part in any of the processes could lead to an increase in marine eutrophication impacts. However, as cited by the European Union., (n.d.), no impact is caused by nitrogen whereas nitrate causes all the impacts. So the marine eutrophication value of the BOF gas fermentation IPA process is considerably higher than the traditional method. Finding an entertainer with a lower impact value could lower the marine eutrophication impact value.

The main impact category would be human carcinogenic toxicity, this impact category implies the possible effects of pollutants, when ingested through the air, water, or soil might have on human health (Ecochain, 2024). The compound's direct effects on people are not adequately quantified. The impact category value is around 0.371 kg 1,4-DCB per kg of IPA produced. Considering the human population with an average of 60 kilograms. The daily limit for them would but the daily limit for the exposure of 1,4-DCB is 0.024 mg/kg body weight/day (EPA, n.d.), and the average 60 kg person's daily limit totals up to 1.44 mg/day. This value might look a bit low for our process as we are considering it for 1kg of IPA, but this value should be assessed or quantified based on several factors like regulatory limits, industrial benchmarks, health risks, and even stakeholder concerns (*Impact category*, n.d.). The major contributor in this impact category would be the steam (84%) and glycerol (47%) inputs for the process. This major impact value is deducted by the emission credit of BOF gas prevented by flaring which contributes to about (-110%), this can be observed in the figure 4.1. Even though the values are within the limits when compared with the traditional IPA value, a huge difference in value can be observed. Finally, the Land use impact category is an impact category to quantify the changes in soil properties like (biotic production, erosion resistance, groundwater regeneration, and mechanical filtration) (Ecochain, 2024). The value is estimated to be 4.801 m^2a crop eq./kg of IPA produced. The major contributor in this land use impact category is the component glycerol with a wide range of greater impact values. The glycerol component in the ecoinvent database is sourced from the rapeseed oil esterification process. Considering this esterification process, the impacts of Land use is greater with a contribution of about 98% to the total value. Sourcing the glycerol from a less environmentally impactful process could significantly lower the impact category values which are dominated by glycerol consumption.

4.3.2. Comparision Study: Biomass waste as Fish feed vs Incineration

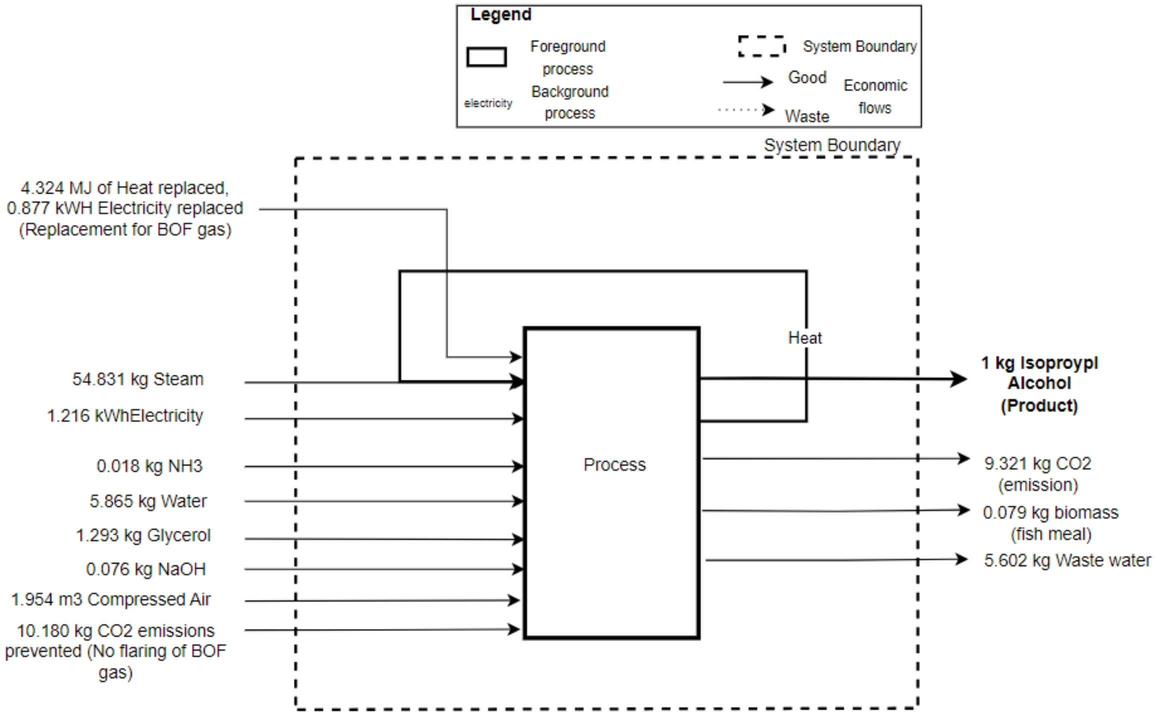

Figure 4.2: LCA study for the scenario of biomass as fish feed (components usage per kg of IPA produced)

Midpoint indicator	Unit	IPA process with Biomass incineration	IPA process with Biomass as fishfeed	Factor Difference
Global warming potential	kg CO_2 eq	27.656	27.586	0.9975
Stratospheric ozone depletion	kg CFC11 eq	2.517E-05	2.516E-05	0.9996
Fine particulate matter formation	kg PM2.5 eq	1.554E-02	1.540E-02	0.9900
Freshwater eutrophication	kg P eq	2.099E-03	2.092E-03	0.9967
Marine eutrophication	kg N eq	8.261E-03	8.258E-03	0.9996
Human carcinogenic toxicity	kg 1,4-DCB	3.709E-01	3.676E-01	0.9911
Land use	m^2a crop eq	4.802	4.801	0.9998

Table 4.8: Comparison of biomass incineration with biomass as fish feed

Impact category	Global warming potential %	Stratospheric ozone depletion %	Fine particulate matter formation %	Freshwater eutrophication %	Marine eutrophication %	Human carcinogenic toxicity %	Land use %
Ammonia	0.185	0.019	0.102	0.133	0.002	0.334	0.000
Water	0.007	0.008	0.019	0.072	0.001	0.057	0.000
Glycerol	13.028	92.846	42.630	53.681	102.519	47.470	98.292
NaOH	0.337	0.348	1.259	2.079	0.047	1.731	0.062
Compressed air	1.885	0.898	11.169	31.401	0.355	54.026	0.417
CO_2 from the process	33.789	0.000	0.000	0.000	0.000	0.000	0.000
Electricity	1.552	0.789	3.727	18.351	0.348	7.451	0.271
Steam (LP,HP)	61.509	7.890	70.714	90.679	2.750	85.174	3.583
Heat replacement	0.700	0.378	1.686	7.299	0.130	3.411	0.104
Electricity replacement	6.210	0.376	0.858	0.112	0.005	0.193	0.000
Chemical heat (during conversion)	10.788	1.560	3.349	2.752	0.065	12.059	0.187
Fishmeal protein	-0.181	-0.049	-0.903	-0.352	-0.028	-0.887	-0.021
BOF prevented from flaring	-29.805	-5.076	-34.591	-106.214	-6.184	-111.017	-2.916

Table 4.9: Percentage of component contribution to the total impact of basecase scenario (biomass as fish feed)

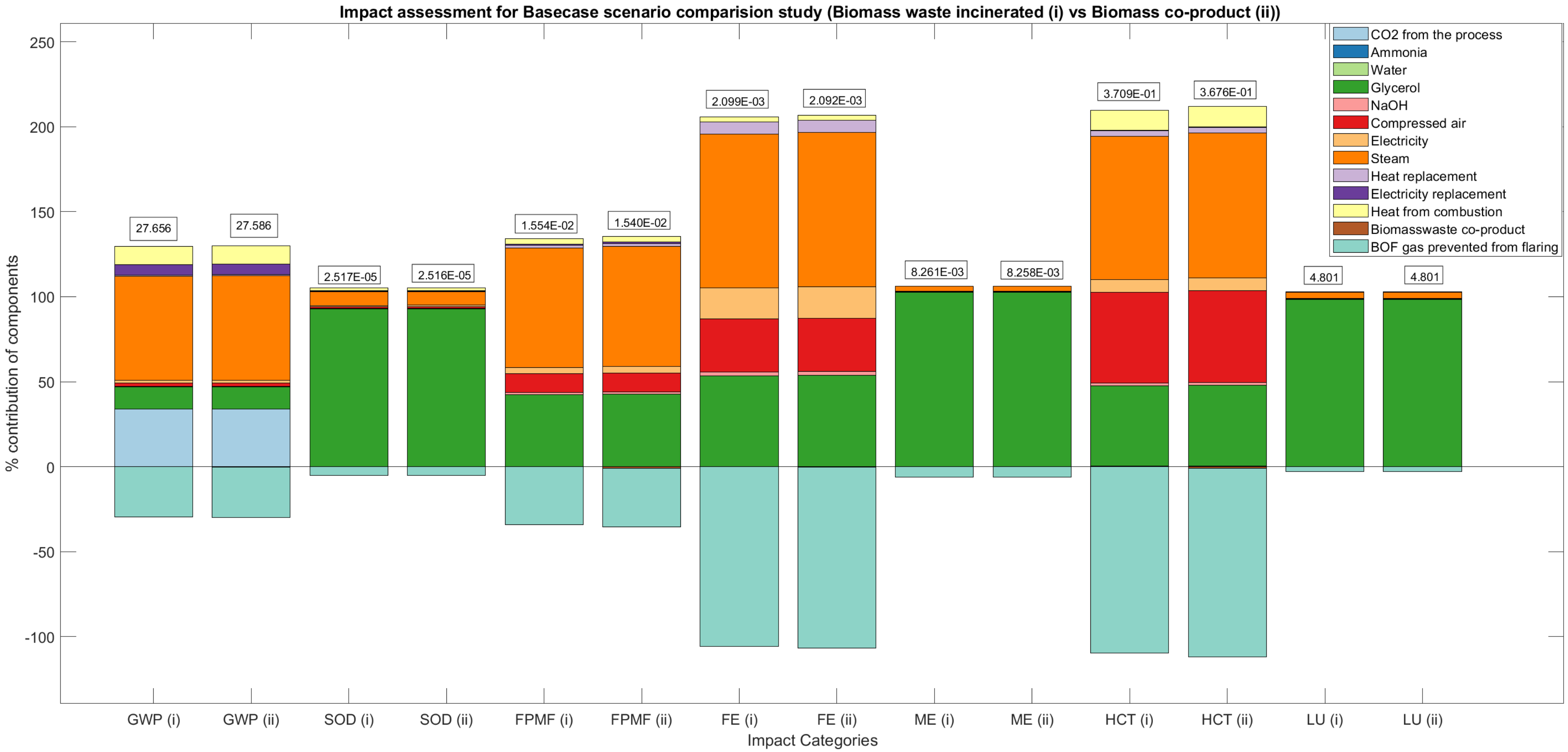

Figure 4.3: Impact assessment for the Basecase scenario comparison study (biomass waste as co-product);(i) represents the scenario of biomass incineration, (ii) represents scenario of biomass as fishmeal co-product; GWP: Global Warming Potential (kg CO_2eq.), SOD: Stratospheric Ozone Depletion (kg CFC11 eq.), FPMF: Fine Particulate Matter Formation (kg PM2.5 eq.), FE: Freshwater Eutrophication (kg Peq.), ME: Marine Eutrophication (kg N eq.), HCT: Human Carcinogenic Toxicity (kg 1,4-DCB), LU: Land Use (m^2 a crop eq.)

The biomass waste is co-produced during the BOF gas fermentation process to produce IPA. Considering its environmental impacts, the LCA for the two scenarios was performed. The first scenario is considering biomass waste as GMO waste and incinerating it. The second scenario is to make it undergo the treatment process (considered within the system boundary) and use it as an alternative to soybean meal in the fish feed sector. In the first scenario of biomass incineration, the Global warming potential is 27.656 kg CO_2 eq./kg IPA, and for the biomass as fish feed, the value is 27.586 kg CO_2 eq./kg IPA which has the % difference of -0.253%, this can be observed in the figure 4.8. This assessment implies that the biomass fish feed scenario has a lower global warming potential value when compared with the incinerating biomass waste which emits CO_2, N_2, and water. This consideration is due to the co-product produced along with the process (biomass out of the system). The impacts for the co-products produced should be deducted from the total impacts because this helps to allocate the impacts between the products and co-products accurately. In our case, the biomass out (considered treated) could potentially replace the conventional, reducing the necessity of that source. The environmental impacts of the total process can be reduced by considering the biomass co-produced as the fish feed alternate.

Soybean meal has 40% protein content, whereas the biomass waste has ±80% (CAP) protein content (Xue et al., 2023). So, the soybean meal can be replaced by biomass co-produced%.

$$\begin{aligned}&\text{Crude protein content of biomass waste (treated)} = 866.7\text{g/kg}\\&\text{Biomass waste available for replacement} = 0.07957\text{kg/ kg IPA}\\&\text{The total protein content in biomass waste} = 0.07957 \times 866.7 = 68.99\text{g}\end{aligned}$$

So the equivalent amount of soybean meal needed to provide the same amount of protein is 0.150 kg. Usually, the fish feed has the composition of 24% soybean meal. In our case, 5% of the soybean meal can be replaced by biomass waste. So the equivalent soybean meal would be 0.1498 kg. The total impact of the IPA process is 27.586 kg CO_2 eq. and the impact value of fishmeal protein per kg is 0.040 kg CO_2 eq. This will be deducted from the total impact value considering the system expansion because biomass as fishmeal protein alternate is a co-product produced along with IPA as the main product.

The steam used in the process has greater contributional effects on the GWP of both processes. The second biggest contributor would be the CO_2 emission out of the system this can be observed in the figure 4.3. From the results of the impact assessment, the midpoint indicator values have the same value for inputs in both scenarios. It is evident both these scenario has the same amount of input consumption although there is a change in the impact assessment values. These differences in GWP values are due to the two different considerations, In the case of biomass incineration the LCA assessment is similar to the base case scenario where the emissions are accounted for along with the deduction of emission credit for BOF gas prevention from flaring. But the second case is considering the biomass as fish feed. In this, biomass waste (considered treated) has the potential to replace the soybean meal in the aquaculture feed (fishmeal protein). This biomass waste is a co-product and the multifunctionality approach of system expansion is applied and the impact value of the co-product is deducted from the total impact value leading to the lower midpoint indicator value when compared with the first case. This change is common for all the seven midpoint categories. The important category would be the GWP, where the change in value is distinct considering the difference in gram CO_2 eq. whereas the other categories do not show a huge change in values. The second case of biomass as fish feed is only performed to estimate the impacts it might cause if this method is applied. The probability of considering this case to be the primary method is too low because the EU Commission has prohibited the use of GMOs in any form.

But on an interesting note, if this scenario was chosen to be the better-suited scenario the biomass waste could be utilized as a good flow for the other process, which has the potential to replace the traditional fish food in the aquaculture sector. So, the calculation was performed in appendix A section, to address whether the treated biomass waste has a market. Considering the global soybean meal market, the total steel production around the world accounts for 1.4 billion tonnes, which could ideally produce ≡ 247.9 kton of IPA, and co-produces ±19.71 kton of biomass waste. If the biomass waste is treated for the waste treatment procedure (assuming no loss in biomass during the procedure) it can replace ≡ 0.0945% of global soybean meal. By this calculation, it is evident that the potential reduction of the amount of soybean meal requirement can be satisfied by the biomass co-produced if the ban has been lifted in the European region.

4.4. Life cycle interpretation for sensitivity analysis cases

In the modeling stage of this BOF gas fermentation process, 11 key performance indicators were chosen to indicate their relative effect on the technical and environmental performances, when they are varied (Brouwer, 2023). The varied values differ for each process. To estimate the environmental impacts by varying these process parameters the impact assessment for all these cases was carried out. For all the sensitivity case scenarios the base-case scenario was set as the benchmark value and process parameters were altered. This impact assessment also compares the impact assessment between each Process parameter and the base case.

4.4.1. Sensitivity analysis: CO conversion

Midpoint indicator	Unit	CO conv Lowerbound	% vary in LB	Basecase	CO conv Upperbound	% vary in UB
Global warming potential	kg CO_2 eq	27.769	0.409	27.656	27.512	-0.521
Stratospheric ozone depletion	kg CFC11 eq	2.518E-05	0.040	2.517E-05	2.520E-05	0.119
Fine particulate matter formation	kg PM2.5 eq	1.542E-02	-0.772	1.554E-02	1.564E-02	0.644
Freshwater eutrophication	kg P eq	2.130E-03	1.477	2.099E-03	2.070E-03	-1.382
Marine eutrophication	kg N eq	8.273E-03	0.145	8.261E-03	8.269E-03	0.097
Human carcinogenic toxicity	kg 1,4-DCB eq	3.818E-01	2.939	3.709E-01	3.611E-01	-2.642
Land use	m^2a crop eq	4.807	0.104	4.802	4.807	0.104

Table 4.10: Sensitivity analysis: CO conversion

Components	GWP LB	GWP UB	SOD LB	SOD UB	FPMF LB	FPMF UB	FE LB	FE UB	ME LB	ME UB	HCT LB	HCT UB	LU UB	LU UB
Ammonia	0.185	0.187	0.019	0.019	0.102	0.101	0.131	0.134	0.002	0.002	0.321	0.340	0.007	0.007
Water	0.007	0.007	0.008	0.008	0.019	0.019	0.070	0.072	0.001	0.001	0.055	0.059	0.001	0.001
Glycerol	12.964	13.074	92.917	92.754	42.633	42.023	52.825	54.287	102.504	102.462	45.781	48.370	98.330	98.243
NaOH	0.333	0.336	0.347	0.347	1.257	1.240	2.042	2.102	0.047	0.047	1.666	1.763	0.054	0.054
Compressed air	2.044	1.740	0.980	0.825	12.173	10.129	33.669	29.209	0.387	0.326	56.760	50.625	0.455	0.384
CO_2 from the process	35.566	32.202	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Electricity	1.641	1.466	0.840	0.742	3.962	3.459	19.195	17.473	0.370	0.328	7.638	7.148	0.286	0.253
Steam (LP.HP)	59.286	63.126	7.648	8.061	68.509	71.297	86.445	93.795	2.664	2.811	79.569	88.760	3.471	3.661
Heat replacement	0.695	0.702	0.378	0.378	1.684	1.661	7.170	7.374	0.129	0.129	3.284	3.472	0.111	0.111
Electricity replacement	6.168	6.225	0.376	0.376	0.857	0.846	0.110	0.113	0.005	0.005	0.186	0.196	0.006	0.006
Chemical heat (during conversion)	10.718	10.819	1.558	1.557	3.343	3.298	2.703	2.780	0.064	0.065	11.610	12.277	0.189	0.189
BOF gas prevented from flaring	-29.607	-29.884	-5.072	-5.067	-34.538	-34.073	-104.361	-107.340	-6.174	-6.176	-106.871	-113.010	-2.909	-2.909

Table 4.11: Percentage of component contribution to the total impact of Lowerbound and Upperbound CO conversion sensitivity case scenario

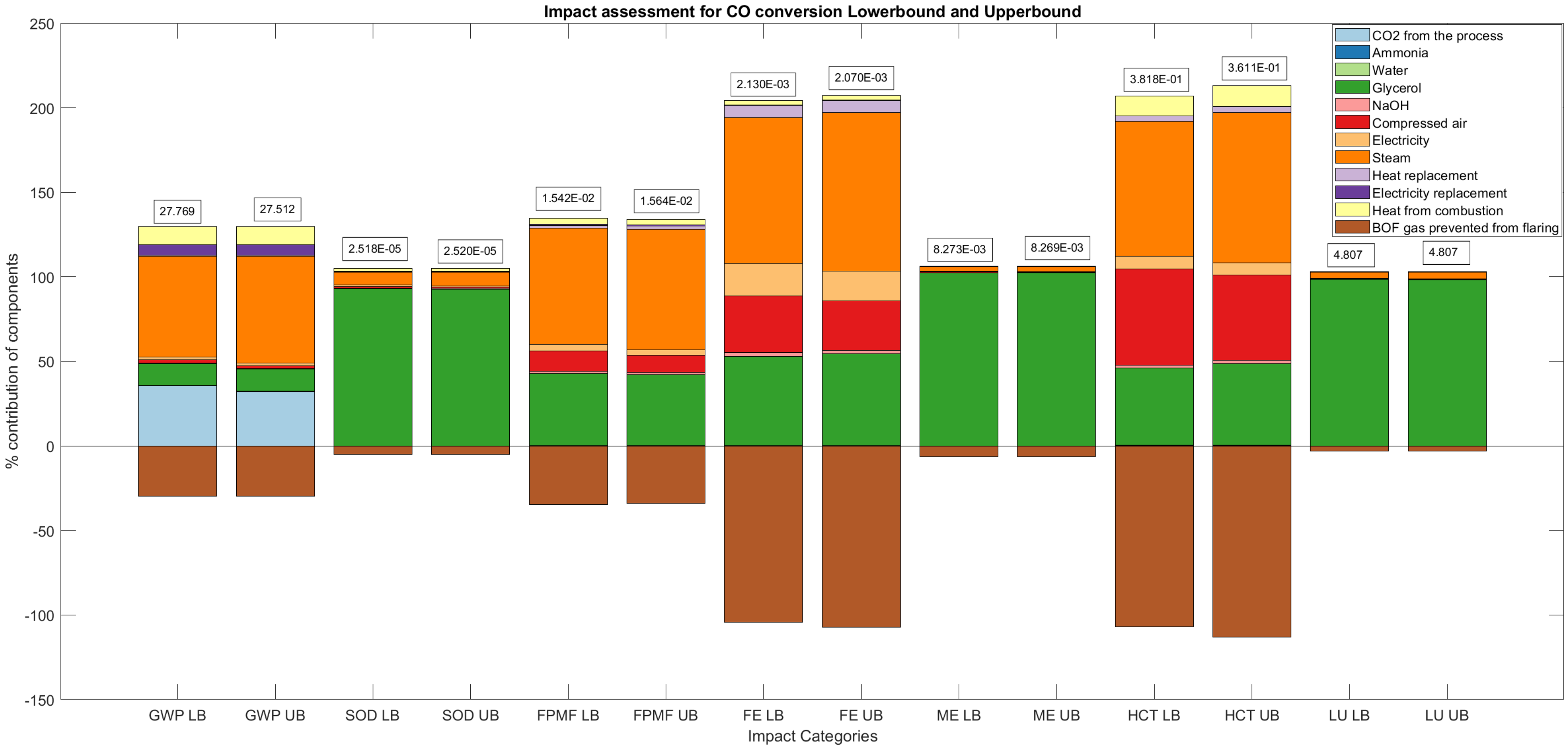

Figure 4.4: Impact assessment for the CO conversion; LB represents the scenario of Lower Bound CO conversion varied by -5%, UB represents scenario of Upper Bound CO conversion varied by +5%; GWP: Global Warming Potential (kg CO_2eq.), SOD: Stratospheric Ozone Depletion (kg CFC11 eq.), FPMF: Fine Particulate Matter Formation (kg PM2.5 eq.), FE: Freshwater Eutrophication (kg Peq.), ME: Marine Eutrophication (kg N eq.), HCT: Human Carcinogenic Toxicity (kg 1,4-DCB), LU: Land Use (m^2 a crop eq.)

The CO conversion is the first process parameter that was considered in the process modeling. Table 4.10 refers to the comparison of impact value between the lower-bound and upper-bound CO conversion analysis for seven midpoint indicators along with the base case. This involvement of the base case for the comparison study is to estimate how much the effects are varied. In this case, the CO conversion fraction of 0.85 was varied by ±5%. This change in the value has some effects on the electricity, steam, compressed air consumption, and CO_2, N_2 emissions from the process.

Considering this GWP impact category, the lower-bound and upper-bound values for the CO conversion vary. For the lower-bound, it is estimated to be around 27.769 kg CO_2 eq. and for the upper-bound is 27.512 kg CO_2 eq. Both these values are compared with the base-case value of 27.656 kg CO_2 eq. and found that varying the CO conversion fraction for about ±5% does not have a much greater impact on the midpoint indicator of Global Warming Potential. But when compared with the conventional IPA production methods, this impact value is huge. Varying the GWP by -5% could observe the percentage change of 0.41% and increasing 5% leads to a decrease in -0.512%. The major contributor to this category for both these lower-bound and upper-bound cases is steam utilization. This steam accounts for $\approx$ 59% of the total impact of this process, and the second most contributor is CO_2 emission from the process. For the CO conversion Process parameter, fluctuating the value results proportionate increase in steam consumption when CO conversion is altered.

In this Stratospheric ozone depletion impact category, the major contributor is the Glycerol for both the CO conversion sensitivity cases. This glycerol contributes approximately 90% of the total impact value of this particular impact category. This increase in glycerol usage is due to the increased broth flow in the extractive distillation when the CO conversion fraction is varied, the glycerol mole fraction is fixed. To maintain the glycerol mole fraction, the glycerol consumption was increased. Although Glycerol is not listed as the main ozone-depleting substance by the environmental agencies (MontrealProtocol, n.d.). However, some processes are related to glycerol, and involve some emissions of CFC-12 and other ODS (Ozone Depleting Substances). This leads to a higher value in the total impacts in the particular impact category.

In the midpoint category of Fine particulate matter formation, the steam is the most contributing component in the total impact value. This HP and LP steam cannot be differentiated in the ecoinvent database. This utility generation process could probably lead to the formation of Fine particulate matter. Because the method used for steam generation could lead to the emission of impurities (Mekonen, 2023). Even some traces of sulfur content in biogas and offgas are also expected (Vitázek, 2016). Also increasing the CO conversion factor increases the utilization of steam. The next biggest contributor would be the compressed air required for the biogas combustion. Compressed air does not have a specific impact but the air sequestrated from the different types of regions with different air pollution index might lead to particulate matter formation.

This freshwater eutrophication is an impact category that deals with the emission of phosphorous in the environment (Shang, 2021). Steam is the major contributor to this midpoint category. Steam does not have any direct emission of phosphorus. The data source from considering the ecoinvent database might include some indirect effects and upstream emissions for steam generation. This major contributor glycerol does change much by varying the CO conversion fraction value. Like freshwater eutrophication, glycerol has the greater contribution in the midpoint indicator of marine eutrophication assessment. But significantly there are no such claims to prove that glycerol usage has direct eutrophication impacts. However, glycerol production might have indirect effects on the characterization factors leading to the eutrophication value. Also, the inventory data for the glycerol involves the complete chain of glycerol, in which something could adversely cause marine eutrophication. In the CO conversion sensitivity cases, glycerol consumption increases with an increase in CO conversion fraction value.

Human Carcinogenic Toxicity is the indicator category that deals with human health out of all the chosen impact categories in our assessment. The major contributor is steam consumption. The steam is not a carcinogen and this impact value for the characterization factor could be due to the upstream processes considered or co-emissions for the steam generation. This higher impact value for steam could be due to fossil usage in the inventory data. This value does change with varying CO conversion values. And the second most impacted contributor would be the heat replacement for the steel mill. This heat replacement does not vary with changes in CO conversion fraction value. The land use midpoint indicator deals with land usage for the process. The major contributor in the category is glycerol with a contribution percentage of ≈ 97%. This is because the glycerol is sourced by the production method of esterification of rapeseed oil (Chilakamarry, 2021). This involves land usage and causes more impact on the process. If the alternate glycerol sourced from the fermentation process is utilized, it might lower the impact category of land use. However, a detailed analysis is required to obtain a conclusion on this. Compressed air holds the next most impactful contribution to this category, but compressed air does not cause any direct effect. It is assumed this value is due to some indirect effects caused by the electricity used for air compression. This electricity could cause an impact because the electricity is a grid mix, and the impacts can't be directly sourced (could be through energy generation which involves huge land use).

4.4.2. Sensitivity analysis: Volumetric mass transfer rate of CO

As cited by the process modeling work performed for the industrial scale BOF gas fermentation to IPA production, this volumetric mass transfer is one of the essential process parameters, demonstrating the change in values in the utilization of the components (Brouwer, 2023). The volumetric mass transfer rate is set at 8 $g_{CO}/\mathrm{L}/\mathrm{H}$ for the base case and varied ±30% for the lower bound and upper bound scenarios. The impact assessment for this particular Process parameter can observe huge variations in the indicator values. From this assessment, it can be interpreted that the most influential VMT_{CO} Process parameter should be altered and the increase in the mass transfer rate can be preferred to lower the total impacts

Midpoint indicator	**Unit**	VMT_{CO} **Lowerbound**	**% vary in LB**	**Basecase**	VMT_{CO} **Upperbound**	**% vary in UB**
Global warming potential	kg CO_2 eq	40.536	46.572	27.656	22.098	-20.097
Stratospheric ozone depletion	kg CFC11 eq	3.998E-05	58.840	2.517E-05	1.906E-05	-24.275
Fine particulate matter formation	kg PM2.5 eq	2.584E-02	66.281	1.554E-02	1.067E-02	-31.338
Freshwater eutrophication	kg P eq	4.128E-03	96.665	2.099E-03	1.118E-03	-46.737
Marine eutrophication	kg N eq	1.335E-02	61.603	8.261E-03	6.187E-03	-25.106
Human carcinogenic toxicity	kg 1,4-DCB eq	0.742	100.000	0.371	0.180	-51.482
Land use	m^2a crop eq	7.661	59.538	4.802	3.633	-24.344

Table 4.12: Sensitivity analysis: Volumetric Mass transfer rate VMT_{CO}

Component	**GWP LB**	**GWP UB**	**SOD LB**	**SOD UB**	**FPMF LB**	**FPMF UB**	**FE LB**	**FE UB**	**ME LB**	**ME UB**	**HCT LB**	**HCT UB**	**LU UB**	**LU UB**
Ammonia	0.141	0.233	0.013	0.025	0.068	0.148	0.075	0.250	0.002	0.003	0.184	0.684	0.005	0.009
Water	0.007	0.007	0.008	0.009	0.017	0.022	0.055	0.106	0.001	0.001	0.043	0.093	0.001	0.001
Glycerol	14.053	12.409	92.593	93.527	40.266	46.932	43.121	76.668	100.531	104.400	37.260	73.966	97.631	99.096
NaOH	0.254	0.420	0.244	0.460	0.836	1.822	1.174	3.903	0.032	0.062	0.955	3.545	0.038	0.071
Compressed air	1.984	1.503	0.874	0.757	10.297	10.293	24.616	37.534	0.340	0.303	41.374	70.438	0.405	0.353
CO_2 from the process	27.979	40.739	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Electricity	1.241	1.878	0.584	1.010	2.611	5.213	10.932	33.304	0.253	0.451	4.337	14.752	0.198	0.344
Steam (LP.HP)	62.579	57.924	7.422	7.858	63.008	76.982	68.714	128.063	2.544	2.769	63.059	131.219	3.356	3.570
Heat replacement	0.476	0.874	0.238	0.500	1.005	2.434	3.699	13.661	0.080	0.173	1.689	6.965	0.070	0.147
Electricity replacement	4.225	7.751	0.237	0.497	0.512	1.239	0.057	0.209	0.003	0.006	0.095	0.394	0.004	0.009
Chemical heat (during conversion)	7.343	13.469	0.981	2.059	1.995	4.832	1.395	5.151	0.040	0.086	5.972	24.626	0.118	0.250
BOF gas prevented from flaring	-20.283	-37.206	-3.194	-6.702	-20.616	-49.916	-53.839	-198.849	-3.826	-8.255	-54.968	-226.682	-1.825	-3.849

Table 4.13: Percentage of component contribution to the total impact of Lowerbound and Upperbound Volumetric mass transfer rate CO sensitivity case scenario

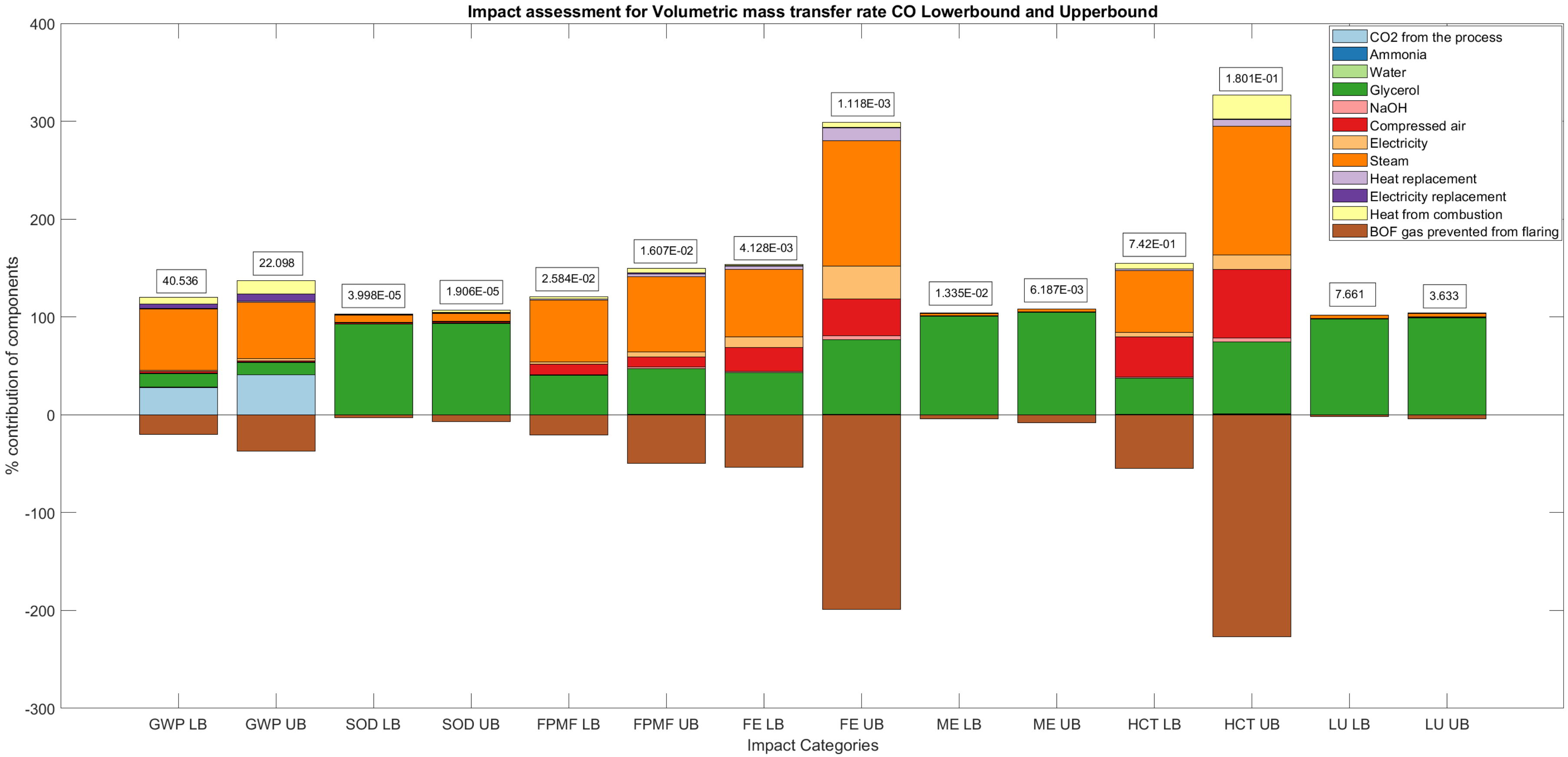

Figure 4.5: Impact assessment for the Volumetric mass transfer rate; LB represents the scenario of Lower Bound Volumetric Mass transfer rate CO conversion varied by -30%, UB represents scenario of Upper Bound Volumetric Mass transfer rate CO varied by +30%; GWP: Global Warming Potential (kg CO_2eq.), SOD: Stratospheric Ozone Depletion (kg CFC11 eq.), FPMF: Fine Particulate Matter Formation (kg PM2.5 eq.), FE: Freshwater Eutrophication (kg Peq.), ME: Marine Eutrophication (kg N eq.), HCT: Human Carcinogenic Toxicity (kg 1,4-DCB), LU: Land Use (m^2 a crop eq.)

Table 4.12 compares impact value between the lower-bound and upper-bound CO volumetric mass transfer rate Process parameter analysis for seven midpoint indicators and the base case. When the impact assessment is performed for this Process parameter VMT_{CO}, fluctuating the mass transfer rate by ±30% could significantly increase the GWP value by 61% for lower bound and 27% decrease for the upper bound cases. The GWP value for the base case is 27.656 kg CO_2 eq. The lower bound VMT_{CO} value is estimated to be 40.536 kg CO_2 eq. and the upper bound value is 22.098 kg CO_2 eq. Steam utilization is the major contributor to both sensitivity cases. But the contribution percentage by steam in the lower bound value is to be ≈ 63% and for the upper bound is ≈ 58%. The change in this contribution percentage is due to the emission credit for preventing the BOF gas from flaring. This emission credit value is common for all the base case and the sensitivity cases. For example, the lower bound uses ≈ 81 kg steam /kg IPA produced, and the upper bound uses ≈ 41 kg steam /kg IPA produced. The base case scenario utilizes ≈ 54 kg steam /kg IPA. Performing this calculation manually could show the same percentage contribution, without including the emission credits. This emission credit holds an important factor in determining the contribution percentage. For the VMT_{CO} Process parameter, fluctuating the value results in the inverse proportionate of steam consumption when altered.

The interpretation of the environmental impacts caused by the components of this process is performed in the subsection 4.3.1 part. The change in the VMT_{CO} Process parameter lowers the Stratospheric ozone depletion value to be 1.906E-02 kg CFC11 eq. for the UB and 3.998E-05 for the LB. Exactly like the base case scenario, glycerol is the most contributional component for the impact in this midpoint indicator. Considering these impact values (kg CFC11 eq.), the glycerol contribution percentage in both cases does not vary significantly. The reason for these minimal contribution changes is due to the impact values in the range of 1E-5 to 1E-9. Likewise, the variation in the process parameter value, lowering it leads to a higher impact value, and increasing the VMT_{CO} results in lower impact values.

This FPMF impact category value has a more or less similar impact value when comparing it with the FPMF value of the conventional IPA method. The major contributor in this sensitivity case would be the steam, this utility generation could lead to greater impact values. The contribution percentage also varies for both sensitivity cases. Similarly, the variation in the process parameter value could alter the impact values for the scenarios. The possible way of causing the environmental effects which contribute to the freshwater eutrophication impact category is explained in the base case scenario's impact assessment in subsection 4.3.1. The major contributor in this impact category is the steam. However, the alteration of the volumetric mass transfer rate by increasing the rate could significantly reduce the steam usage and for the lower mass transfer rate the the impacts are vice versa. Likewise, marine eutrophication's major contributor is the glycerol used in the extractive distillation process. Lowering the volumetric mass transfer rate could potentially increase the eutrophication effects for this process parameter. So it is suggested that the higher volumetric mass transfer rate should be maintained to reduce the impact category value significantly.

It can be interpreted that the process for the BOF gas to IPA production does not utilize carcinogens in any form. Since the lower bound value for the VMT_{CO} process parameter has the human carcinogenic toxicity value to be around 0.742 kg 1,4-DCB. This estimated value for the lower bound is a 100% increase compared with the base case. However, the upper bound value is compared with the traditional IPA method, and the impact value of the upper bound is considerably better for this impact category. The major contributor to this indicator would be the steam followed by the compressed air. The impact category of land use is employed to quantify the effects on the land. Similarly, the upper bound values for this impact category lead to the lower midpoint indicator values. The impact value is estimated to be 3.633 m^2 crop eq. This lower sensitivity value is very high when the traditional method for IPA production is taken into consideration.

4.4.3. Sensitivity analysis: Product selectivity

Midpoint indicator	**Unit**	**Product selectivity LB**	**% vary in LB**	**Basecase**	**Product selectivity UB**	**% vary in UB**
Global warming potential	kg CO_2 eq	28.713	3.822	27.656	26.607	-3.793
Stratospheric ozone depletion	kg CFC11 eq	2.657E-05	5.562	2.517E-05	2.419E-05	-3.894
Fine particulate matter formation	kg PM2.5 eq	1.635E-02	5.212	1.554E-02	1.477E-02	-4.955
Freshwater eutrophication	kg P eq	2.310E-03	10.052	2.099E-03	1.913E-03	-8.861
Marine eutrophication	kg N eq	8.733E-03	5.714	8.261E-03	7.947E-03	-3.801
Human carcinogenic toxicity	kg 1,4-DCB eq	4.129E-01	11.324	3.709E-01	3.355E-01	-9.544
Land use	m^2a crop eq	5.066	5.498	4.802	4.626	-3.665

Table 4.14: Sensitivity analysis: Product selectivity

Component	**GWP LB**	**GWP UB**	**SOD LB**	**SOD UB**	**FPMF LB**	**FPMF UB**	**FE LB**	**FE UB**	**ME LB**	**ME UB**	**HCT LB**	**HCT UB**	**LU UB**	**LU UB**
Ammonia	0.196	0.178	0.019	0.018	0.106	0.099	0.132	0.134	0.002	0.002	0.326	0.338	0.007	0.006
Water	0.007	0.007	0.008	0.008	0.019	0.019	0.068	0.076	0.001	0.001	0.053	0.061	0.001	0.001
Glycerol	13.202	13.026	92.712	93.104	42.356	42.874	51.273	56.614	102.238	102.722	44.577	50.167	98.249	98.379
NaOH	0.634	0.052	0.648	0.054	2.333	0.198	3.704	0.343	0.087	0.007	3.032	0.286	0.101	0.008
Compressed air	2.031	1.792	0.954	0.857	11.798	10.684	31.882	31.493	0.376	0.338	53.917	54.285	0.444	0.398
CO_2 from the process	34.828	33.404	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Electricity	1.592	1.531	0.798	0.781	3.749	3.700	17.748	19.107	0.352	0.345	7.085	7.774	0.272	0.266
Steam (LP.HP)	59.141	62.560	7.476	8.049	66.675	72.358	82.192	97.298	2.603	2.804	75.893	91.571	3.397	3.647
Heat replacement	0.672	0.726	0.358	0.394	1.589	1.759	6.609	7.982	0.123	0.135	3.037	3.738	0.105	0.115
Electricity replacement	5.965	6.437	0.356	0.391	0.809	0.895	0.101	0.122	0.004	0.005	0.172	0.211	0.006	0.007
Chemical heat (during conversion)	10.366	11.187	1.477	1.622	3.154	3.492	2.492	3.009	0.061	0.067	10.736	13.215	0.179	0.196
BOF gas prevented from flaring	-28.635	-30.901	-4.806	-5.279	-32.589	-36.080	-96.202	-116.179	-5.848	-6.426	-98.827	-121.647	-2.760	-3.023

Table 4.15: Percentage of component contribution to the total impact of Lowerbound and Upperbound Product selectivity sensitivity case scenario

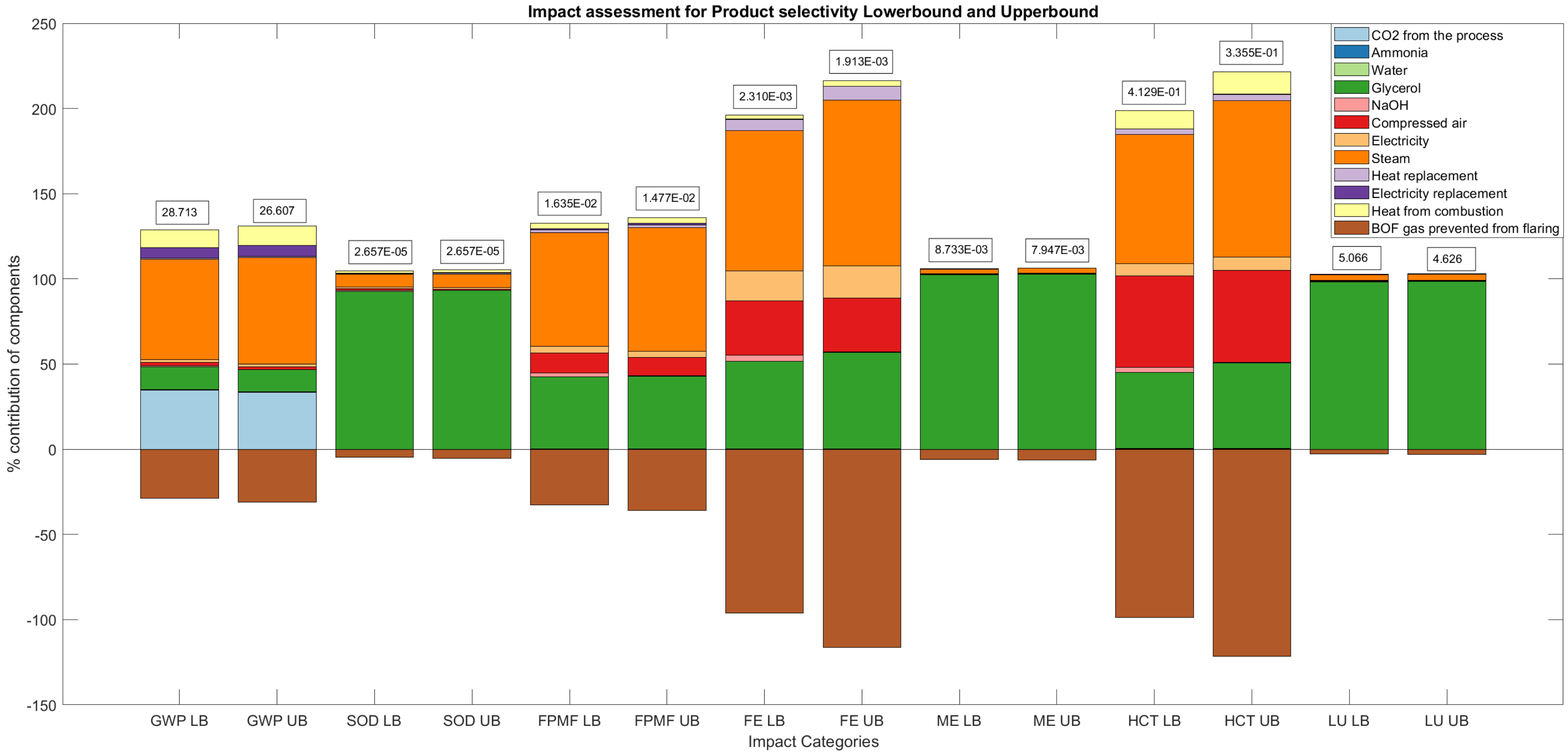

Figure 4.6: Impact assessment for the Product selectivity; LB represents the scenario of Lower Bound Product selectivity varied by -5%, UB represents scenario of Upper Bound Product selectivity varied by +5%; GWP: Global Warming Potential (kg CO_2eq.), SOD: Stratospheric Ozone Depletion (kg CFC11 eq.), FPMF: Fine Particulate Matter Formation (kg PM2.5 eq.), FE: Freshwater Eutrophication (kg Peq.), ME: Marine Eutrophication (kg N eq.), HCT: Human Carcinogenic Toxicity (kg 1,4-DCB), LU: Land Use (m^2 a crop eq.)

Table 4.14 refers to the comparison of impact value between the lower-bound and upper-bound Product selectivity for seven midpoint indicators along with the base case. Product selectivity is also considered one of the main process parameters in its impact assessment study. Varying this process parameter value for the range ±5%, results in the higher accumulation of IPA. As cited by the previous modeling study (Brouwer, 2023), this process parameter variation leads to a decrease in the $NaOH$ requirement for the process. Similar to process parameter VMT_{CO}, this product selectivity also has the inverse proportionate impact results when the process parameter is altered by 5%. The Global warming potential impact category of this process parameter is increasing with the decrease in product selectivity. This is because product selectivity also shows big effects on water consumption and NaOH feed. The major contributor for this process is the steam for both the cases and the contribution percentage ranges are nearly 59-62%. The stratospheric ozone depletion impact category impact value also decreases when the product selectivity is increased, the major contributor is the glycerol. The impact caused only by the glycerol is very high when it is compared with the conventional IPA process. So, optimizing the process to lower the glycerol consumption could drastically lower the ozone depletion impact category value of the process.

The fine particulate matter formation impact category is addressed to prevalent emission-related diseases. The component steam consumption for the process is the major contributor to this midpoint indicator with no direct particulate matter emissions. Steam is the major contributor to this impact category. This higher impact category value for steam is assumed, but the information to prove this is not coherent. Next, the eutrophication impacts cause on the freshwater and the marine environment are assessed by altering the process parameter of product selectivity. The major contribution to the eutrophication of freshwater is the steam used in the system, likewise for marine eutrophication. The glycerol used in extractive distillation is the major contributor to the eutrophication of freshwater. It observed that traces of glycerol can be found in the waste liquid coming out of the system. The values are in minimum but considering the eutrophication potential in minimum values, this is a factor that should be taken into consideration. Finally, the Land use impact category values also change with the change in product selectivity process parameter. Even from analyzing this impact category, it can be claimed that increasing the product selectivity value is the better approach for the lower impact value consideration.

4.4.4. Sensitivity analysis: Dilution rate

Midpoint indicator	Unit	Dilution rate LB	% vary in LB	Basecase	Dilution rate UB	% vary in UB
Global warming potential	kg CO_2 eq	20.464	-26.005	27.656	37.375	35.142
Stratospheric ozone depletion	kg CFC11 eq	1.720E-05	-31.665	2.517E-05	3.618E-05	43.743
Fine particulate matter formation	kg PM2.5 eq	9.618E-03	-38.108	1.554E-02	2.319E-02	49.228
Freshwater eutrophication	kg P eq	9.853E-04	-53.059	2.099E-03	3.623E-03	72.606
Marine eutrophication	kg N eq	5.531E-03	-33.047	8.261E-03	1.204E-02	45.745
Human carcinogenic toxicity	kg 1,4-DCB eq	1.733E-01	-53.276	3.709E-01	6.517E-01	75.708
Land use	m^2a crop eq	3.265	-32.007	4.802	6.927	44.252

Table 4.16: Sensitivity analysis: Dilution rate

Component	GWP LB	GWP UB	SOD LB	SOD UB	FPMF LB	FPMF UB	FE LB	FE UB	ME LB	ME UB	HCT LB	HCT UB	LU UB	LU UB
Ammonia	0.213	0.153	0.023	0.014	0.139	0.076	0.239	0.085	0.003	0.002	0.600	0.209	0.008	0.005
Water	0.007	0.007	0.009	0.008	0.022	0.017	0.110	0.057	0.001	0.001	0.088	0.045	0.001	0.001
Glycerol	12.066	13.798	93.493	92.635	46.893	40.625	78.308	44.475	105.154	100.875	69.195	38.425	99.298	97.751
NaOH	0.453	0.275	0.510	0.269	2.019	0.930	4.422	1.335	0.070	0.036	3.679	1.086	0.079	0.042
Compressed air	2.011	2.001	1.042	0.898	14.157	10.667	52.773	26.068	0.420	0.350	90.708	43.811	0.486	0.416
CO_2 from the process	43.167	29.630	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Electricity	1.993	1.321	1.102	0.633	5.685	2.855	37.126	12.222	0.496	0.276	15.062	4.848	0.376	0.215
Steam (LP.HP)	56.410	61.752	7.867	7.462	77.038	63.891	131.008	71.228	2.794	2.566	122.948	65.360	3.583	3.377
Heat replacement	0.944	0.517	0.555	0.263	2.701	1.120	15.496	4.214	0.194	0.089	7.236	1.924	0.163	0.077
Electricity replacement	8.370	4.583	0.552	0.262	1.375	0.570	0.237	0.065	0.007	0.003	0.409	0.109	0.009	0.004
Chemical heat (during conversion)	14.545	7.964	2.286	1.084	5.361	2.224	5.843	1.589	0.096	0.044	25.586	6.803	0.278	0.131
BOF gas prevented from flaring	-40.177	-21.998	-7.440	-3.530	-55.389	-22.976	-225.564	-61.339	-9.234	-4.241	-235.512	-62.620	-4.283	-2.019

Table 4.17: Percentage of component contribution to the total impact of Lowerbound and Upperbound Dilution rate sensitivity case scenario

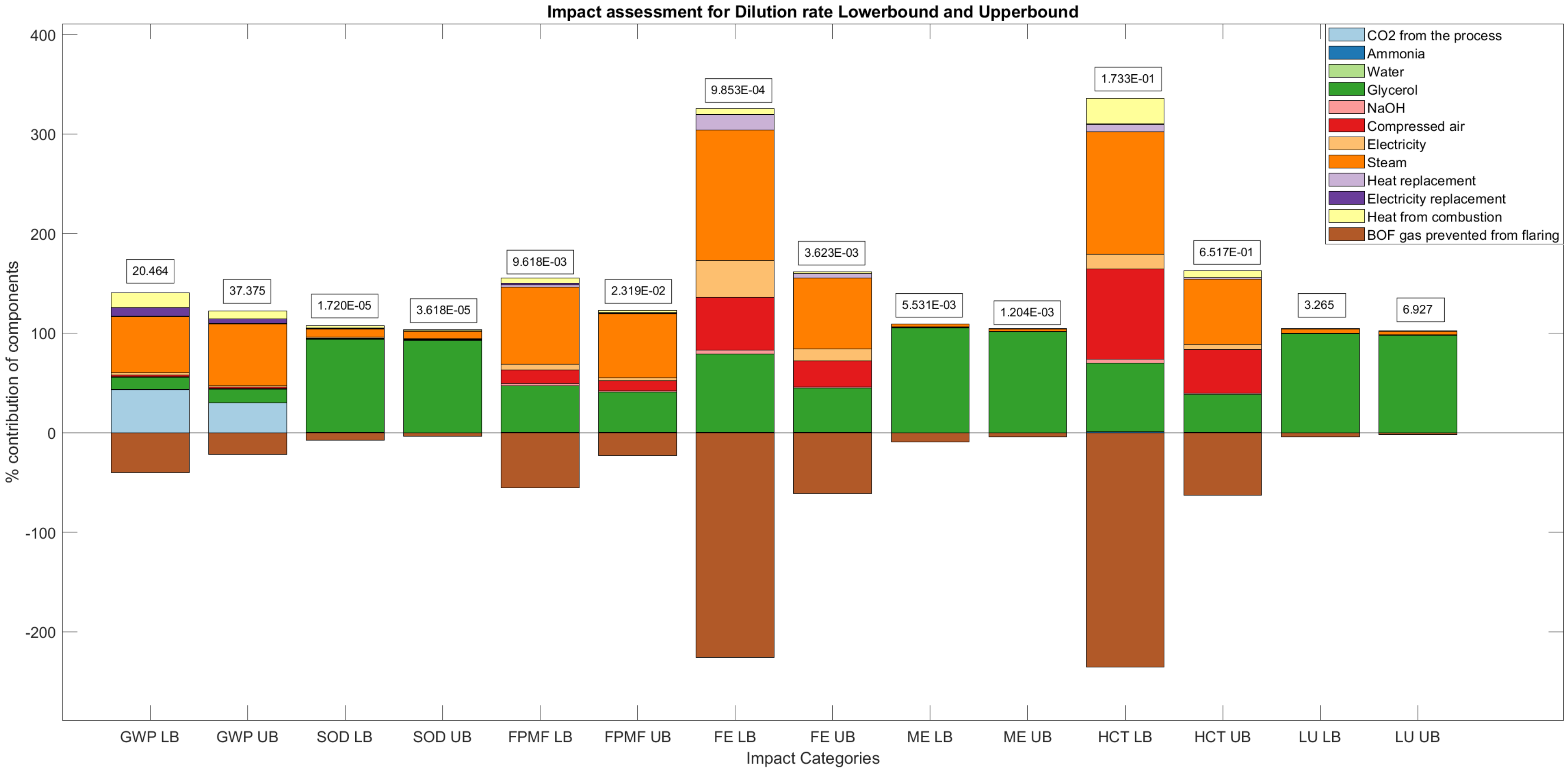

Figure 4.7: Impact assessment for the Dilution rate; LB represents the scenario of Lower Bound Dilution rate varied by -30%, UB represents scenario of Upper Bound Dilution rate varied by +30%; GWP: Global Warming Potential (kg CO_2eq.), SOD: Stratospheric Ozone Depletion (kg CFC11 eq.), FPMF: Fine Particulate Matter Formation (kg PM2.5 eq.), FE: Freshwater Eutrophication (kg Peq.), ME: Marine Eutrophication (kg N eq.), HCT: Human Carcinogenic Toxicity (kg 1,4-DCB), LU: Land Use (m^2 a crop eq.)

The table 4.16 represents the sensitivity case for the Dilution rate process parameter. This Dilution rate is one of the most influential process parameters, which shows lower impact values in all the midpoint indicator categories. This category shows sensitivity for both the lowering and increasing the dilution rate of the process. The dilution rate is varied by ±30% The broth outflow is less in the low dilation rate (-30%), and the BOF gas conversion leads to a higher IPA titer. The dilution rate lower bound is the most ideal situation since the utility consumption is significantly lower when compared with the base case and the upper bound (+30%). Initially, the GWP midpoint indicator results are obtained for the dilution rate scenarios. The impact value for the lower bound is 20.464 kg CO_2 eq. and for the upper bound is 37.375 kg CO_2 eq. The steam is a huge contributor to the sensitivity cases, which contributes about $\approx$ 56% of the total impact values for the lower bound case. The other components' contribution is added up to the total impact value, and the deduction of value for the emission credit by preventing the BOF gas from flaring. For the upper bound value, the contribution of steam is $\approx$ 61%. The change in value for the contribution is explained in the previous parts of the report. The second most influential component to the total impact value is the contribution of carbon dioxide emissions. Lowering the utility usage in the lower bound Dilution rate sensitivity case and optimizing the process can further lower the environmental effects for the impact category of global warming potential.

The stratospheric ozone depletion is the next impact category for the impact assessment. Even in this category, the minimal value is by the lower bound dilution rate. The huge contributional impact is caused by the glycerol followed by the steam. Comparing the lowest obtained impact value for the BOF gas fermentation process with the fossil IPA production method, still the impact value is exceptionally higher for the BOF gas-IPA production method. The impact category value for 1 kg of steam is lower, but considering the total kg of steam utilization this impact value contributes more to the overall process. There is no involvement of ODS present in the process, Next the fine particulate matter formation impact category is interpreted. The lower bound dilution rate appears to be the ideal process to produce IPA, as it has the lowest impact value. This lowest impact value is also contributed by the utilization of steam followed by glycerol and compressed air for the overall process. The value is considerably high, but there are no direct particulate matter emitting components in this process. It may be due to the indirect effects.

Next, the eutrophication of freshwater and marine was assessed, and steam is the major contributor to the freshwater eutrophication and glycerol for the marine eutrophication midpoint indicators. For the eutrophication, the steam utility contribution percentage of 130% for the lower bound and 71% for the upper bound case. The major change in impact category value is due to the emission credit preventing the BOF from flaring process. But this emission credit is constant for all the sensitivity and base cases. So, the next major contributor would be steam consumption. For the impact category of human carcinogenic toxicity, the value is measured in kg 1,4 dichlorobenzene (DCB). For this impact category, the values have appeared to be very high when compared with the conventional IPA production method and this major contribution is by the use of the glycerol for the distillation process to obtain pure IPA. It's likely achievable to get a negative impact value by finding an entertainer with a lower impact value. The last impact category of Land use is considered, and the values of glycerol dominate the total impact value of the process. The impact value of glycerol is about 3.242 m^2 crop eq. and the total value for the lower bound is 3.265 m^2 crop eq. The Ecoinvent database's glycerol component comes from the esterification of rapeseed oil. This might increase the impact value if it is compared with the glycerol via fermentation.

4.4.5. Sensitivity analysis: Extractive distillation Glycerol mole fraction

Midpoint indicator	Unit	Gly mol frac. LB	% vary in LB	Basecase	Gly mol frac. UB	% vary in UB
Global warming potential	kg CO_2 eq	27.653	-0.011	27.656	28.184	1.909
Stratospheric ozone depletion	kg CFC11 eq	1.860E-05	-26.103	2.517E-05	3.260E-05	29.519
Fine particulate matter formation	kg PM2.5 eq	1.414E-02	-9.009	1.554E-02	1.730E-02	11.326
Freshwater eutrophication	kg P eq	1.808E-03	-13.864	2.099E-03	2.504E-03	19.295
Marine eutrophication	kg N eq	5.862E-03	-29.040	8.261E-03	1.096E-02	32.672
Human carcinogenic toxicity	kg 1,4-DCB eq	3.124E-01	-15.772	3.709E-01	4.560E-01	22.944
Land use	m^2a crop eq	3.467	-27.801	4.802	6.305	31.299

Table 4.18: Sensitive analysis: Glycerol mole fraction

Component	GWP LB	GWP UB	SOD LB	SOD UB	FPMF LB	FPMF UB	FE LB	FE UB	ME LB	ME UB	HCT LB	HCT UB	LU UB	LU UB
Ammonia	0.194	0.181	0.027	0.014	0.117	0.091	0.161	0.111	0.003	0.002	0.412	0.268	0.009	0.005
Water	0.007	0.007	0.012	0.006	0.021	0.017	0.086	0.060	0.002	0.001	0.070	0.046	0.002	0.001
Glycerol	9.297	16.834	89.744	94.697	33.214	50.107	44.438	59.219	103.314	101.944	39.959	50.520	97.371	98.801
NaOH	0.351	0.327	0.492	0.268	1.437	1.117	2.521	1.732	0.069	0.035	2.134	1.391	0.078	0.041
Compressed air	1.600	2.325	1.032	0.875	10.349	12.532	30.907	33.062	0.426	0.337	54.061	54.866	0.492	0.401
CO_2 from the process	33.711	34.921	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Electricity	1.549	1.587	1.067	0.637	4.063	3.467	21.257	16.023	0.491	0.274	8.776	6.276	0.372	0.214
Steam (LP.HP)	65.367	55.666	11.357	5.636	82.059	58.222	111.803	70.072	4.128	1.916	106.776	63.490	5.284	2.522
Heat replacement	0.698	0.685	0.511	0.292	1.837	1.502	8.446	6.099	0.183	0.098	4.013	2.750	0.154	0.085
Electricity replacement	6.194	6.077	0.509	0.291	0.935	0.764	0.129	0.093	0.006	0.003	0.227	0.155	0.009	0.005
Chemical heat (during conversion)	10.763	10.561	2.107	1.205	3.647	2.981	3.184	2.299	0.091	0.049	14.190	9.721	0.262	0.144
BOF gas prevented from flaring	-29.732	-29.172	-6.859	-3.922	-37.678	-30.801	-122.933	-88.771	-8.713	-4.659	-130.619	-89.485	-4.034	-2.218

Table 4.19: Percentage of component contribution to the total impact of Lowerbound and Upperbound glycerol mole fraction sensitivity case scenario

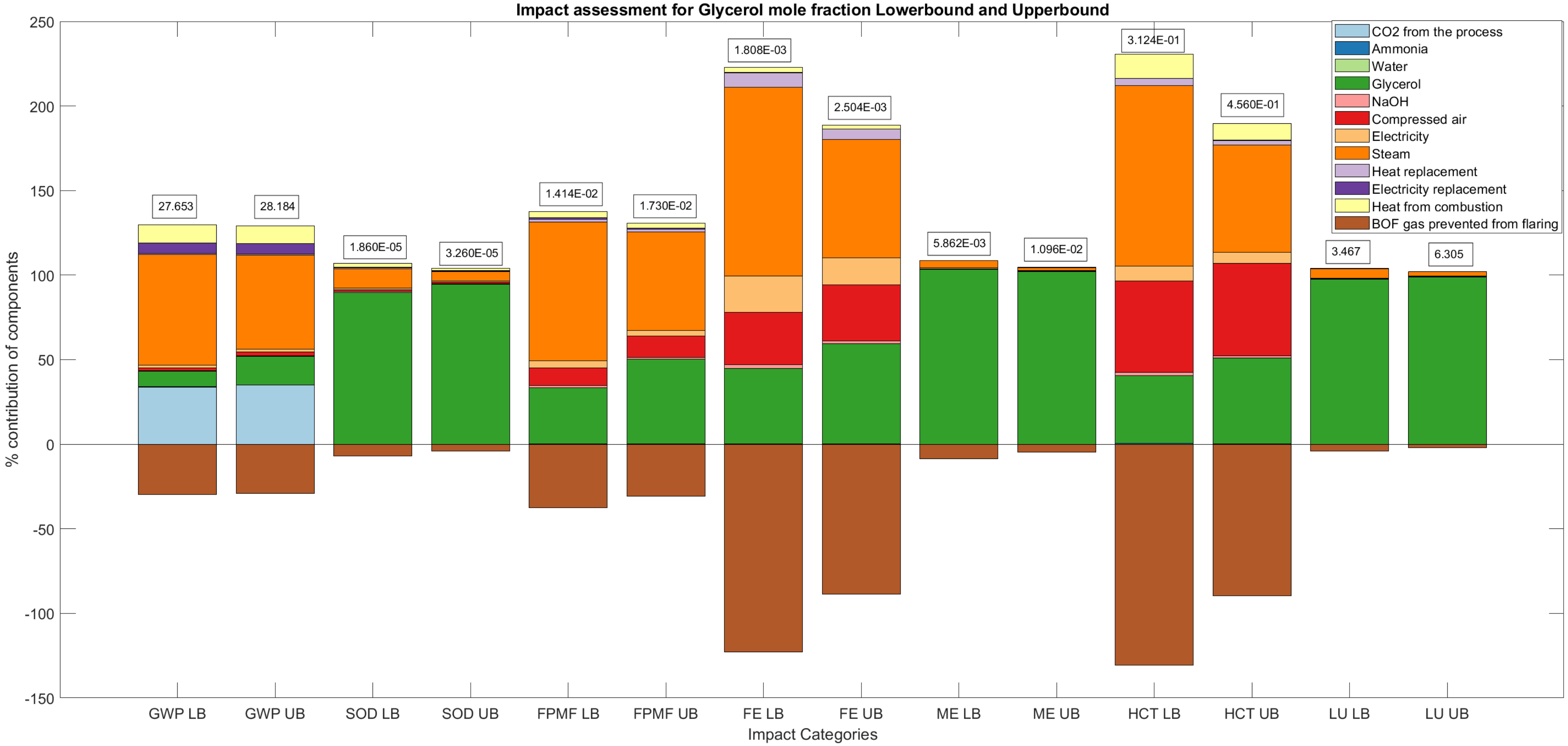

Figure 4.8: Impact assessment for the Glycerol mole fraction; LB represents the scenario of Lower Bound Glycerol mole fraction varied by -30%, UB represents scenario of Upper Bound GLycerol mole fraction varied by +30%; GWP: Global Warming Potential (kg CO_2eq.), SOD: Stratospheric Ozone Depletion (kg CFC11 eq.), FPMF: Fine Particulate Matter Formation (kg PM2.5 eq.), FE: Freshwater Eutrophication (kg Peq.), ME: Marine Eutrophication (kg N eq.), HCT: Human Carcinogenic Toxicity (kg 1,4-DCB), LU: Land Use (m^2 a crop eq.)

The table 4.18 represents the sensitivity case for the Glycerol mole fraction process parameter. The impact study interpretation was performed for the process parameter of glycerol mole fraction during extractive distillation by varying ±30%. Lowering this mole fraction value by -30% results in a big increase in the IPA titer. The impact assessment study shows a significant change when the contribution to the particular impact category is varied. For the global warming potential, the value for the lower bound is 27.653 kg CO_2 eq., and for the upper bound is 28.184 kg CO_2 eq. These GWP values for both these cases are comparatively similar when compared with the base, but very high compared to the traditional IPA method. The change in impact values is much observed because the major contributor to the impact value is the steam and not glycerol. However, in the midpoint category of stratospheric ozone depletion, a huge difference in the impact values can be observed when compared with the base case. This difference in this indicator is due to the major contributor glycerol. Thus lowering the glycerol mole fractions lowers the glycerol usage and a lesser impact value can be obtained. But if the glycerol mole fraction is increased, there is a huge spike in the impact value considering the base case. Increasing the glycerol mole fraction elevates the impact value of SOD.

The fine particulate matter formation is the next impact category considered. In this impact category, the lower bound glycerol mole fraction lowers the glycerol usage resulting in a lesser impact value. As already discussed, the change in contributing component utilization results is the total impact value of the process. For the freshwater and marine eutrophication impact category, steam is the main contributor to the freshwater category, with a much smaller impact on freshwater eutrophication. The effects of marine eutrophication are also lessened due to the decreased use of glycerol for the lower-bound cases. In the upper-bound scenario, the higher freshwater eutrophication effect is caused by the steam, and marine eutrophication is by the glycerol. Human carcinogenic toxicity is the only impact category that focuses on human health. The change in the glycerol mole fraction by -30% significantly diminished the overall impact of this category. Raising the glycerol mole fraction by 30% leads to increased carcinogenic toxicity effects. Finally, for the land use impact category, the lowest impact value is obtained by lowering the glycerol mole fraction by -30%. The production of glycerol mainly affects land use impact. The land use impact value is decreased to 3.467 m^2 crop eq. in the lower bound, as there is less demand for glycerol. The increase in impact for the upper bound reflects the increased usage of glycerol for the extractive distillation process.

4.4.6. Sensitivity analysis: Temperature Offgas condenser

Midpoint indicator	Unit	Offgas condenser LB	% vary in LB	Basecase	Offgas condenser UB	% vary in UB
Global warming potential	kg CO_2 eq	27.518	-0.499	27.656	27.397	-0.937
Stratospheric ozone depletion	kg CFC11 eq	2.520E-05	0.119	2.517E-05	2.510E-05	-0.278
Fine particulate matter formation	kg PM2.5 eq	1.546E-02	-0.515	1.554E-02	1.534E-02	-1.287
Freshwater eutrophication	kg P eq	2.088E-03	-0.524	2.099E-03	2.029E-03	-3.335
Marine eutrophication	kg N eq	8.260E-03	-0.012	8.261E-03	8.239E-03	-0.266
Human carcinogenic toxicity	kg 1,4-DCB eq	3.686E-01	-0.620	3.709E-01	3.634E-01	-2.022
Land use	m^2a crop eq	4.801	-0.021	4.802	4.789	-0.271

Table 4.20: Sensitivity analysis: Temperature Offgas condenser

Component	GWP LB	GWP UB	SOD LB	SOD UB	FPMF LB	FPMF UB	FE LB	FE UB	ME LB	ME UB	HCT LB	HCT UB	LU UB	LU UB
Ammonia	0.186	0.187	0.019	0.019	0.102	0.103	0.133	0.137	0.002	0.002	0.333	0.337	0.007	0.007
Water	0.007	0.007	0.008	0.008	0.019	0.019	0.072	0.075	0.001	0.001	0.057	0.059	0.001	0.001
Glycerol	13.062	13.094	92.866	92.970	42.473	42.725	53.793	55.241	102.500	102.560	47.347	47.938	98.304	98.345
NaOH	0.336	0.337	0.348	0.348	1.254	1.263	2.083	2.142	0.047	0.047	1.726	1.750	0.054	0.054
Compressed air	1.890	1.893	0.898	0.899	11.129	11.188	31.465	32.290	0.355	0.355	53.872	54.506	0.418	0.418
CO_2 from the process	33.945	34.054	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Electricity	1.575	1.380	0.799	0.699	3.759	3.305	18.618	16.710	0.353	0.308	7.524	6.658	0.272	0.238
Steam (LP.HP)	61.134	61.237	7.823	7.826	69.855	70.215	90.094	92.450	2.726	2.726	84.221	85.208	3.551	3.550
Heat replacement	0.702	0.705	0.378	0.380	1.680	1.694	7.313	7.524	0.130	0.130	3.401	3.451	0.111	0.111
Electricity replacement	6.224	6.252	0.377	0.378	0.855	0.862	0.112	0.115	0.005	0.005	0.192	0.195	0.006	0.006
Chemical heat (during conversion)	10.816	10.864	1.560	1.565	3.336	3.362	2.757	2.837	0.065	0.065	12.026	12.200	0.189	0.189
BOF gas prevented from flaring	-29.877	-30.009	-5.077	-5.092	-34.463	-34.736	-106.440	-109.521	-6.183	-6.199	-110.700	-112.303	-2.913	-2.920

Table 4.21: Percentage of component contribution to the total impact of Lowerbound and Upperbound temperature offgas condenser sensitivity case scenario

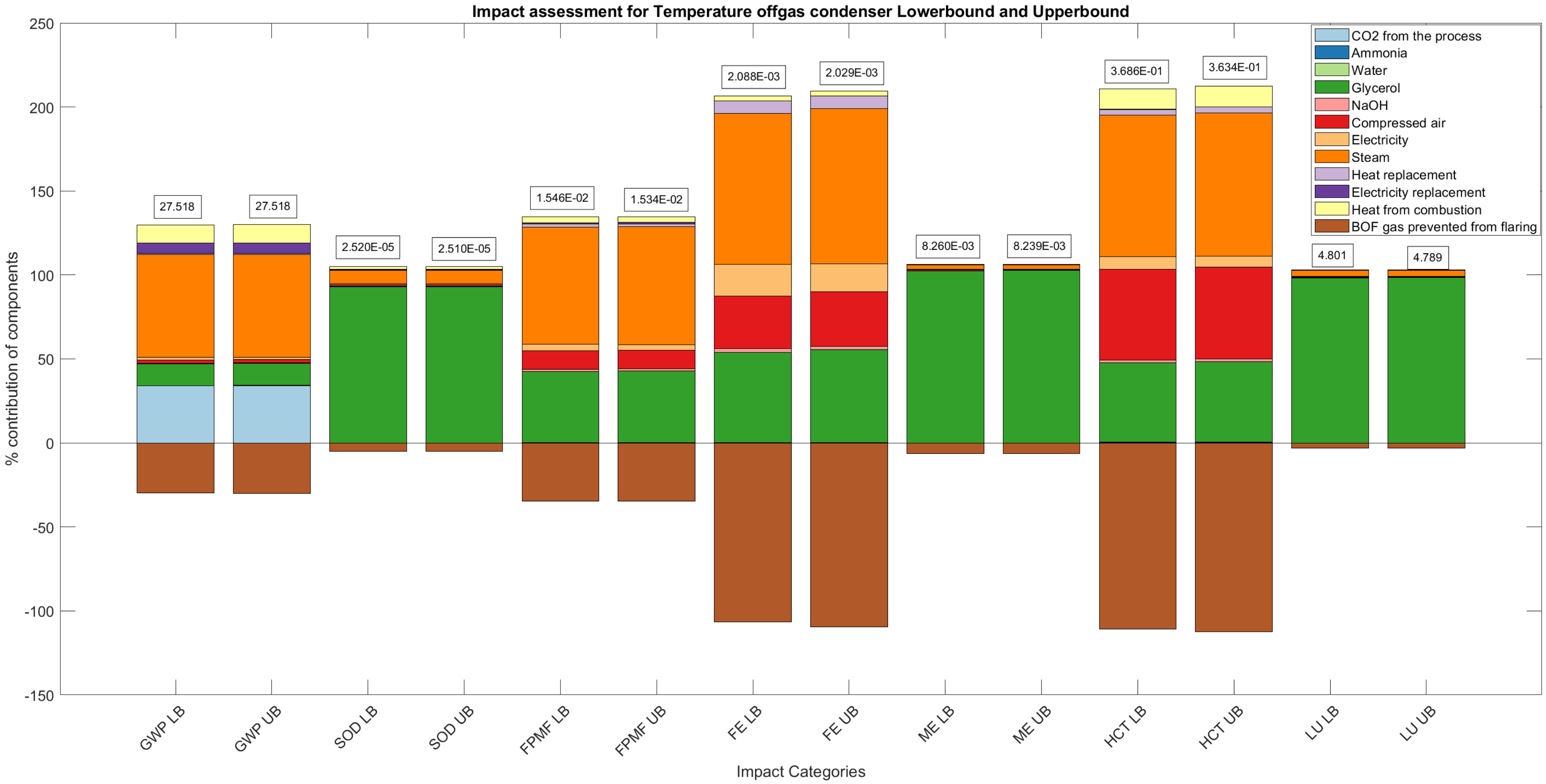

Figure 4.9: Impact assessment for the Temperature Offgas condenser; LB represents the scenario of Lower Bound Temperature offgas condenser varied by -1.80%, UB represents scenario of Upper Bound Temperature offgas condenser varied by +11.50%; GWP: Global Warming Potential (kg CO_2eq.), SOD: Stratospheric Ozone Depletion (kg CFC11 eq.), FPMF: Fine Particulate Matter Formation (kg PM2.5 eq.), FE: Freshwater Eutrophication (kg Peq.), ME: Marine Eutrophication (kg N eq.), HCT: Human Carcinogenic Toxicity (kg 1,4-DCB), LU: Land Use (m^2 a crop eq.)

The table 4.20 represents the sensitivity case for the Temperature Offgas condenser process parameter. The temperature of the offgas condenser process parameter is not a critical parameter for the process. This process parameter parameter is varied by -1.80% and 11.50%. Increasing the off-gas condenser temperature results in pure IPA production. This also results in lowering the usage of utilities like steam and electricity consumption (Brouwer, 2023). It was expected by Brouwer (2023) that increasing the temperature of off-gas could increase the technical performance. Similarly for the impact category of global warming potential, increasing the off-gas temperature leads to the lower impact value but the difference between the lowering temperature is not very high. The difference in value is negligible. The major contributor is the steam for the GWP impact values followed by the carbon dioxide emissions from the process. The stratospheric ozone depletion does not show any change in values by varying the temperature of the off-gas. The major reason for this no variation is the major contributor to the impact category. Glycerol is the major contributor to this value. The process parameter of off-gas condenser temperature does not cause any effect on the extractive distillation part and the glycerol usage for the process remains unchanged. The impact category of fine particulate matter formation is considered. In this, the steam is the major contributor, and increasing the temperature of the off-gas condenser could lower the electricity and steam consumption which results in the lower impact values for the upper bound process parameter. The difference values are very minimal.

Next, the eutrophication of freshwater and marine is considered. In this category both the lower bound and upper bound impact values do not have a difference in values. Very minimal differences in values are only observed. Varying the temperature of the system does have a significant effect on these case scenarios. The major contributors to freshwater eutrophication are the steam and glycerol for marine eutrophication. The human carcinogenic toxicity indicator values appear to be the same for both the increase and decrease of the temperature value. the change in value is very negligible and this value is contributed majorly by the glycerol. Lastly, the land use impact category value remains the same for the sensitivity cases, and the major contributor to this impact category is glycerol usage. This impact assessment implies that altering the temperature of this off-gas condenser does contribute much to lowering the environmental impact value.

4.4.7. Sensitivity analysis: Anaerobic waste conversion fraction

Midpoint indicator	Unit	Anaerobic waste conv. LB	% vary in LB	Basecase	Anaerobic waste conv. UB	% vary in UB
Global warming potential	kg CO_2 eq	27.639	-0.061	27.656	27.337	-1.153
Stratospheric ozone depletion	kg CFC11 eq	2.520E-05	0.119	2.517E-05	2.510E-05	-0.278
Fine particulate matter formation	kg PM2.5 eq	1.553E-02	-0.064	1.554E-02	1.534E-02	-1.287
Freshwater eutrophication	kg P eq	2.063E-03	-1.715	2.099E-03	2.097E-03	-0.095
Marine eutrophication	kg N eq	8.261E-03	0.000	8.261E-03	8.256E-03	-0.061
Human carcinogenic toxicity	kg 1,4-DCB eq	3.581E-01	-3.451	3.709E-01	3.773E-01	1.726
Land use	m^2a crop eq	4.802	0.000	4.802	4.798	-0.083

Table 4.22: Sensitivity analysis: Anaerobic waste conversion fraction

Component	GWP LB	GWP UB	SOD LB	SOD UB	FPMF LB	FPMF UB	FE LB	FE UB	ME LB	ME UB	HCT LB	HCT UB	LU UB	LU UB
Ammonia	0.186	0.188	0.019	0.019	0.102	0.103	0.135	0.133	0.002	0.002	0.343	0.325	0.007	0.007
Water	0.007	0.007	0.008	0.008	0.019	0.019	0.073	0.072	0.001	0.001	0.059	0.056	0.001	0.001
Glycerol	13.004	13.146	92.798	92.972	42.267	42.804	54.430	53.563	102.480	102.538	48.736	46.251	98.269	98.354
NaOH	0.335	0.338	0.348	0.348	1.248	1.264	2.108	2.075	0.047	0.047	1.777	1.686	0.054	0.054
Compressed air	1.726	2.057	0.823	0.973	10.157	12.132	29.198	33.889	0.326	0.384	50.855	56.922	0.383	0.452
CO_2 from the process	33.116	34.847	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Electricity	1.525	1.589	0.777	0.802	3.638	3.799	18.320	18.589	0.343	0.354	7.532	7.370	0.265	0.273
Steam (LP.HP)	62.185	60.043	7.987	7.643	71.024	68.699	93.139	87.544	2.785	2.661	88.573	80.285	3.627	3.467
Heat replacement	0.699	0.706	0.378	0.379	1.672	1.694	7.399	7.283	0.130	0.130	3.501	3.323	0.111	0.111
Electricity replacement	6.197	6.265	0.376	0.377	0.851	0.862	0.113	0.112	0.005	0.005	0.198	0.188	0.006	0.006
Chemical heat (during conversion)	10.769	10.888	1.559	1.562	3.320	3.362	2.790	2.746	0.065	0.065	12.380	11.750	0.189	0.189
BOF gas prevented from flaring	-29.747	-30.075	-5.073	-5.083	-34.297	-34.737	-107.706	-106.004	-6.182	-6.186	-113.953	-108.156	-2.912	-2.915

Table 4.23: Percentage of component contribution to the total impact of Lowerbound and Upperbound anaerobic waste conversion sensitivity case scenario

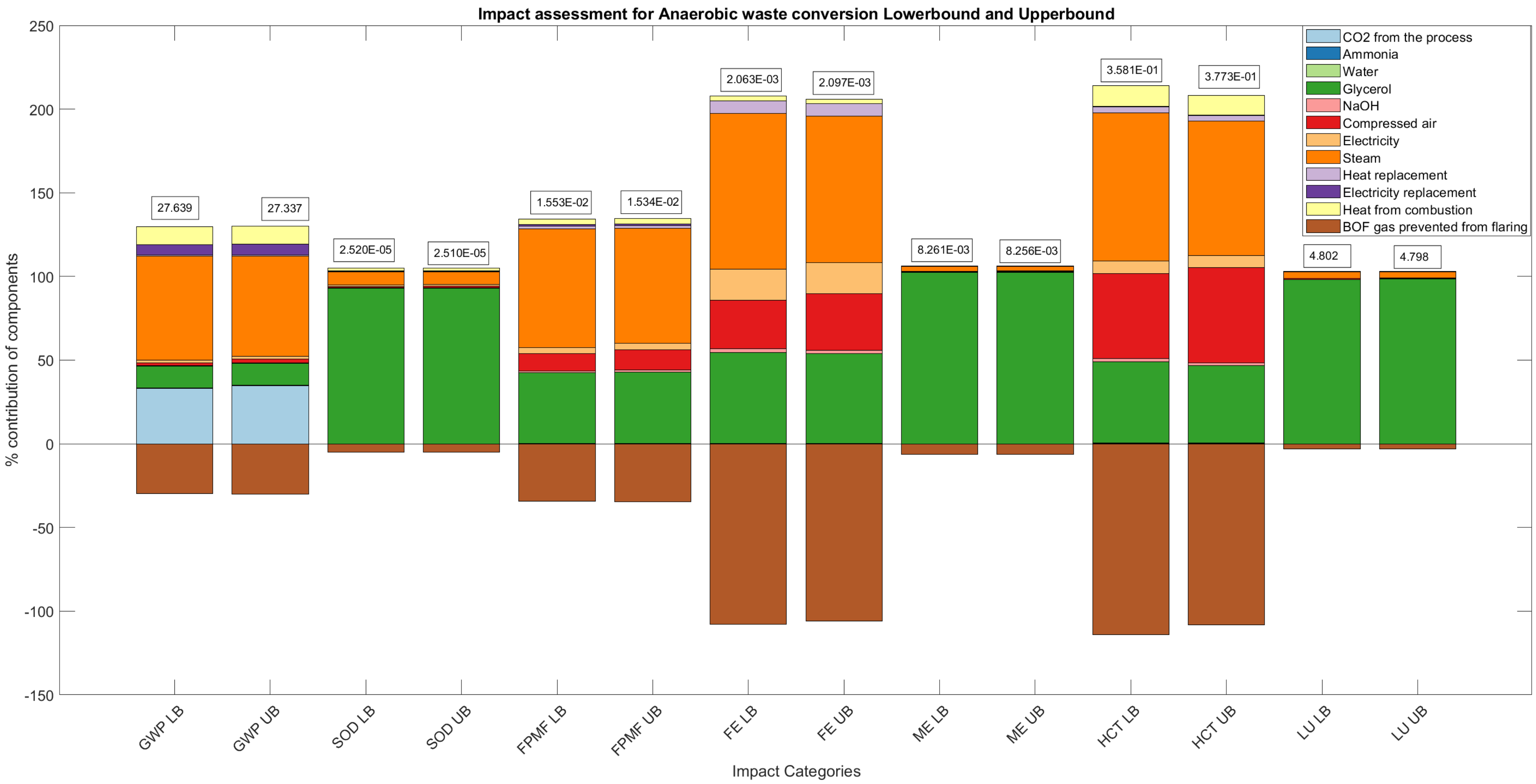

Figure 4.10: Impact assessment for the Anaerobic waste conversion; LB represents the scenario of Lower Bound Anaerobic waste conversion varied by -10%, UB represents scenario of Upper Bound Anaerobic waste conversion varied by +10%; GWP: Global Warming Potential (kg CO_2eq.), SOD: Stratospheric Ozone Depletion (kg CFC11 eq.), FPMF: Fine Particulate Matter Formation (kg PM2.5 eq.), FE: Freshwater Eutrophication (kg Peq.), ME: Marine Eutrophication (kg N eq.), HCT: Human Carcinogenic Toxicity (kg 1,4-DCB), LU: Land Use (m^2 a crop eq.)

The table 4.22 represents the sensitivity case for the Anaerobic waste conversion fraction process parameter. The anaerobic waste conversion is the process parameter that has the least effect on the process (Brouwer, 2023). Increasing the waste conversion fraction appears to lower the impact on the process. This minimal difference in value can be seen in the impact category of global warming potential. The major contributor to this impact category is steam, which consumption is decreased by increasing the waste conversion fraction. Varying the conversion fraction by ±10% does not affect the utilization of major feeds for this process like glycerol, NaOH, water, and so on. So the next impact category of stratospheric ozone depletion values shows no huge difference in values for varying the waste conversion fraction even when compared with the base case scenario. The fine particulate matter also exhibits a minimal difference in value. The upper bound (+10%) change has a minimalist lower value when compared with the lower bound.

In the case of freshwater and marine eutrophication, the very minimum change in the impact value is exhibited in the category of freshwater eutrophication, with the lowest impact value for the upper bound. In the case of marine eutrophication, no significant change is observed as the major contributor to this is glycerol, and the freshwater category is the steam. Next, the human carcinogenic toxicity and land use impact category also shows a minute deviation in values. It can be implied that increasing the waste conversion fraction by 10% can lower the impact values by a negligible amount.

4.4.8. Sensitivity analysis: Extractive distillation molar reflux ratio

Midpoint indicator	Unit	Molar Reflux Ratio LB	% vary in LB	Basecase	Molar Reflux Ratio UB	% vary in UB
Global warming potential	kg CO_2 eq	26.432	-4.426	27.656	28.745	3.938
Stratospheric ozone depletion	kg CFC11 eq	2.520E-05	0.119	2.517E-05	2.530E-05	0.516
Fine particulate matter formation	kg PM2.5 eq	1.475E-02	-5.084	1.554E-02	1.624E-02	4.505
Freshwater eutrophication	kg P eq	1.970E-03	-6.146	2.099E-03	2.220E-03	5.765
Marine eutrophication	kg N eq	8.295E-03	0.412	8.261E-03	8.274E-03	0.157
Human carcinogenic toxicity	kg 1,4-DCB eq	3.509E-01	-5.392	3.709E-01	3.908E-01	5.365
Land use	m^2a crop eq	4.817	0.312	4.802	4.812	0.208

Table 4.24: Sensitivity analysis: Extractive distillation molar reflux ratio

Component	GWP LB	GWP UB	SOD LB	SOD UB	FPMF LB	FPMF UB	FE LB	FE UB	ME LB	ME UB	HCT LB	HCT UB	LU UB	LU UB
Ammonia	0.196	0.178	0.019	0.019	0.108	0.097	0.142	0.125	0.002	0.002	0.353	0.314	0.007	0.007
Water	0.007	0.007	0.008	0.008	0.020	0.018	0.077	0.067	0.001	0.001	0.061	0.054	0.001	0.001
Glycerol	13.679	12.501	93.413	92.343	44.773	40.412	57.351	50.575	102.679	102.300	50.040	44.651	98.557	98.051
NaOH	0.353	0.322	0.351	0.346	1.326	1.193	2.227	1.958	0.047	0.047	1.830	1.628	0.054	0.054
Compressed air	2.003	1.806	0.915	0.892	11.872	10.575	33.946	29.543	0.360	0.354	57.613	50.736	0.424	0.416
CO_2 from the process	35.691	32.477	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Electricity	1.633	1.488	0.796	0.785	3.924	3.532	19.654	17.284	0.350	0.348	7.874	7.006	0.270	0.268
Steam (LP,HP)	59.072	62.839	7.261	8.355	67.941	71.385	88.624	90.976	2.520	2.922	82.126	85.306	3.285	3.804
Heat replacement	0.730	0.672	0.378	0.376	1.761	1.599	7.750	6.877	0.129	0.129	3.574	3.209	0.111	0.111
Electricity replacement	6.480	10.355	0.377	1.551	0.896	3.175	0.119	2.593	0.005	0.064	0.202	11.345	0.006	0.188
Chemical heat (during conversion)	11.261	5.959	1.560	0.375	3.496	0.814	2.922	0.105	0.064	0.005	12.635	0.181	0.188	0.006
BOF gas prevented from flaring	-31.106	-28.603	-5.077	-5.050	-36.115	-32.801	-112.813	-100.104	-6.157	-6.173	-116.308	-104.430	-2.903	-2.906

Table 4.25: Percentage of component contribution to the total impact of Lowerbound and Upperbound extractive distillation molar reflux ratio sensitivity case scenario

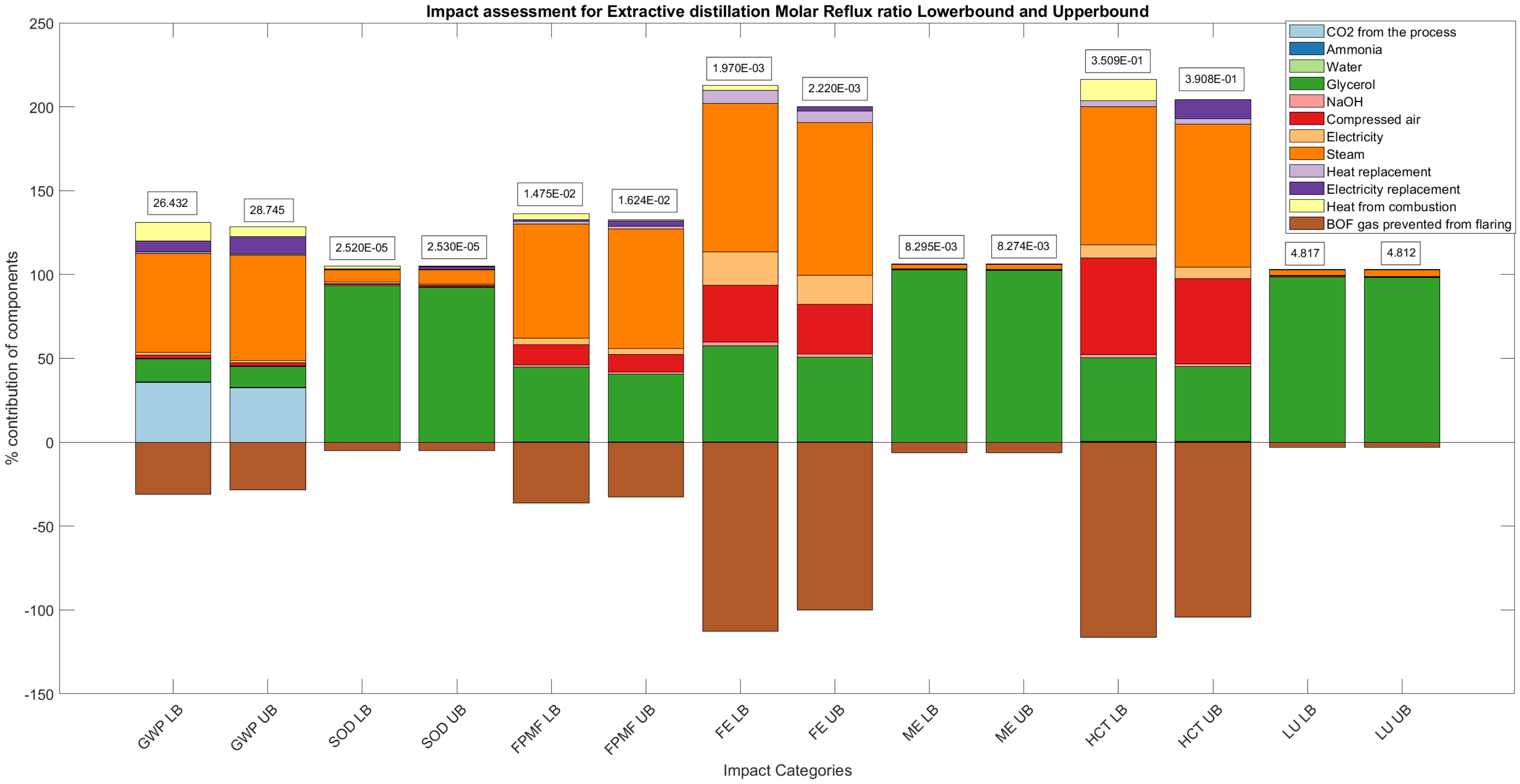

Figure 4.11: Impact assessment for the Extractive distillation molar reflux ratio; LB represents the scenario of Lower Bound Molar reflux ratio varied by -30%, UB represents scenario of Upper Bound Molar reflux raio varied by +30%; GWP: Global Warming Potential (kg CO_2eq.), SOD: Stratospheric Ozone Depletion (kg CFC11 eq.), FPMF: Fine Particulate Matter Formation (kg PM2.5 eq.), FE: Freshwater Eutrophication (kg Peq.), ME: Marine Eutrophication (kg N eq.), HCT: Human Carcinogenic Toxicity (kg 1,4-DCB), LU: Land Use (m^2 a crop eq.)

Table 4.24 represents the sensitivity case for the Extractive distillation molar reflux ratio process parameter. The molar reflux ratio of the extractive distillation for the process is varied by ±30% and the sensitivity cases were performed. This change in the ratio value alters the steam consumption reported (Brouwer, 2023). So the impact categories, for which the major contributor is steam only show a deflection in the impact values. For example, the impact categories like global warming potential, fine particulate matter formation, freshwater eutrophication, and human carcinogenic toxicity show a huge change in values as the major contributor is steam. Lowering the molar reflux ratio of the extractive distillation lowers the impact value for these categories. And for the other categories of stratospheric ozone depletion, marine eutrophication, and land use the major contributor is glycerol. This glycerol usage is not affected by the change in molar reflux ratios. So the overall impact values for these impact categories remain in the range of negligible amounts.

4.4.9. Sensitivity analysis: Biomass filtration liq-liq mole fraction

Midpoint indicator	Unit	Biomass liq-liq mol.frac LB	% vary in LB	Basecase	Biomass liq-liq mol.frac UB	% vary in UB
Global warming potential	kg CO_2 eq	27.604	-0.188	27.656	27.395	-0.944
Stratospheric ozone depletion	kg CFC11 eq	2.520E-05	0.119	2.517E-05	2.510E-05	-0.278
Fine particulate matter formation	kg PM2.5 eq	1.547E-02	-0.450	1.554E-02	1.541E-02	-0.837
Freshwater eutrophication	kg P eq	2.089E-03	-0.476	2.099E-03	2.074E-03	-1.191
Marine eutrophication	kg N eq	8.272E-03	0.133	8.261E-03	8.241E-03	-0.242
Human carcinogenic toxicity	kg 1,4-DCB eq	3.689E-01	-0.539	3.709E-01	3.672E-01	-0.998
Land use	m^2a crop eq	4.807	0.104	4.802	4.790	-0.250

Table 4.26: Sensitivity analysis: Biomass filtration liq-liq mole fraction

Component	GWP LB	GWP UB	SOD LB	SOD UB	FPMF LB	FPMF UB	FE LB	FE UB	ME LB	ME UB	HCT LB	HCT UB	LU UB	LU UB
Ammonia	0.188	0.185	0.019	0.019	0.103	0.101	0.135	0.133	0.002	0.002	0.336	0.331	0.007	0.006
Water	0.339	0.007	0.351	0.008	1.266	0.017	2.103	0.066	0.047	0.001	1.743	0.053	0.054	0.001
Glycerol	13.039	13.092	92.869	92.886	42.487	42.518	53.828	54.049	102.495	102.519	47.376	47.435	98.304	98.313
NaOH	0.008	0.334	0.009	0.345	0.020	1.245	0.078	2.076	0.001	0.046	0.062	1.715	0.001	0.053
Compressed air	1.882	1.901	0.896	0.902	11.107	11.178	31.412	31.720	0.354	0.356	53.780	54.151	0.417	0.419
CO_2 from the process	34.088	33.843	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Electricity	1.564	1.549	0.795	0.784	3.741	3.692	18.535	18.354	0.351	0.346	7.490	7.396	0.271	0.267
Steam (LP.HP)	60.991	61.280	7.819	7.825	69.838	69.931	90.101	90.526	2.725	2.727	84.224	84.380	3.549	3.552
Heat replacement	0.699	0.705	0.378	0.379	1.679	1.686	7.307	7.363	0.129	0.130	3.399	3.415	0.111	0.111
Electricity replacement	6.205	6.252	0.376	0.377	0.854	0.858	0.112	0.113	0.005	0.005	0.192	0.193	0.006	0.006
Chemical heat (during conversion)	10.783	10.865	1.558	1.563	3.332	3.346	2.755	2.776	0.064	0.065	12.017	12.074	0.189	0.189
BOF gas prevented from flaring	-29.785	-30.011	-5.070	-5.089	-34.428	-34.573	-106.366	-107.175	-6.174	-6.197	-110.619	-111.143	-2.909	-2.919

Table 4.27: Percentage of component contribution to the total impact of Lowerbound and Upperbound biomass filtration liq-liq fraction sensitivity case scenario

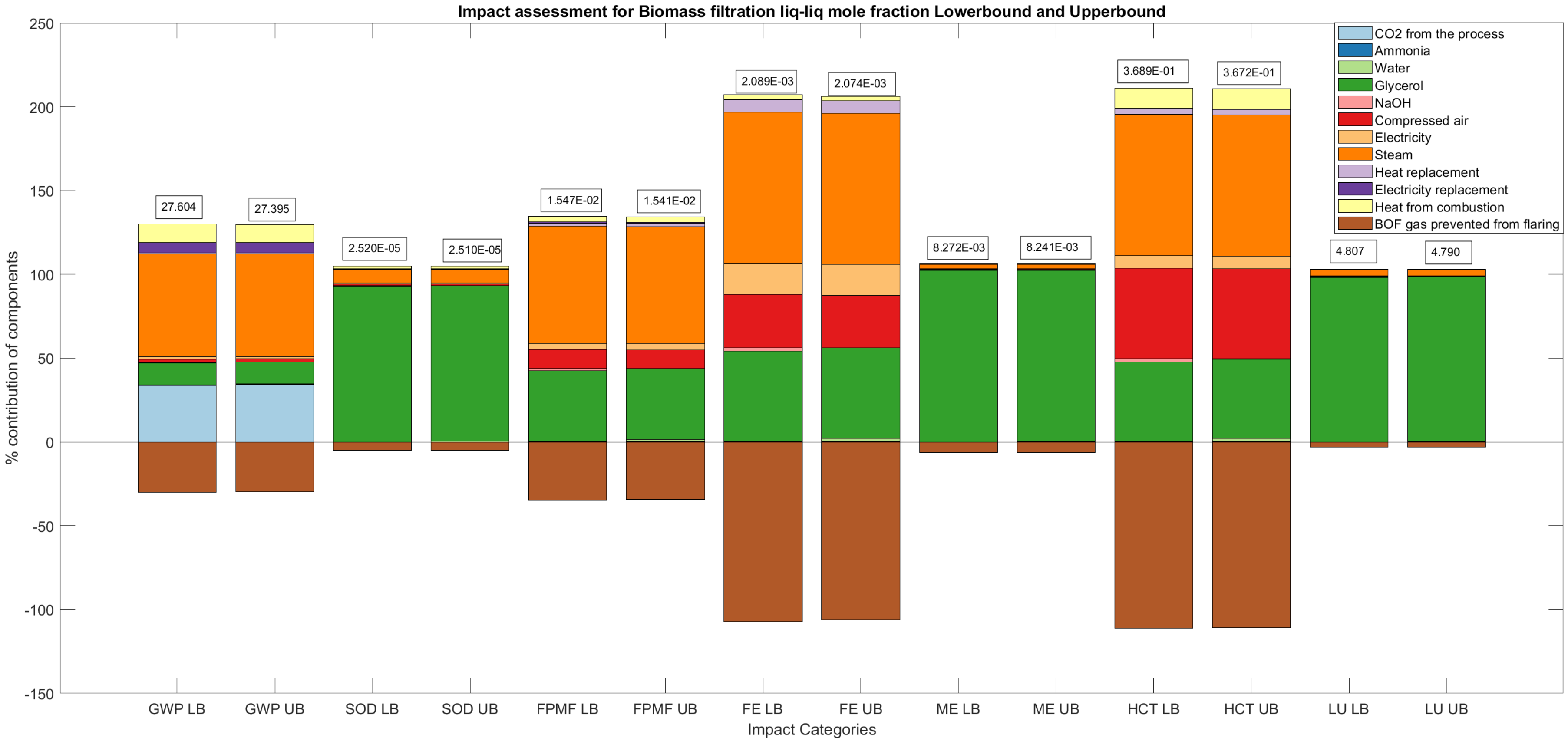

Figure 4.12: Impact assessment for the Biomass filtration liq-liq mole fraction; LB represents the scenario of Lower Bound Biomass filtration liq-liq mole fraction varied by -1%, UB represents scenario of Upper Bound Biomass filtration liq-liq mole fraction varied by +1%; GWP: Global Warming Potential (kg CO_2eq.), SOD: Stratospheric Ozone Depletion (kg CFC11 eq.), FPMF: Fine Particulate Matter Formation (kg PM2.5 eq.), FE: Freshwater Eutrophication (kg Peq.), ME: Marine Eutrophication (kg N eq.), HCT: Human Carcinogenic Toxicity (kg 1,4-DCB), LU: Land Use (m^2 a crop eq.)

The table 4.26 represents the sensitivity case for the Biomass filtration liq-liq mole fraction process parameter. This particular process parameter of biomass filtration liq-lip mole fraction is varied by ±1% (Brouwer, 2023) and the impact assessment is performed. This process parameter does not show any significant change in the impact values for lower bound and upper bound values. Lowering the mole fraction by -1% shows a small change only for the consumption of steam. No other significant changes can be observed. So the impact values for the midpoint categories of GWP, SOD, FPMF, FE, ME, HCT, and LU do not show a huge deflection, and the values also remain in the same range considering the base case scenario.

4.4.10. Sensitivity analysis: Purges

Midpoint indicator	Unit	Broth purge LB	% vary in LB	Basecase	Broth purge UB	% vary in UB
Global warming potential	kg CO_2 eq	27.265	-1.414	27.656	27.679	0.083
Stratospheric ozone depletion	kg CFC11 eq	2.490E-05	-1.073	2.517E-05	2.530E-05	0.516
Fine particulate matter formation	kg PM2.5 eq	1.527E-02	-1.737	1.554E-02	1.557E-02	0.193
Freshwater eutrophication	kg P eq	2.056E-03	-2.049	2.099E-03	2.097E-03	-0.095
Marine eutrophication	kg N eq	8.192E-03	-0.835	8.261E-03	8.299E-03	0.460
Human carcinogenic toxicity	kg 1,4-DCB eq	3.649E-01	-1.618	3.709E-01	3.690E-01	-0.512
Land use	m^2a crop eq	4.763	-0.812	4.802	4.823	0.437

Table 4.28: Sensitivity analysis: Broth purge

Component	GWP LB	GWP UB	SOD LB	SOD UB	FPMF LB	FPMF UB	FE LB	FE UB	ME LB	ME UB	HCT LB	HCT UB	LU UB	LU UB
Ammonia	0.188	0.186	0.019	0.019	0.103	0.101	0.135	0.133	0.002	0.002	0.336	0.333	0.007	0.006
Water	0.005	0.009	0.006	0.010	0.015	0.023	0.055	0.089	0.001	0.002	0.044	0.071	0.001	0.002
Glycerol	13.083	13.044	92.919	92.841	42.668	42.370	54.224	53.801	102.560	102.470	47.460	47.510	98.339	98.285
NaOH	0.339	0.335	0.350	0.346	1.268	1.247	2.114	2.077	0.047	0.046	1.742	1.726	0.054	0.054
Compressed air	1.930	1.847	0.917	0.879	11.402	10.867	32.345	30.801	0.362	0.347	55.068	52.908	0.426	0.409
CO_2 from the process	34.287	33.683	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Electricity	1.568	1.545	0.795	0.785	3.754	3.685	18.656	18.298	0.351	0.346	7.497	7.419	0.271	0.267
Steam (LP.HP)	60.848	61.416	7.779	7.868	69.734	70.102	90.247	90.647	2.711	2.742	83.892	85.016	3.530	3.572
Heat replacement	0.708	0.698	0.382	0.377	1.701	1.669	7.428	7.281	0.131	0.129	3.436	3.398	0.112	0.111
Electricity replacement	6.282	6.188	0.380	0.375	0.866	0.849	0.114	0.112	0.005	0.005	0.194	0.192	0.006	0.006
Chemical heat (during conversion)	10.917	10.754	1.573	1.552	3.377	3.313	2.800	2.745	0.065	0.064	12.148	12.014	0.190	0.188
BOF gas prevented from flaring	-30.155	-29.704	-5.119	-5.053	-34.887	-34.227	-108.117	-105.983	-6.234	-6.154	-111.816	-110.587	-2.936	-2.899

Table 4.29: Percentage of component contribution to the total impact of Lowerbound and Upperbound Broth purge sensitivity case scenario

The table 4.28 represents the sensitivity case for the broth purge process parameter. The broth purge is a process parameter for which the value is varied for about ±30%. The water feed was considered to be more sensitive to the process parameter, and the rest of the components' usage had negligible changes. The impact categories like GWP, SOD, FPMF, FE, ME, HCT, and LU values appear to be slightly lower when compared with the base case. These minimal changes can be observed due to the change in water feed into the system. The rest component impact values differ by a very low significant amount. These negligible minimal changes are because the variation in the process parameter does not affect the most contributing components of steam consumption and glycerol usage.

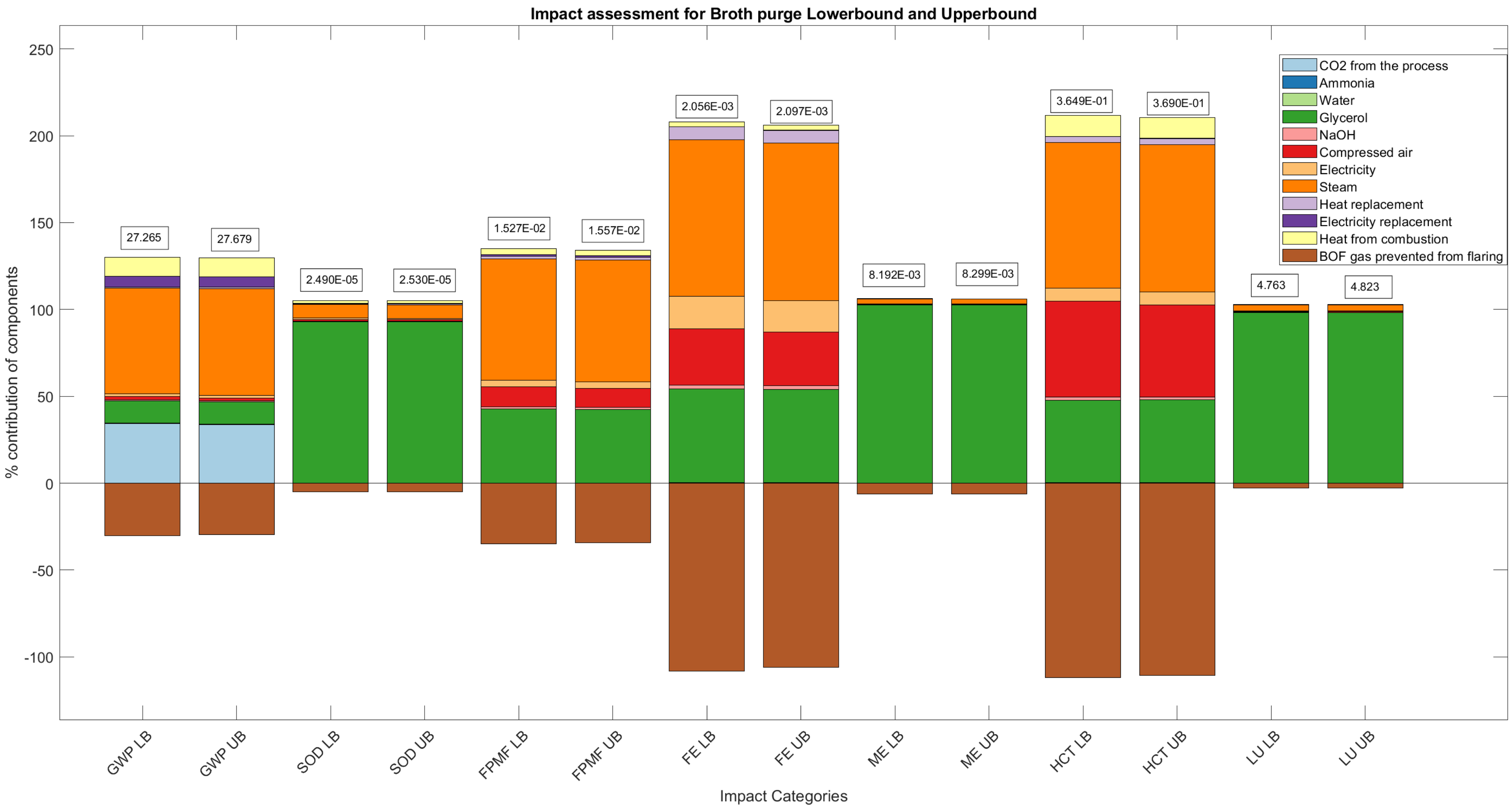

Figure 4.13: Impact assessment for the Broth purge; LB represents the scenario of Lower Bound Broth purge varied by -30%, UB represents scenario of Upper Bound Broth purge varied by +30%; GWP: Global Warming Potential (kg CO_2eq.), SOD: Stratospheric Ozone Depletion (kg CFC11 eq.), FPMF: Fine Particulate Matter Formation (kg PM2.5 eq.), FE: Freshwater Eutrophication (kg Peq.), ME: Marine Eutrophication (kg N eq.), HCT: Human Carcinogenic Toxicity (kg 1,4-DCB), LU: Land Use (m^2 a crop eq.)

Midpoint indicator	Unit	Glycerol purge LB	% vary in LB	Basecase	Glycerol purge UB	% vary in UB
Global warming potential	kg CO_2 eq	26.692	-3.486	27.656	28.137	1.739
Stratospheric ozone depletion	kg CFC11 eq	1.824E-05	-27.533	2.517E-05	3.208E-05	27.453
Fine particulate matter formation	kg PM2.5 eq	1.365E-02	-12.162	1.554E-02	1.714E-02	10.296
Freshwater eutrophication	kg P eq	1.686E-03	-19.676	2.099E-03	2.465E-03	17.437
Marine eutrophication	kg N eq	5.744E-03	-30.468	8.261E-03	1.079E-02	30.614
Human carcinogenic toxicity	kg 1,4-DCB eq	2.875E-01	-22.486	3.709E-01	4.473E-01	20.599
Land use	m^2a crop eq	3.400	-29.196	4.802	6.208	29.279

Table 4.30: Sensitivity analysis: Glycerol purge

Component	GWP LB	GWP UB	SOD LB	SOD UB	FPMF LB	FPMF UB	FE LB	FE UB	ME LB	ME UB	HCT LB	HCT UB	LU UB	LU UB
Ammonia	0.192	0.182	0.026	0.015	0.116	0.092	0.165	0.113	0.003	0.002	0.427	0.274	0.009	0.005
Water	0.007	0.007	0.011	0.007	0.021	0.017	0.089	0.061	0.002	0.001	0.073	0.047	0.002	0.001
Glycerol	9.458	16.598	89.935	94.620	33.774	49.769	46.791	59.197	103.531	101.978	42.634	50.698	97.495	98.784
NaOH	0.347	0.329	0.480	0.273	1.421	1.131	2.581	1.764	0.067	0.036	2.214	1.422	0.076	0.042
Compressed air	1.519	2.273	0.966	0.866	9.822	12.342	30.376	32.769	0.398	0.334	53.838	54.591	0.460	0.397
CO_2 from the process	33.158	34.950	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Electricity	1.539	1.585	1.044	0.645	4.033	3.488	21.852	16.225	0.481	0.278	9.142	6.380	0.364	0.217
Steam (LP.HP)	66.291	55.945	11.346	5.740	83.182	58.946	117.354	71.399	4.124	1.953	113.566	64.944	5.274	2.570
Heat replacement	0.723	0.686	0.522	0.297	1.902	1.515	9.056	6.193	0.186	0.099	4.361	2.803	0.157	0.086
Electricity replacement	6.417	6.087	0.519	0.295	0.968	0.771	0.139	0.095	0.007	0.004	0.247	0.158	0.009	0.005
Chemical heat (during conversion)	11.151	10.578	2.151	1.223	3.777	3.008	3.414	2.335	0.093	0.049	15.418	9.911	0.267	0.146
BOF gas prevented from flaring	-30.802	-29.220	-7.000	-3.981	-39.017	-31.080	-131.817	-90.149	-8.891	-4.734	-141.919	-91.229	-4.113	-2.253

Table 4.31: Percentage of component contribution to the total impact of Lowerbound and Upperbound glycerol purge sensitivity case scenario

The table 4.30 represents the sensitivity case for the glycerol purge process parameter. The glycerol purge is the final process parameter considered for this impact assessment study. This change in the process parameter value by ±30% shows a huge variation in glycerol usage. So the impact categories of global warming potential, fine particulate matter formation, freshwater eutrophication, and human carcinogenic toxicity do not show any huge change in values. Lowering the glycerol purge by ±30% could obtain drastic changes for the midpoint indicators of stratospheric ozone depletion, marine eutrophication, and land use when compared with the base case scenario. This change in the impact values is caused by the main contributor glycerol usage.

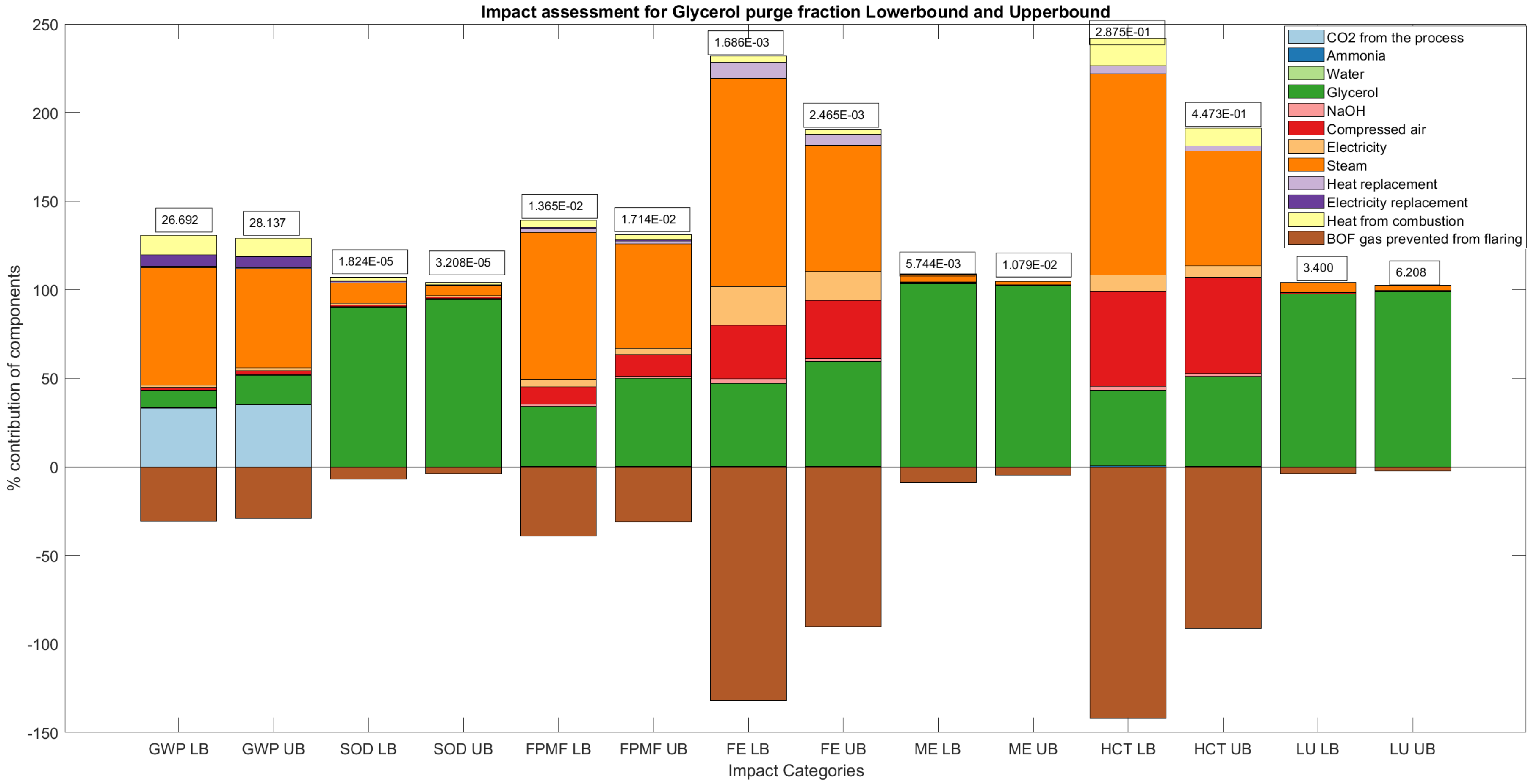

Figure 4.14: Impact assessment for the Glycerol purge; LB represents the scenario of Lower Bound Glycerol purge varied by -30%, UB represents scenario of Upper Bound Glycerol purge varied by +30%; GWP: Global Warming Potential (kg CO_2eq.), SOD: Stratospheric Ozone Depletion (kg CFC11 eq.), FPMF: Fine Particulate Matter Formation (kg PM2.5 eq.), FE: Freshwater Eutrophication (kg Peq.), ME: Marine Eutrophication (kg N eq.), HCT: Human Carcinogenic Toxicity (kg 1,4-DCB), LU: Land Use (m^2 a crop eq.)

4.5. Verification methodology

Based on the methodology explained in the section section 3.9, the calculations were performed for all the case scenarios including the cases from the base case to all the 11 process parameters (lower bound & upper bound for all the process parameters). The procedure is done by calculating the inputs and outputs of the process by normalizing them with reference to the functional unit. All the inputs and units are calculated for per kg of isopropyl alcohol. For example, the inputs like glycerol and electricity total usage are regulated and changed to kg glycerol used/ kg IPA produced, and for kWh electricity consumed/ kg IPA produced. In all the cases, the inputs that are altered by the process parameters like glycerol, water, $NaOH$, NH_3, electricity for the process, and steam consumption were only taken into account.

This selective component modification is because, these components change concerning the variation in the process parameters like CO conversion, product selectivity, and so on. But other components like the electricity, and heat replacement for steel mills, and the emissions from the process can be neglected to undergo this verification methodology to authenticate this methodology procedure. The major reason for not considering the electricity and heat replacement is because these replacements can be related directly based on the BOF gas usage in the steel mill. This BOF gas feedstock usage does not vary for different process parameters, and the calculations for the replacement consider only 1 kg of IPA production. So, no change in values between the base case and the sensitivity cases can be observed because both these assessments are for 1 kg of IPA. Secondly, emissions like wastewater, CO_2, and N_2 are not considered, because the 7 midpoint indicator category does not include the category that majorly focuses the water consumption, so the wastewater emission is neglected. The N_2 stays inert in the environment. The impacts caused by the emissions cannot be accounted for in the total impact assessment. The CO_2 is emitted along with the main product and varies accordingly with the outputs of the total process.

Then the impact assessment for the base case scenario is performed using the SimaPro tool and the midpoint indicator category impact value for the components mentioned above were collected. Then the component usage for both cases (scenarios varying process parameters) was interpreted and the percentage change in the component usage for both the lower bound and upper bound were calculated. Then the data collected for the base case midpoint indicator value is varied with the same percentage change. Then predicted values for the process parameters can be performed with this method. The impact assessment for these sensitivity cases was also performed using the SimaPro tool. The main objective of this verification method is to minimize the usage of the SimaPro tool if the impact assessment has to be performed for the sensitivity analysis cases for the same process. The results of this comparison between the predicted and calculated values are coherent and the maximum variation between these values is observed to be in the range of 1E-05 to 1E-07. If the values exceed this range then this method is not effective and cannot be utilized for the assessments.

The verification methodology for all the process parameter, the % change in the values for the impact categories when comparing the predicted values and the calculated values are in the range of 2E-06 % to 1E-05 (negligible percent). This implies that the methodology proposed can be utilized if the sensitivity cases are considered for the LCA. This potentially reduces the reliance on the SimaPro tool to perform all the calculations.

The graphs representing the percentage change in the comparison for the rest of the sensitivity cases can be found in Appendix C.

4.6. Comparison of assessments across midpoint indicators

In this comparison study, the sensitivity cases were compared across the seven midpoint indicators. Performing this scenario, it will be able to identify the most impact case and the least impact case. Considering the case with lower GWP, might not have the lower impacts for other midpoint indicators like SOD, FPMF, FE, ME, HCT, and LU. With this method, the process parameters that have to be considered for lowering the impacts can be identified.

Considering the space constraints the x-axis is displayed with the alphabet the representation for these alphabets are

1. **a**- Base case
2. **b**- CO conv LB
3. **c**- CO conv UB
4. **d**- CO vol. mass transfer LB
5. **e**- CO vol. mass transfer UB
6. **f**- Product selectivity LB
7. **g**- Product selectivity UB
8. **h**- Dilution rate LB
9. **i**- Dilution rate UB
10. **j**- Gly mol frac LB
11. **k**- Gly mol frac UB
12. **l**- Offgas condenser LB
13. **m**- Offgas condenser UB
14. **n**- Anaerobic waste conv LB
15. **o**- Anaerobic waste conv UB
16. **p**- Molar RR LB
17. **q**- Molar RR UB
18. **r**- Biomassconcfrac LB
19. **s**- Biomassconcfrac UB
20. **t**- Broth Purge LB
21. **u**- Broth Purge UB
22. **v**- Glycerol purge fraction LB
23. **w**- Glycerol purge fraction UB

4.6.1. Global warming potential

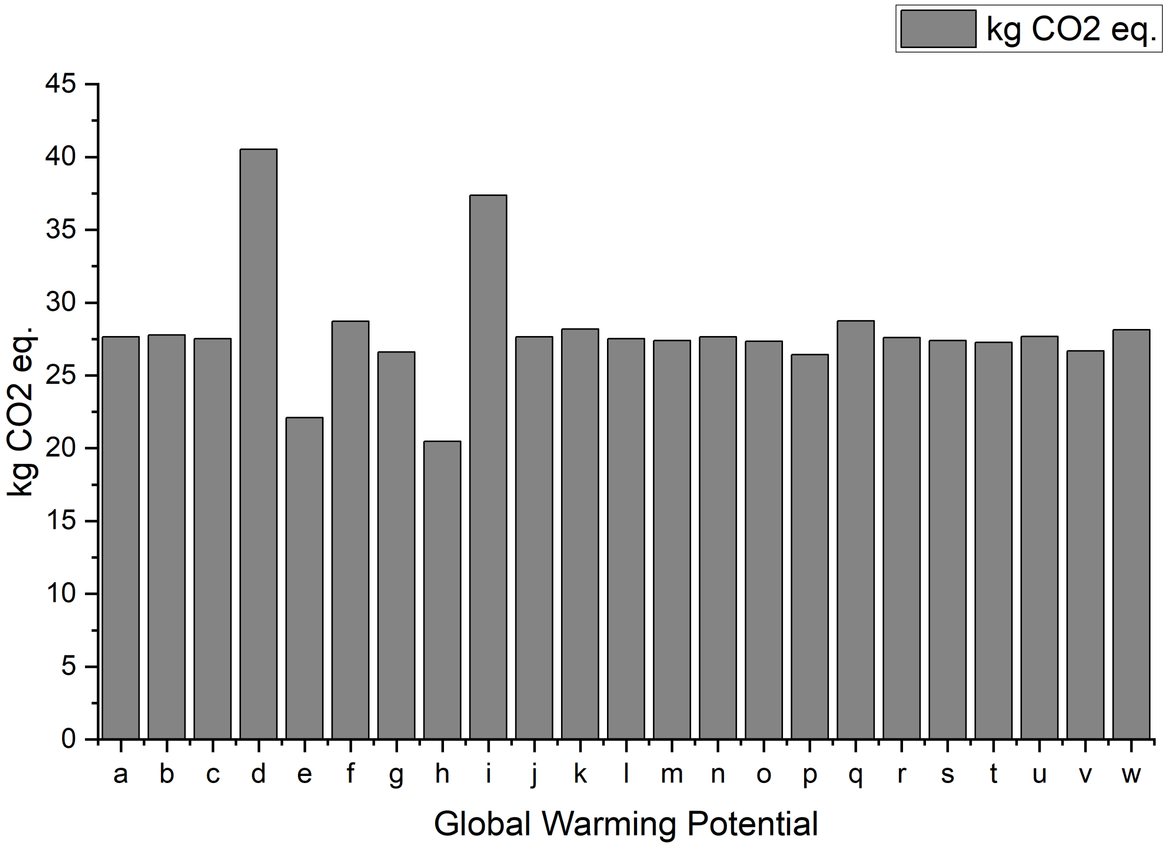

Figure 4.15: Comparison study: Global Warming Potential
a- Base case, **b**- CO conv LB (varied by -5%) , **c**- CO conv UB (varied by +5%), **d**- CO vol. mass transfer LB (varied by -30%), **e**- CO vol. mass transfer UB (varied by +30%), **f**- Product selectivity LB (varied by -5%), **g**- Product selectivity UB (varied by +5%), **h**- Dilution rate LB (varied by -30%), **i**- Dilution rate UB (varied by +30%), **j**- Gly mol frac LB (varied by -30%), **k**- Gly mol frac UB (varied by +30%), **l**- Temperature Offgas condenser LB (varied by -1.80%),**m**- Offgas condenser UB (varied by +11.5%), **n**- Anaerobic waste conv LB (varied by -10%), **o**- Anaerobic waste conv UB (varied by +10%), **p**- Molar RR LB (varied by -30%), **q**- Molar RR UB (varied by +30%), **r**- Biomass liq-liq moll frac LB (varied by -1%), **s**- Biomass liq-liq moll frac UB (varied by +10%), **t**- Broth Purge LB (varied by -30%), **u**- Broth Purge UB (varied by +30%), **v**- Glycerol purge fraction LB (varied by -30%), **w**- Glycerol purge fraction UB (varied by +30%)

The impact assessment for all the process parameters was performed and the ideal scenario can be identified from the fig4.15. The scenario with the least Global warming impact is the process parameter of Lower bound Dilution rate. In this sensitivity case, the dilution rate is altered by ±30%. Lowering the dilution rate for the process lowers the Global warming potential of the process to 20.464 kg CO_2 eq. The major contributor is the utility of steam, the complete interpretation can be found in the section 4.4.4. This case has a lower GWP value for this impact category. So it is implied that lowering the dilution rate for the base case by ±30% results in a significantly minimal Global Warming Potential impact value. On the other hand, the sensitivity cases of (**e** - CO volumetric mass transfer upper bound) and (**p** - molar reflux ratio lower bound) also show lower impact values considering the base case scenario. This implies that the combination of these certain process parameters like lowering the Dilution rate, extractive distillation molar reflux ratio, and increasing the Volumetric mass transfer rate CO will lead to to overall decrease in the total impact value of this process. This comparison study helps to identify the essential process parameters that can be adapted to obtain the bare minimum value in terms of the environmental impact category.

4.6.2. Stratospheric ozone depletion

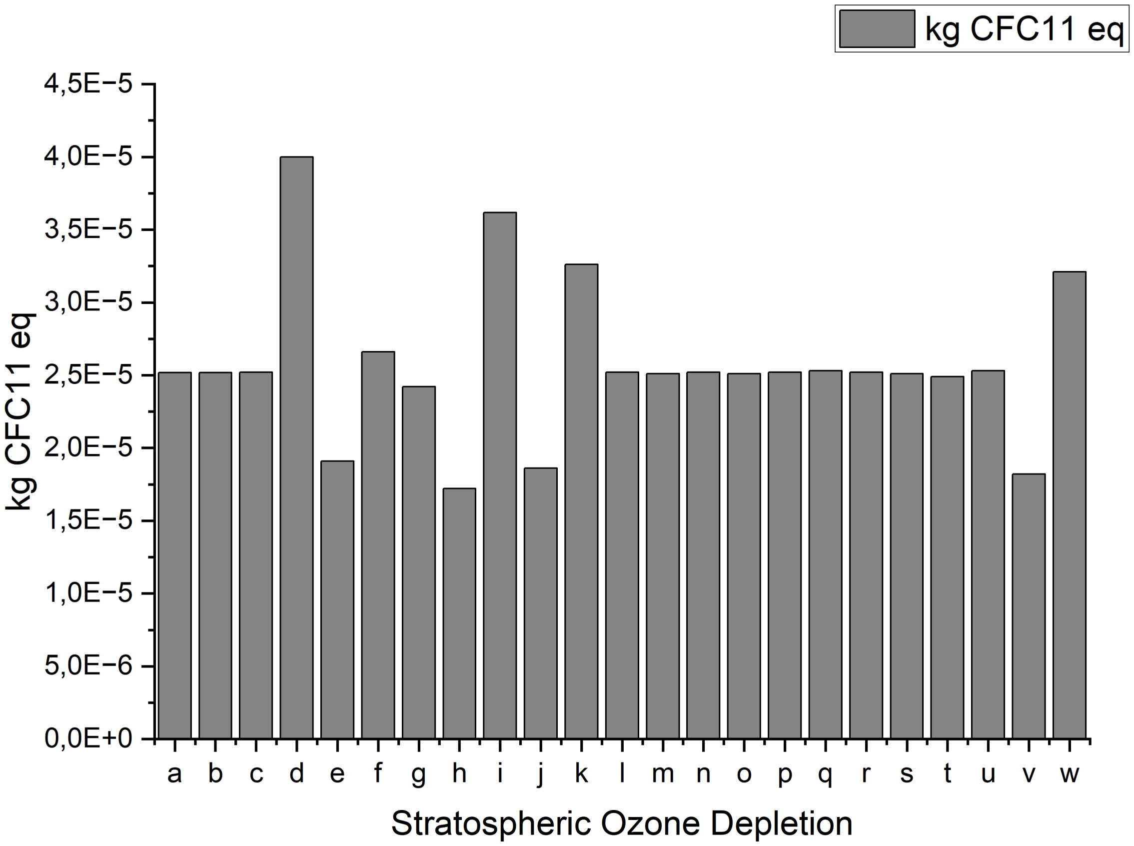

Figure 4.16: Comparison study: Stratospheric ozone depletion
a- Base case, **b**- CO conv LB (varied by -5%) , **c**- CO conv UB (varied by +5%), **d**- CO vol. mass transfer LB (varied by -30%), **e**- CO vol. mass transfer UB (varied by +30%), **f**- Product selectivity LB (varied by -5%), **g**- Product selectivity UB (varied by +5%), **h**- Dilution rate LB (varied by -30%), **i**- Dilution rate UB (varied by +30%), **j**- Gly mol frac LB (varied by -30%), **k**- Gly mol frac UB (varied by +30%), **l**- Temperature Offgas condenser LB (varied by -1.80%),**m**- Offgas condenser UB (varied by +11.5%), **n**- Anaerobic waste conv LB (varied by -10%), **o**- Anaerobic waste conv UB (varied by +10%), **p**- Molar RR LB (varied by -30%), **q**- Molar RR UB (varied by +30%), **r**- Biomass liq-liq moll frac LB (varied by -1%), **s**- Biomass liq-liq moll frac UB (varied by +10%), **t**- Broth Purge LB (varied by -30%), **u**- Broth Purge UB (varied by +30%), **v**- Glycerol purge fraction LB (varied by -30%), **w**- Glycerol purge fraction UB (varied by +30%)

Figure 4.16 represents the comparison to observe the minimal Stratospheric ozone depletion impact value. Similar to the GWP, this lower bound Dilution rate (varied by -30%) has the lower impact value for this midpoint indicator. The major contributor to this scenario is the utilization of glycerol in the extractive distillation process followed by steam consumption. As already implied, the lowered dilution rate for the IPA production process has a significant minimal change in impact value when compared with the upper bound volumetric mass transfer rate. The sensitivity case scenario:(**e** - CO volumetric mass transfer upper bound), sensitivity case scenario:(**j** - Glycerol mole fraction lower bound), and sensitivity case scenario:(**v** - glycerol purge fraction lower bound) show less impactful sensitivity cases when comparing with the base case scenario. These sensitivity cases minimize glycerol usage in their process. Considering the comparison across the GWP in the previous section, the sensitivity cases that obtain lower impact values are different in the stratospheric ozone depletion impact category. Because glycerol is the major component in this category the sensitivity cases in which glycerol usage is minimized are identified. Combining the process parameters of lowering dilution rate, extractive distillation glycerol mole fraction, glycerol purge fraction, and increasing the volumetric mass transfer rate will result in lower stratospheric ozone depletion impact values.

4.6.3. Fine particulate matter formation

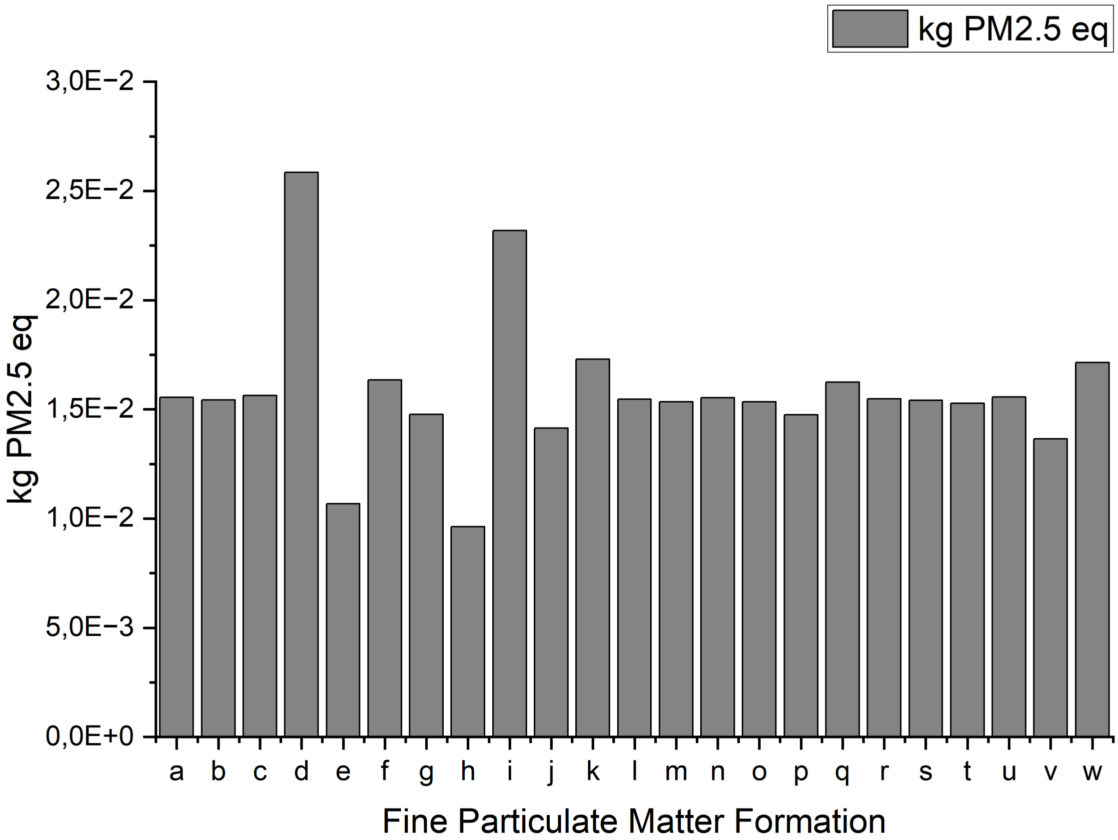

Figure 4.17: Comparison study: Fine particulate matter formation
a- Base case, **b**- CO conv LB (varied by -5%) , **c**- CO conv UB (varied by +5%), **d**- CO vol. mass transfer LB (varied by -30%), **e**- CO vol. mass transfer UB (varied by +30%), **f**- Product selectivity LB (varied by -5%), **g**- Product selectivity UB (varied by +5%), **h**- Dilution rate LB (varied by -30%), **i**- Dilution rate UB (varied by +30%), **j**- Gly mol frac LB (varied by -30%), **k**- Gly mol frac UB (varied by +30%), **l**- Temperature Offgas condenser LB (varied by -1.80%),**m**- Offgas condenser UB (varied by +11.5%), **n**- Anaerobic waste conv LB (varied by -10%), **o**- Anaerobic waste conv UB (varied by +10%), **p**- Molar RR LB (varied by -30%), **q**- Molar RR UB (varied by +30%), **r**- Biomass liq-liq moll frac LB (varied by -1%), **s**- Biomass liq-liq moll frac UB (varied by +10%), **t**- Broth Purge LB (varied by -30%), **u**- Broth Purge UB (varied by +30%), **v**- Glycerol purge fraction LB (varied by -30%), **w**- Glycerol purge fraction UB (varied by +30%)

In this figure 4.17, the impact category of fine particulate matter formation for all the sensitivity cases and the base case are performed. Even in this particular impact category, the lower bound dilution rate shows a huge difference in values when compared with the lower bound volumetric mass transfer rate. Steam utility used in the process has the most contributional effect to the total impact of this process. Relatively the emission credit lowers the contributional effect caused by the steam consumption. The sensitivity case scenario:(**e** - CO volumetric mass transfer upper bound) shows a similar less impact case like the dilution rater lower bound and the scenario of The value changes are in negligible amounts, but when considering the range in 0.1E-2 the dilution rate is observed to be very minimal in all the impact cases. Similarly, the sensitivity case:(**v** - Glycerol purge fraction) also resembles a lower impact value. However, a wide range of sensitivity scenarios with minimal impact values is observed due to low steam consumption in the impact categories of CO volumetric mass transfer lower bound, molar reflux ratio lower bound, product selectivity lower bound, and glycerol purge fraction lower bound. So by combining all the process parameters in the process model the environmental impact value for this impact category can be minimized.

4.6.4. Freshwater eutrophication

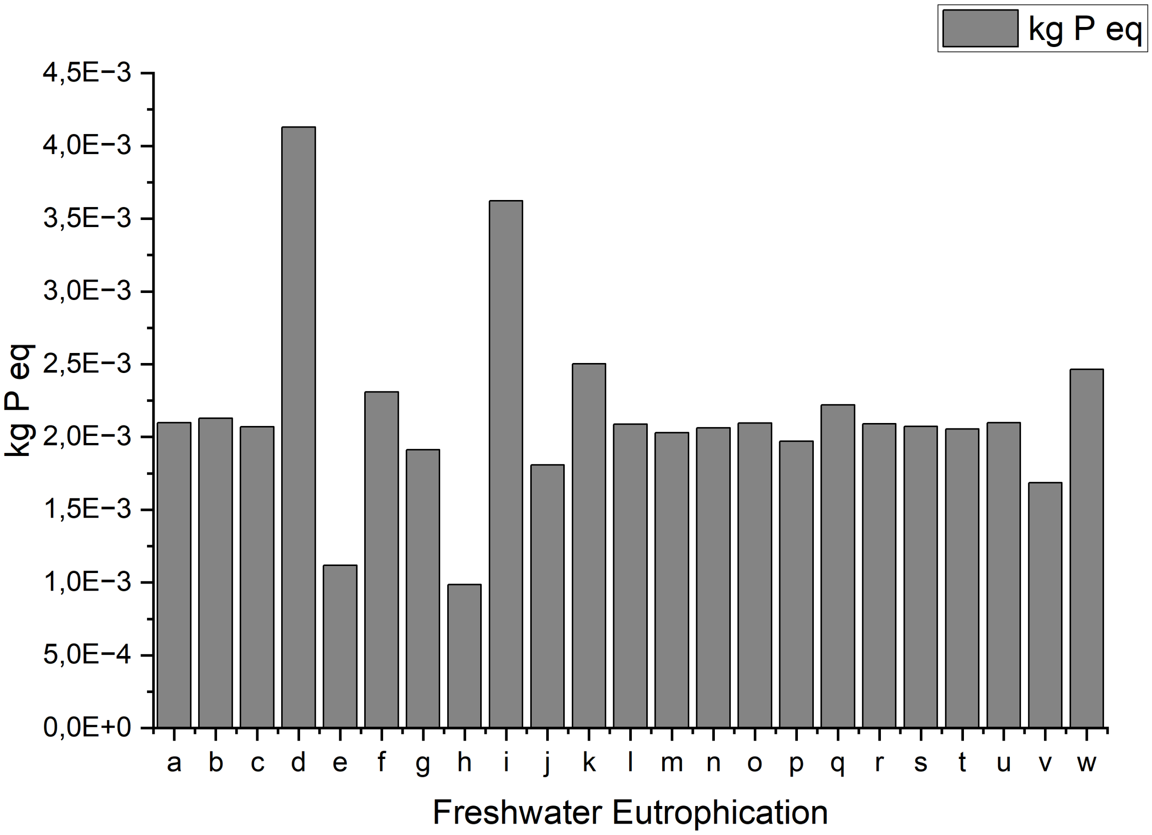

Figure 4.18: Comparison study: Freshwater eutrophication
a- Base case, **b**- CO conv LB (varied by -5%) , **c**- CO conv UB (varied by +5%), **d**- CO vol. mass transfer LB (varied by -30%), **e**- CO vol. mass transfer UB (varied by +30%), **f**- Product selectivity LB (varied by -5%), **g**- Product selectivity UB (varied by +5%), **h**- Dilution rate LB (varied by -30%), **i**- Dilution rate UB (varied by +30%), **j**- Gly mol frac LB (varied by -30%), **k**- Gly mol frac UB (varied by +30%), **l**- Temperature Offgas condenser LB (varied by -1.80%),**m**- Offgas condenser UB (varied by +11.5%), **n**- Anaerobic waste conv LB (varied by -10%), **o**- Anaerobic waste conv UB (varied by +10%), **p**- Molar RR LB (varied by -30%), **q**- Molar RR UB (varied by +30%), **r**- Biomass liq-liq moll frac LB (varied by -1%), **s**- Biomass liq-liq moll frac UB (varied by +10%), **t**- Broth Purge LB (varied by -30%), **u**- Broth Purge UB (varied by +30%), **v**- Glycerol purge fraction LB (varied by -30%), **w**- Glycerol purge fraction UB (varied by +30%)

This figure 4.18 represents the impact study for all the sensitivity analyses across the midpoint indicator of freshwater eutrophication. In this comparison study two different scenarios: the upper bound volumetric mass transfer rate and the lower bound dilution rate have very low impact values for freshwater eutrophication. But considering both these processes, the dilution rate: LB appears to be the most minimal impact value. The lowered impact value for this process is due to the minimal consumption of steam utility to produce 1 kg IPA. The eutrophication characterization factor for the steam is not so high, but considering the usage in kg per kg of steam produced. The contributional effect of this steam exceeds the total impact value and the emission credit of BOF gas prevented from flaring potentially lowers the kg P eq. of 1 kg IPA. Similarly, the impact values of the sensitivity cases of CO volumetric mass transfer upper bound, molar reflux ratio lower bound, product selectivity lower bound, and glycerol purge fraction lower bound. The lower impact value for these cases is due to the minimal utilization of glycerol for the process. So adapting the process parameters by lowering the molar reflux ratio and glycerol purge fraction and by increasing the volumetric mass transfer rate, product selectivity could lead to the optimal process model with lower impact values.

4.6.5. Marine eutrophication

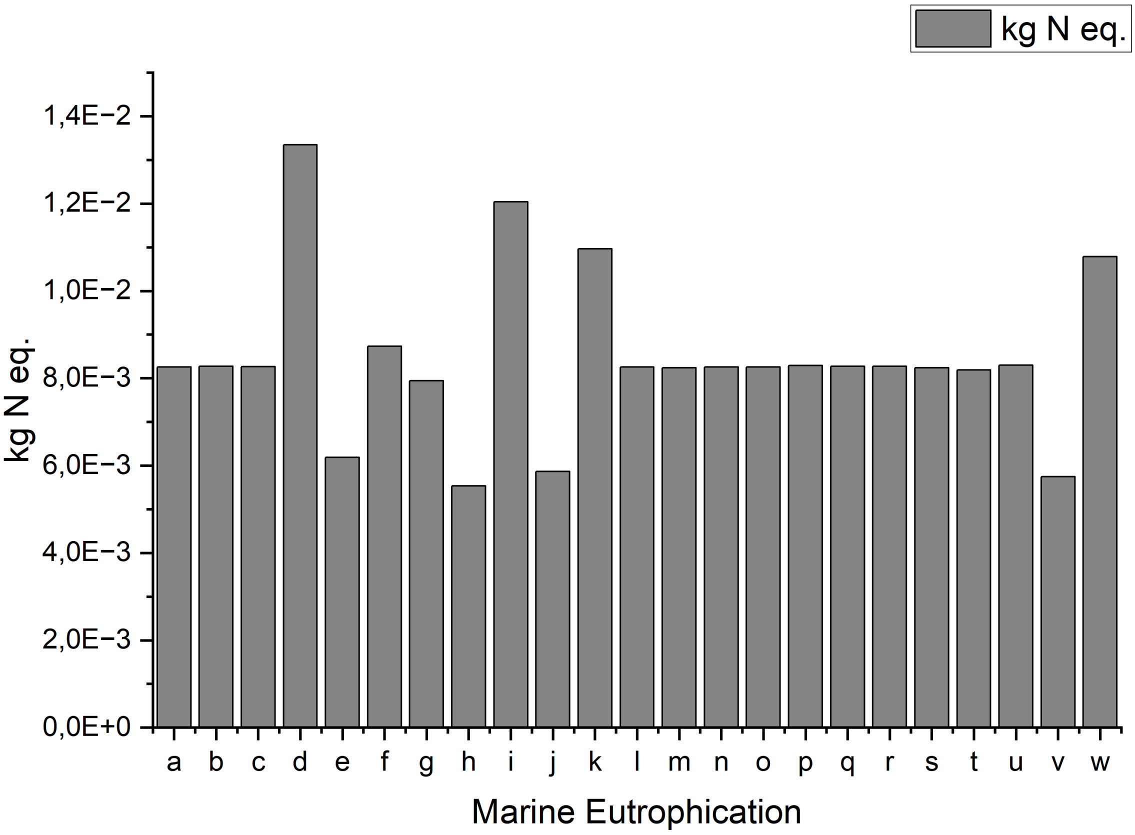

Figure 4.19: Comparison study: Marine eutrophication
a- Base case, **b**- CO conv LB (varied by -5%) , **c**- CO conv UB (varied by +5%), **d**- CO vol. mass transfer LB (varied by -30%), **e**- CO vol. mass transfer UB (varied by +30%), **f**- Product selectivity LB (varied by -5%), **g**- Product selectivity UB (varied by +5%), **h**- Dilution rate LB (varied by -30%), **i**- Dilution rate UB (varied by +30%), **j**- Gly mol frac LB (varied by -30%), **k**- Gly mol frac UB (varied by +30%), **l**- Temperature Offgas condenser LB (varied by -1.80%),**m**- Offgas condenser UB (varied by +11.5%), **n**- Anaerobic waste conv LB (varied by -10%), **o**- Anaerobic waste conv UB (varied by +10%), **p**- Molar RR LB (varied by -30%), **q**- Molar RR UB (varied by +30%), **r**- Biomass liq-liq moll frac LB (varied by -1%), **s**- Biomass liq-liq moll frac UB (varied by +10%), **t**- Broth Purge LB (varied by -30%), **u**- Broth Purge UB (varied by +30%), **v**- Glycerol purge fraction LB (varied by -30%), **w**- Glycerol purge fraction UB (varied by +30%)

Similar to freshwater eutrophication, this impact category of marine eutrophication also has two different cases with impact values nearby. The first case is the lower bound dilution rate and the second case is the lower bound Glycerol purge fraction. Out of these two lower impact values, the lower bound dilution rate still has the lower impact values minimizing the indirect nutrient runoff into the water body followed by the sensitivity cases of CO volumetric mass transfer lower bound, molar reflux ratio lower bound, product selectivity lower bound, and glycerol purge fraction lower bound. Therefore, the ideal process model with reduced impact values may be reached by modifying the process parameters by lowering the molar reflux ratio and glycerol purge percentage and by raising the volumetric mass transfer rate, and product selectivity.

4.6.6. Human carcinogenic toxicity

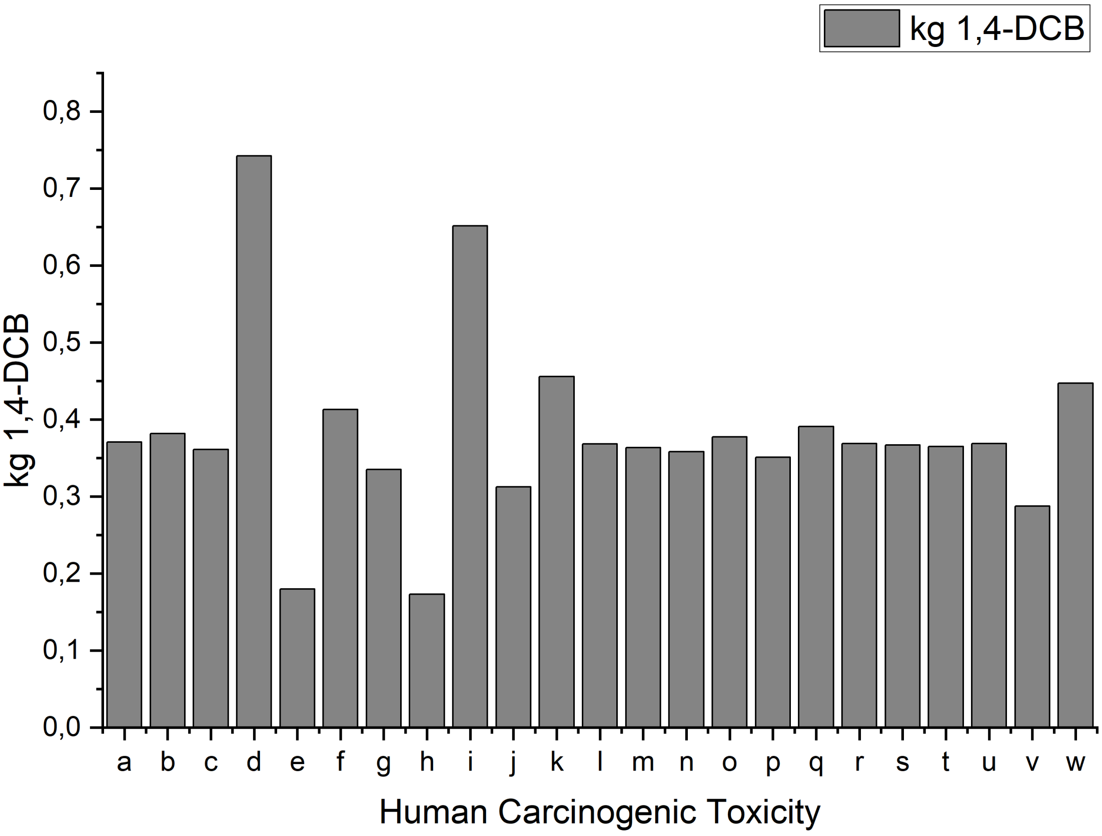

Figure 4.20: Comparison study: Human carcinogenic toxicity
a- Base case, **b**- CO conv LB (varied by -5%) , **c**- CO conv UB (varied by +5%), **d**- CO vol. mass transfer LB (varied by -30%), **e**- CO vol. mass transfer UB (varied by +30%), **f**- Product selectivity LB (varied by -5%), **g**- Product selectivity UB (varied by +5%), **h**- Dilution rate LB (varied by -30%), **i**- Dilution rate UB (varied by +30%), **j**- Gly mol frac LB (varied by -30%), **k**- Gly mol frac UB (varied by +30%), **l**- Temperature Offgas condenser LB (varied by -1.80%),**m**- Offgas condenser UB (varied by +11.5%), **n**- Anaerobic waste conv LB (varied by -10%), **o**- Anaerobic waste conv UB (varied by +10%), **p**- Molar RR LB (varied by -30%), **q**- Molar RR UB (varied by +30%), **r**- Biomass liq-liq moll frac LB (varied by -1%), **s**- Biomass liq-liq moll frac UB (varied by +10%), **t**- Broth Purge LB (varied by -30%), **u**- Broth Purge UB (varied by +30%), **v**- Glycerol purge fraction LB (varied by -30%), **w**- Glycerol purge fraction UB (varied by +30%)

Figure 4.20 displays the sensitivity analysis cases across the human carcinogenic toxicity indicator. The scenario with the lower impact values is performed by altering the -30% dilution rate for the production process. Since there are no carcinogens that are directly used in this process, the impact value of 0.173 kg 1,4 DCB is contributed by the steam utility for the process. Even the utility effect is compensated by preventing the BOF gas from flaring in the steel mill. This prevention heavily lowers the impact value of this particular indicator. The sensitivity case of CO volumetric mass transfer upper bound showed a similar value when compared with the dilution rate. Even though the values are in negligible amounts, the dilution rate appears to be the lowest of all the cases. However, the lower values compared to the base case are observed for the sensitivity cases of CO volumetric mass transfer lower bound, molar reflux ratio lower bound, product selectivity lower bound, and glycerol purge fraction lower bound. The process model which incorporates the process parameters by lowering the dilution rate, molar reflux ratio, glycerol purge fraction, and by increasing the volumetric mass transfer rate, product selectivity,might result in the minimal impact value of marine eutrophication.

4.6.7. Land use

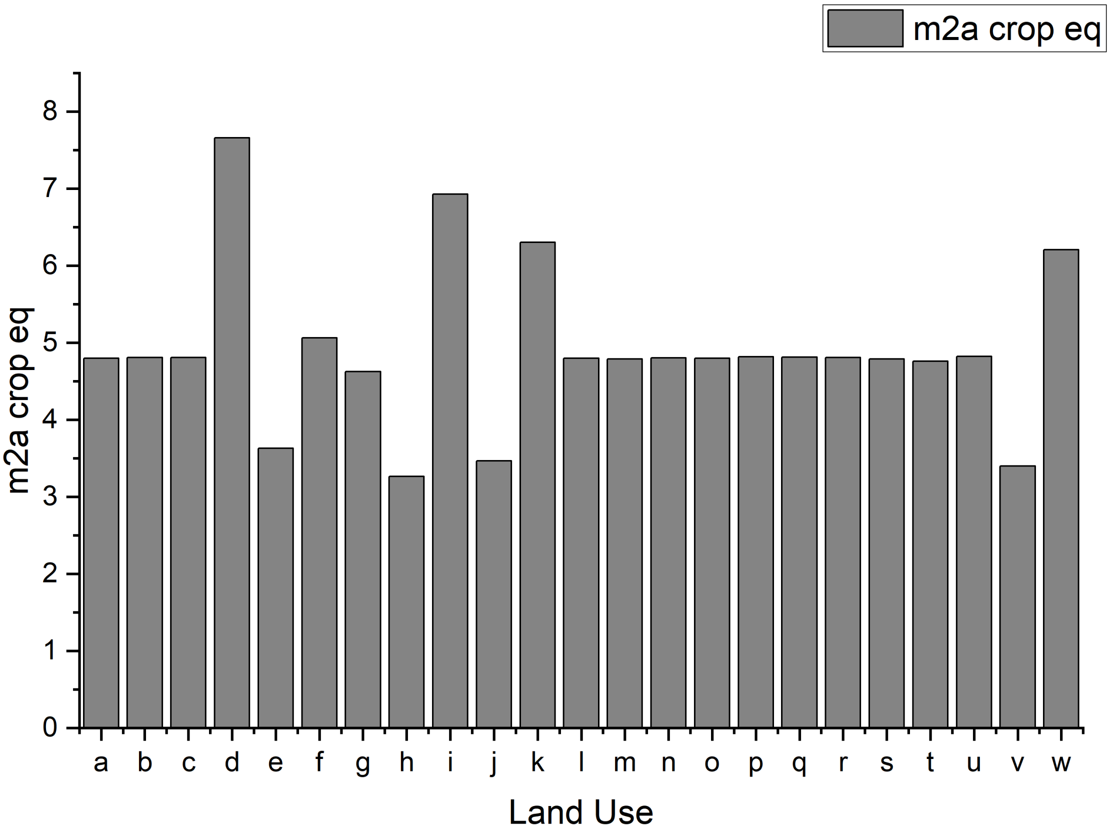

Figure 4.21: Comparison study: Land use **a**- Base case, **b**- CO conv LB (varied by -5%) , **c**- CO conv UB (varied by +5%), **d**- CO vol. mass transfer LB (varied by -30%), **e**- CO vol. mass transfer UB (varied by +30%), **f**- Product selectivity LB (varied by -5%), **g**- Product selectivity UB (varied by +5%), **h**- Dilution rate LB (varied by -30%), **i**- Dilution rate UB (varied by +30%), **j**- Gly mol frac LB (varied by -30%), **k**- Gly mol frac UB (varied by +30%), **l**- Temperature Offgas condenser LB (varied by -1.80%),**m**- Offgas condenser UB (varied by +11.5%), **n**- Anaerobic waste conv LB (varied by -10%), **o**- Anaerobic waste conv UB (varied by +10%), **p**- Molar RR LB (varied by -30%), **q**- Molar RR UB (varied by +30%), **r**- Biomass liq-liq moll frac LB (varied by -1%), **s**- Biomass liq-liq moll frac UB (varied by +10%), **t**- Broth Purge LB (varied by -30%), **u**- Broth Purge UB (varied by +30%), **v**- Glycerol purge fraction LB (varied by -30%), **w**- Glycerol purge fraction UB (varied by +30%)

The midpoint indicator Land use is compared for all the sensitivity cases in figure 4.21. The scenario with the minimal impact value is the lower bound dilution rate scenario. The calculated value is 3.265 m^2a crop eq./kg of generated IPA. Glycerol, a molecule having a wide range of increased effect values, is the main contributor to this land use impact category. The esterification of rapeseed oil provides the source of the glycerol component found in the Ecoinvent database and is assumed to be the main reason for the increase in impact value. hence, by lowering the molar reflux ratio, glycerol purge fraction, while raising the volumetric mass transfer rate, and product selectivity, the ideal process model with lower impact values may be reached.

On the whole, all the sensitivity cases were compared across seven impact categories. A particular scenario of the dilution rate: lower bound was identified to be the category with the least environmental impact. Generally, it was estimated that for every impact category different scenarios will have lower impact values. Usually, only the global warming potential is the only impact category that will be considered for the environmental impact assessment, due to its wide acceptance and as the criteria in all the protocols formulated. So the other impact categories for the process are not assessed. This is a trade-off because if we consider only the GWP for our process, minimizing the steam utility could significantly lower the impact value of GWP would be the interpretation we could identify from the results. However, the results of the other six impact categories show that glycerol is also an environmentally effective component that should also be minimized. So, the process model should be adapted considering the lower bound Dilution rate and the overall process to lower the steam and glycerol utilization could lower the impact values for all the opted impact categories.

4.7. Contributional effects of components on the process model

The Base case process model was performed with the Life Cycle Impact assessment study and the most influential components that account for the major impact value are identified. Namely, steam is the major contributional component for the midpoint impact categories of Global Warming Potential, Fine Particulate Matter Formation, Freshwater Eutrophication, and Human Carcinogenic Toxicity, and the glycerol for the midpoint categories of Stratospheric Ozone Depletion, Marine Eutrophication, and Land Use.

4.7.1. Percentage effects of Steam on the process model

Global Warming Potential

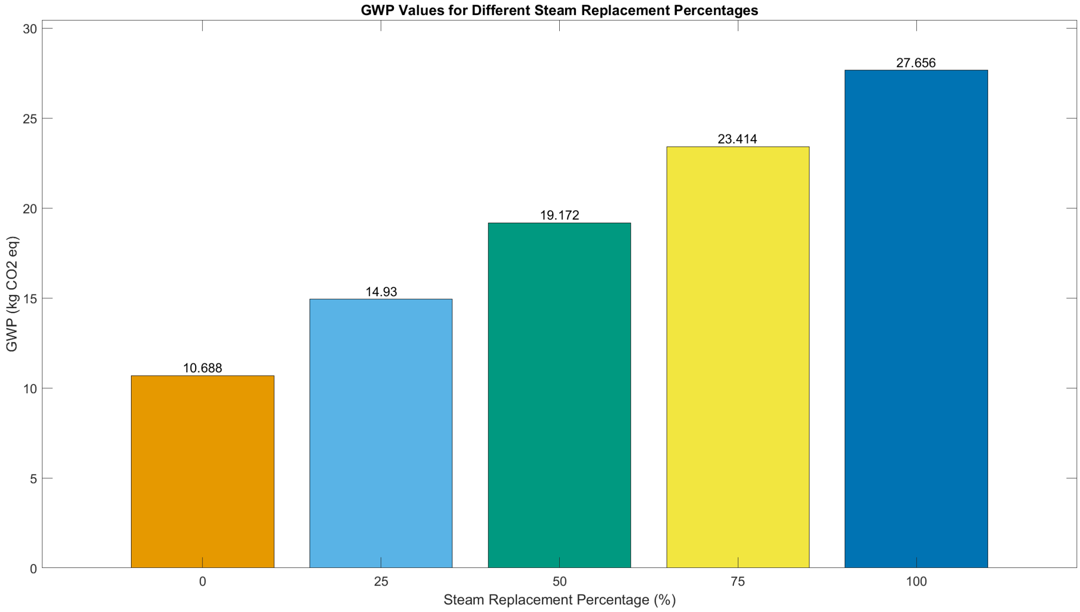

Figure 4.22: Effect of Steam utility on the Global Warming Potential impact category

In this figure 4.22, the steam utility was reduced by a certain percentage from the total utilization, and the impact value for the impact category of GWP was estimated. The 100% represents the base case model. Similarly, the percentage reduction for 75%, 50%, 25%, and 0% were estimated. The steam comparison study implies that the steam might be a major contributor to the impact category value of GWP, but reducing the steam utility to 0% still results in 10.688 kg CO_2 eq. but a 61% reduction from the total value can be observed showing that this value is still higher than the conventional IPA value of 2.026 kg CO_2 eq.

Fine Particulate Matter Formation

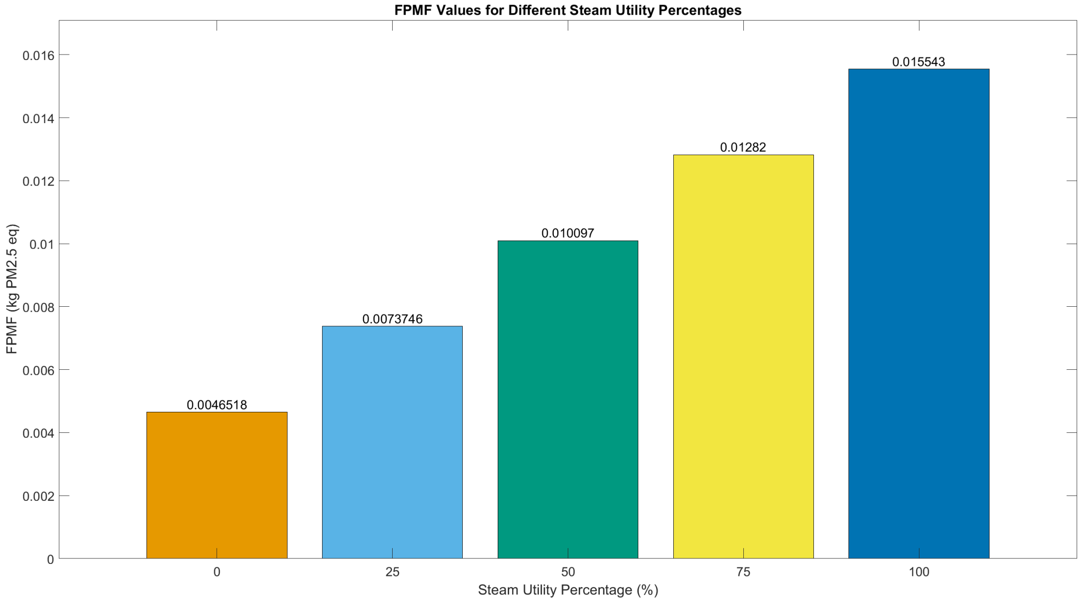

Figure 4.23: Effect of Steam utility on the Fine Particulate Matter Formation impact category

Figure 4.23 illustrates the contribution of steam to the impact category of fine particulate matter formation. By reducing the percentages from 100% to 0% (steam utility contribution in process model), approximately 18% of the impact values are deducted for decreasing ±25% (steam utility contribution in process model). Comparing the 0% glycerol usage value of 0.004 kg PM2.5 eq. is twice the total impact value of the conventional IPA method.

Freshwater Eutrophication

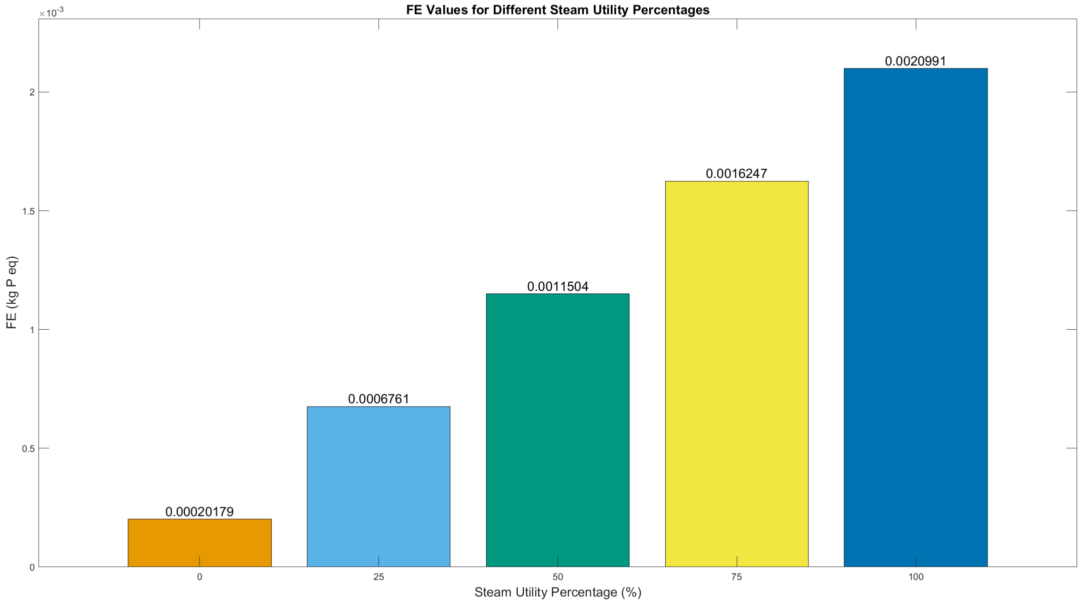

Figure 4.24: Effect of Steam utility on the Freshwater Eutrophication impact category

Figure 4.24 represents the contribution of steam to the freshwater eutrophication impact category. In this, reducing the steam utilization by 75% (25% usage) could result in a lower impact value for the FE impact category. So, steam should be lower to reduce the overall impact on the water bodies as the eutrophication deals with the impact on water bodies.

Human Carcinogenic Toxicity

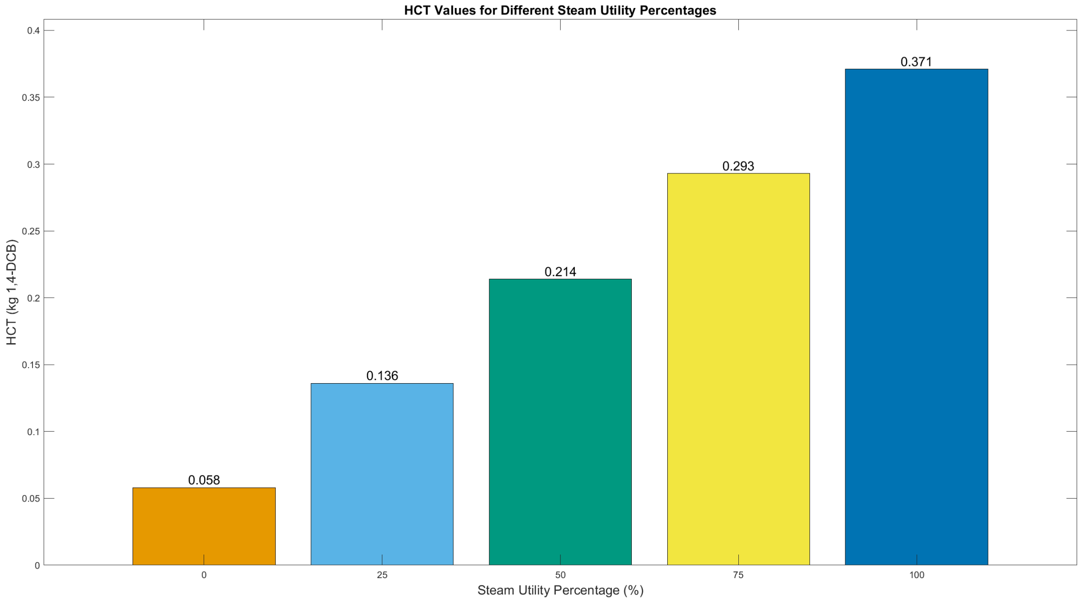

Figure 4.25: Effect of Steam utility on the Fine Particulate Matter Formation impact category

In this figure 4.25, the contribution of steam to the impact category of fine particulate matter formation graph is plotted. The complete reduction of the usage of steam utility results in 0.058 kg 1,4-DCB. This value is approximately similar to the impact value of the conventional production method. But steam is an essential utility for the process, so minimizing the total usage by 75% could result in the value of 0.136 kg 1,4-DCB, which is twice as the conventional value.

4.7.2. Percentage effects of Glycerol on the process model

Stratospheric Ozone Depletion

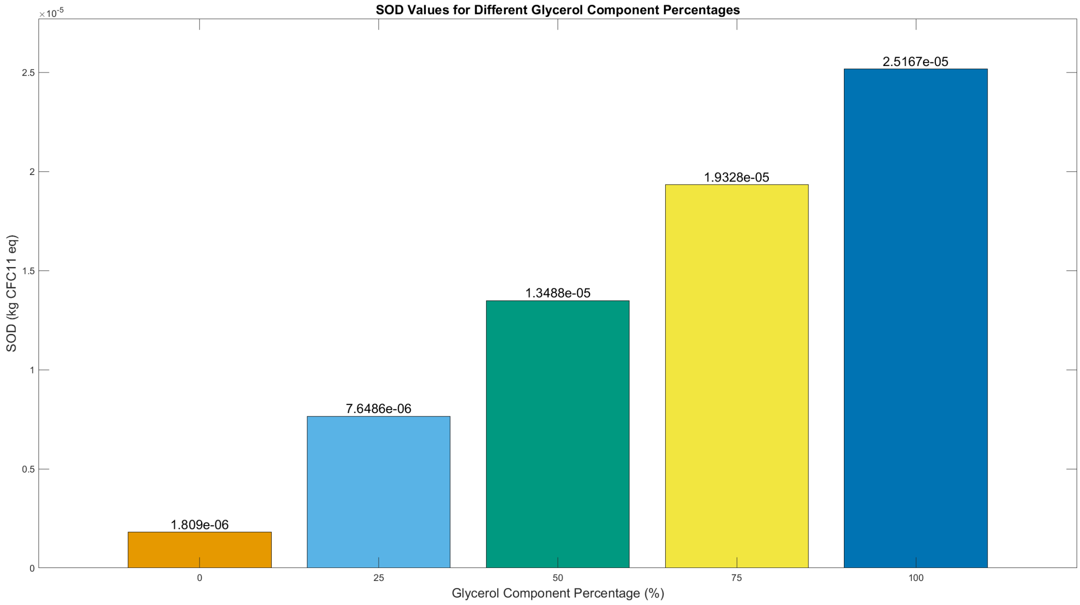

Figure 4.26: Effect of Glycerol component on the Stratospheric Ozone Depletion impact category

Figure 4.26 represents the contribution of the glycerol component to the impact category of stratospheric ozone depletion. Reducing the component percentage by 25% from 100 to 0% leads to the percentage change of the value of about approximately ±28% for depreciation of each 25%. Still, the complete reduction of glycerol usage in the process model of about 1.809E-06 is higher than the conventional IPA value of 1.47E-07. This implies that glycerol plays a major role in obtaining the lower values but has other components which have higher impact values, but lesser than glycerol.

Marine Eutrophication

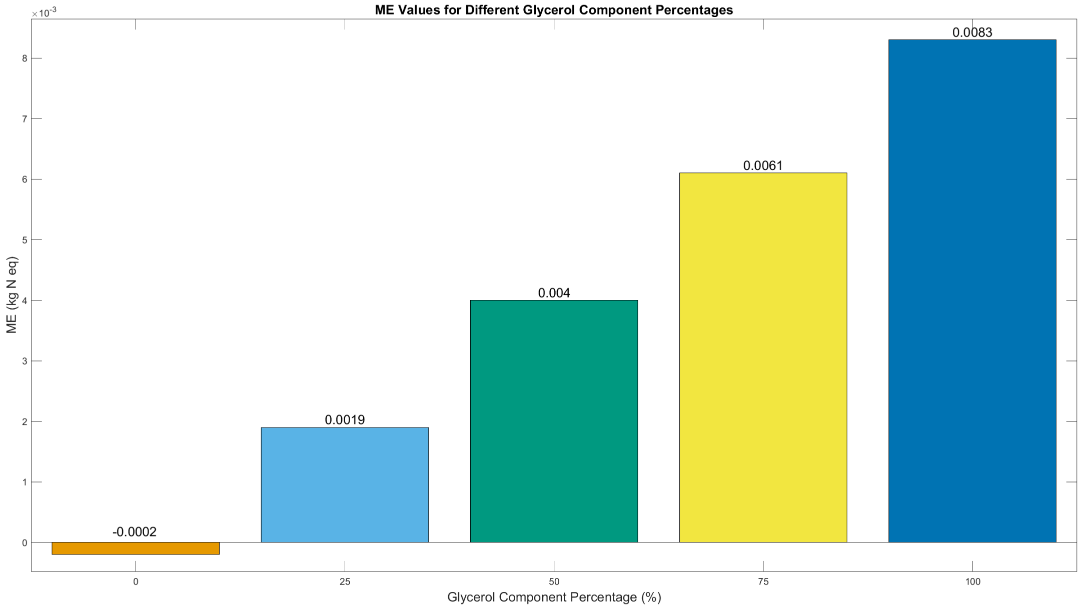

Figure 4.27: Effect of Steam utility on the Marine Eutrophication impact category

In this figure 4.27, the contribution of the glycerol component to the marine eutrophication impact category is visualized. Reducing the glycerol usage from 100 to 0% results in a negative value for the marine eutrophication category. For this impact category, Glycerol is the crucial component by less than 25% usage can obtain values equivalent to the conventional IPA method. However, the component of glycerol is essential for the extractive distillation process.

Land Use

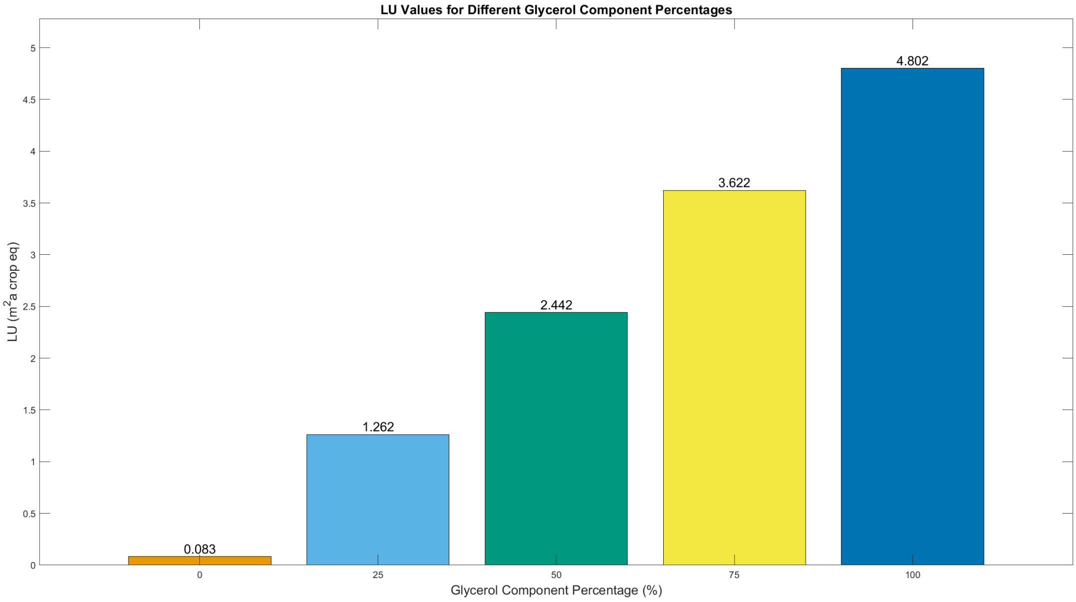

Figure 4.28: Effect of Steam utility on the Land Use impact category

Figure 4.28 illustrates the contribution of the glycerol component to the Land use impact category. The 0% usage of glycerol results in the impact value of 0.083 m^2a crop eq. which is a 153% increase from the conventional value. But the base case uses 100% of glycerol which estimates about 4.802 m^2a crop eq.. It can be inferred that lowering the glycerol usage from 100% to 0% shows a 98% decrease in the impact category value of Land use.

4.7.3. Percentage effects of combined (Glycerol and Steam) on the process model

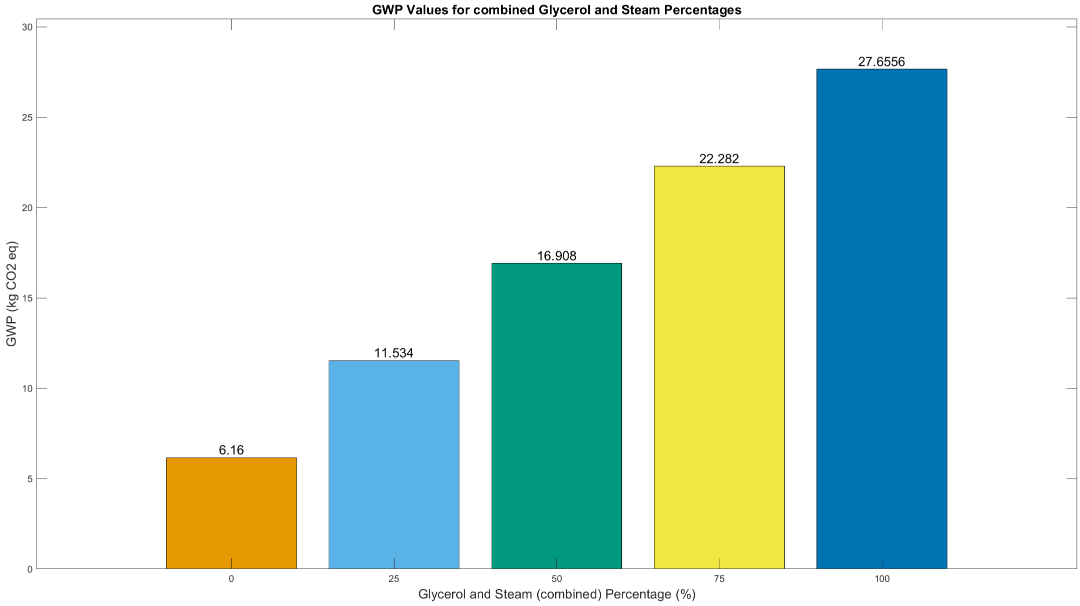

Figure 4.29: Effects of Glycerol and Steam on the Global Warming Potential Impact category

Figure 4.29 illustrates the effects by combining the reduction of glycerol and steam utilization in the process model. Completely cutting off the total usage (0% usage) of glycerol and steam still results in the value of about 6.16 kg CO_2 eq. which is a 204% increase when compared with the conventional IPA value of about 2.1026 kg CO_2 eq. So, the other components excluding the glycerol and steam still lead to high impact value, so the major contributors of steam and glycerol usage should be optimized and reduced. However, the negative kg CO_2 eq. value for the process model cannot be obtained with these process model steps.

4.7.4. Percentage effects of Energy replacement on the process model

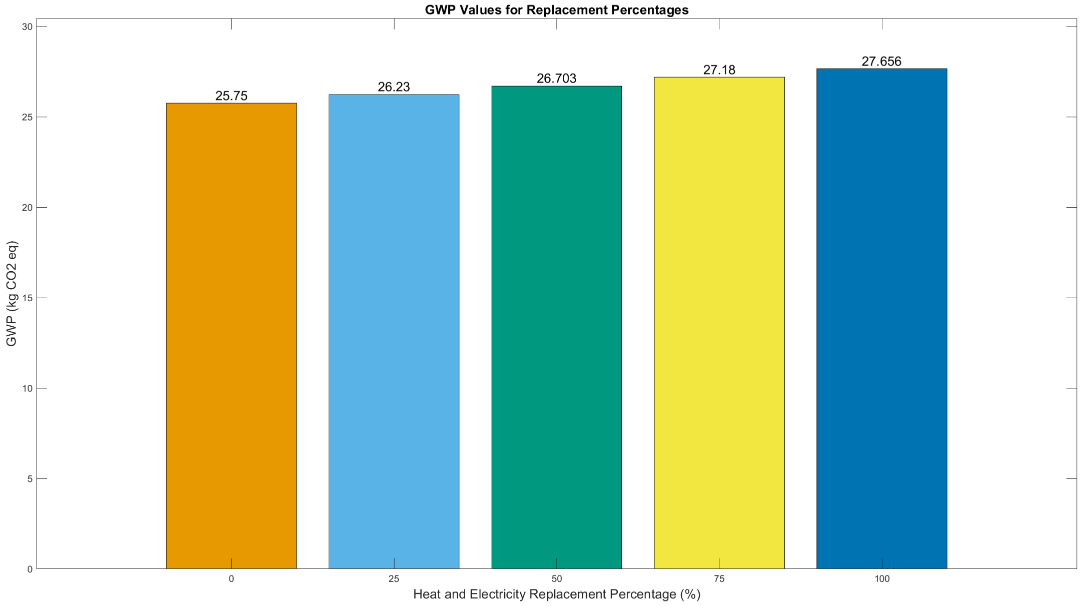

Figure 4.30: Effects of Energy Replacement on the Global Warming Potential Impact category

The effects of energy replacement for the impact category of global warming potential are illustrated in the figure 4.30. In this figure, it is evident that the varying ±25% of the total energy replacement does not result in a huge decrease in the overall GWP impact value of about 25.75 kg CO_2 eq. Reducing the energy replacement from 100 to 0% results in a percentage change of -6.9%, which has no effect in terms of comparison with the conventional IPA value of 2.026 kg CO_2 eq.

4.8. Reflection on this life cycle impact assessments

4.8.1. Discussions to reduce the environmental effects of this process

The LCA was performed for the commercial process using the Liew et al.,(2022) method and compared the carbon profile for both the pilot scale plant and the commercial scale model. This method is not so accurate that it does not consider the multifunctionality criteria like substitution and system expansion. The components that contribute less than 5% to the GWP were excluded from the impact assessment and the reduction in emissions (-163%) was achieved in the plot scale plant (Liew et al., 2022). If the same Liew et al.,(2022) method is applied to the commercial scale model an increase in emissions is observed (+261.5% increase). So this impact assessment does not provide a clear GWP profile. And the fossil IPA emission value of 1.85 kg CO_2/kg IPA was not so coherent. So the LCA study considering the cradle-to-gate was performed to estimate the environmental impacts caused by the commercial process. The comparison data for the conventional IPA production was used from the ecoinvent 3.9 database.

The impact assessment performed for the base case scenario has the higher impact values across all the impact values. The major contributors to the impact assessment apart from the essential inputs like NH_3, water, etc., are the impact values from heat and electricity that have to be replaced for the steel mill instead of internal utilization of BOF gas. The overall impact of the system was significantly reduced by the emission credit. This credit is for the role of preventing the BOF gas from flaring in the environment. After performing all the impact assessments for this process, it is evident that the impact values for the base case scenario of BOF gas-IPA production are comparatively very high compared with the conventional method for IPA production (direct/indirect hydration of propylene) method. There could be a few reasons why this lower impact value of the conventional method. Firstly, the IPA is produced as a main product in the hydration process along with many co-products like Diisopropyl ether, C6 olefins, hydrogen (H_2), and trace amounts of n-propyl alcohol (Shimizua, Takahashib, & Ikushimac, n.d.). So maybe system expansion is considered and the impacts of these co-products are deducted from the total impact resulting in lower impact value. Secondly, the overview regarding the type of LCA (like cradle-to-gate, gate-to-gate) is not available. Lastly, the emission credit could have been considered because this hydration process produces hydrogen which can be used as a feedstock for other processes. So the total impact could be significantly reduced. The major drawbacks to the impact assessment performed were the exclusion of the impacts of acetogenic microbes *C. Autoethanogenum* and the traces of components like acetic acid and others were also avoided. If these components impact are included, the effective overall impact of the LCA system can be estimated.

The glycerol used in the process for the extractive distillation step is continuously fed into the system in a very minimal amount. Because the glycerol after the recovery would contain impurities of acetic acid and sodium salt so, the 10% of the glycerol stream is purged. This purging of glycerol results in the formation of biogas with a composition of 63.4% CO_2, 32.5% CH_4, and rest traces. This biogas is further combusted and the CO_2 is emitted in the environment. This CO_2 emission accounts for 10.3% of total CO_2 emission from the process. This accounts for the major reason that the BOF gas prevented from flaring is comparatively lower when the CO_2 emission from the process is considered.

The impact assessments for the sensitivity cases of Volumetric mass transfer rate CO lowerbound, Dilution rate upperbound, and Product selectivity lowerbound imply that the CO_2 emission from the process is huge compared with the base case and other sensitivity cases. This is because these scenarios utilize glycerol. The anaerobic digestion and biogas combustion are huge, hence the higher emission of CO_2 from the process. This increase in the CO_2 emissions can be observed in fig 4.15 because the CO_2 accounts only for the impact category of Global Warming Potential. The increase in glycerol consumption is increased as described by (Brouwer, 2023) when the volumetric mass transfer rate is lowered by -30%, +30% increase in Dilution rate, and -30% decrease in product selectivity. On the other hand, scenarios like upperbound CO conversion, and lowerbound Dilution rate shows low CO_2 emission value due to minimal glycerol consumption.

Similarly, steam utility consumption is observed to be higher in the impact categories of GWP, FPMF, FE, and HCT. The sensitivity case of lowerbound volumetric mass transfer rate CO shows the huge steam utility consumption and the lowerbound Dilution rate sensitivity case shows the lower utilization of steam for the process model. For the impact categories of FPMF, FE, and HCT, the steam utilization is minimal in the case of lower bound Dilution rate varied -30%. Because the overall process model for this sensitivity case has a minimal steam requirement.

4.8.2. Reflection on the LCA model

The impact assessment for the two scenarios of considering the biomass waste as fishmeal and the incineration is performed. As predicted, the impact value for the scenario of biomass waste as fish meal was lower than the biomass incineration scenario. However, the biomass incineration scenario is considered to be the ideal situation to treat the biomass waste generated. Since there is a ban on the products produced via microorganisms (GMOs). So this biomass incineration scenario was set as the base and all the sensitivity cases also consider the biomass waste to be incinerated. The impact assessment for the sensitivity cases was performed and the impact values varied when the process parameters were varied by the lower bound and upper bound values. Based on these impact assessments the most essential process parameters was identified. By varying the dilution rate by -30% results in lower impact values across all the seven midpoint indicators. So this Process parameter is suggested to be the ideal sensitivity analysis scenario to obtain lower impact values.

From the comparison of sensitivity cases across the midpoint indicators, it is observed that the process parameter of dilution rate obtains the minimal impact value. But the comparison study also reveals that the other scenarios by lowering the extractive distillation molar reflux ratio and by increasing the product selectivity and volumetric mass transfer rate results in overall lower impact values. The major reason for this consideration of three sensitivity cases along with the prominent dilution rate process parameter is due to its impact on all the impact categories like GWP, SOD, FPMF, FE, ME, HCT, and LU. The impact categories like SOD, ME, and HCT have the major contributor as glycerol, so the sensitivity case of glycerol purge fraction, and glycerol mole fraction are also considered essential process parameters along with the previously mentioned four process parameters. The overall process model can be further modeled based on the process parameters by lowering the dilution rate by (-30%), molar reflux ratio (-30%), glycerol purge fraction (-30%), and by increasing the parameters of volumetric mass transfer rate by +30% and product selectivity by +5% would result in the lower overall impact values.

The effects of glycerol and steam on the overall impact value of the process model were performed. The percentage utilization of steam and glycerol varied from full utilization to zero utilization (with a decrement of 25%). As the major component of steam is for the impact categories of GWP, FPMF, FE, and HCT results in the value of lower impact values for the zero utilization. Other cases of GWP, FPMF, and HCT except FE have a zero utilization value higher than the conventional IPA method value, whereas for the freshwater eutrophication reducing the overall usage by 75% (25% utilization) can obtain an impact value of 0.0006 kg P eq. lower than the conventional production method. In the case of glycerol, the impact categories of SOD, ME, and LU are considered as the glycerol is the major contributor. Out of these three categories, the zero utilization of glycerol results in a negative value for the impact category of Marine eutrophication, the other two categories still have higher impact values even if the glycerol is not even utilized.

The combined glycerol and steam replacement scenarios estimate about 6.16 kg CO_2 eq. value for the zero utilization. So, it can be inferred that the components other than steam and glycerol result in a higher value. For the case of the energy replacement study, a change in impact value of 6.9% is identified by varying the utilization from 100 to 0% by the decrement value of ±25%. From this percentage effect study, it can be implied that, even zero utilization of steam and glycerol results in a higher impact value of 6.16 kg CO_2 eq. On an interesting note, the other impact categories of freshwater eutrophication and marine eutrophication values can be lowered by reducing the total usage of steam and glycerol by 75%, thus obtaining an impact value lower than the conventional IPA method. Rest 5 other midpoint indicators have the impact values way over the conventional method.

The SimaPro is the tool used for the impact assessment of the commercial scale process. The base case was performed by altering the inputs and outputs of the process with reference to the functional unit. A new project must be created for every sensitivity case, which involves using the SimaPro tool for more time. So it was proposed that only the base case impact assessment be performed using the SimaPro tool and the sensitivity cases be performed with the help of an Excel sheet. Because this sensitivity case has the same inputs and outputs as the base case, calculating the percentage change between the base case and the (lower bound/ upper bound) impact values across different midpoint indicators can be obtained by similarly varying the percentage change for the impact values of the base case. This method was performed to verify the applicability of the impact assessments performed for sensitivity cases. This method results are verified with the results using the SimaPro tool and the percentage change in values is in the range of 1E-07% to 1E-05%.

Most of the life cycle assessments performed around the globe concentrate mostly on the CO_2 emissions (GWP) alone. So to provide overall effects on the environment by the process on the areas of ecosystem, human health, and resources, seven different midpoint indicators were chosen. The major drawback in this selection of impact category is that the water consumption impact category is not used for the impact assessment of all the cases. The major reason for this is that during biomass incineration the water emitted as a result of this process is not well defined and properties/ quality cannot be assumed. So this consideration is not made. The CO_2 emitted from the biogas combustion is considered anaerobic, but still, the emission should be considered emission irrespective of the type of CO_2 like biogenic or fossil. This biogenic consideration is another reason to reduce the total impact value of the process. The initial consideration of the CO_2 emission from the process could be considered biogenic because of the carbon fixture procedure by the gas-fermentation process but the source of the feedstock of the BOF gas is derived from the natural ores, which has a long carbon cycle. So, this emission from the process could be identified as the fossil carbon dioxide which contributes to the global warming potential impact value of this process. The possible arguments favoring both the biogenic and fossil CO_2 are the major limitation of this process. Considering biogenic emission of CO_2 could lower the GWP value of the process when compared with the fossil emission of CO_2.

The major contributors like glycerol used as the component for the impact assessment are produced via the esterification process, which might have some direct effects on the impact category values. But the glycerol has been opted as the best entrainer in the modeling work done by Brouwer et al., (2023) based on the consideration of glycerol production by fermentation of biomass. It might significantly lower the impact value by a considerable amount. However, the syngas fermentation process can be coined as a green way of producing Isopropyl alcohol, but it involves a huge consumption of steam. This steam requirement can be satisfied by electricity. Unless the electricity production is green, any process involving carbon sequestration is not green anymore. In some cases, the region is set as the European landscape and the most suitable components are synthesized in the different parts of the world and an alternate has to be identified that suits the landscape requirements. This also accounts for some additional impact values.

5

Conclusion

To conclude, the life cycle assessment was performed for the process of "Industrial scale BOF gas fermentation to synthesize Isopropyl alcohol using *C.Autoethanogenum*". The main objective of this topic is to estimate the cumulative effects caused by this process across different midpoint indicators. So, the eleven process parameters were chosen based on the previous modeling work, and the sensitivity analysis was performed on the 11 process parameters. The major feedstock for the gas fermentation process is the BOF gas which is the steel mill emission. This BOF gas is utilized internally for heat and electricity requirements. In case of redirecting them for the IPA production this has to be replaced by an alternate method. The gas fermentation process also accounts for the impacts caused by these replacements. For 1 kg of IPA produced nearly 4.324 MJ of heat and 0.877 kWh of electricity has to be replaced for internal usage in the steel mill.

The components utilized for the gas fermentation are re-calibrated based on the functional unit of 1 kg IPA along with the steel mill replacements and emission credits. This re-calibration is done for all the sensitivity analysis cases to perform the impact assessments. Usually, the global warming potential is alone chosen for the LCA assessments which is the trade-off to the process as it does not account for the most impactful components that contribute to different indicators.

In our case, seven different midpoint impact categories were chosen to estimate the overall impacts of this production process model. The impact assessments were performed and the major contributor to the process is the usage of HP and LP steam utility and the glycerol usage for the extractive distillation process. The steam utility is the major contributor to impact categories of global warming potential, fine particulate matter formation, freshwater eutrophication, and human carcinogenic toxicity, and for the other impact categories like stratospheric ozone depletion, marine eutrophication, and land use, the glycerol is the major contributor. For the 11 process parameters of CO conversion, Volumetric mass transfer rate of CO, Product selectivity, Dilution rate, Extractive distillation glycerol mole fraction, Temperature offgas condenser, Anaerobic waste conversion, Extractive distillation molar reflux ratio, Biomass liq-liq mole fraction and the broth and glycerol purges, the same assessments are performed and the process parameter with the minimal impact value is identified. The dilution rate is the most influential process parameter, lowering the dilution rate of this process by -30% could significantly reduce the contributional utilization of steam (56.410%) and glycerol (12.066%) for the process when compared with the glycerol (12.990%) and steam (61.345%) of the base case scenario for the impact category of GWP. This process parameter could reach the GWP value of 20.464 kg CO_2 eq. which is a 26% decrease. lower than the base case. This lower value is estimated across all the midpoint indicators resulting in the overall least impactful process model. The emission credit for preventing the BOF gas from flaring plays a crucial role in reducing the impact values because if no exact requirements are met for the BOF gas, the BOF gas is flared which results in the emission of carbon dioxide. The CO_2 emission from the system is higher than the BOF gas needed for the process because the recovered glycerol from the distillation process is anaerobically digested and combusted resulting in higher CO_2 emission from the process of about 9.34 kg CO_2 eq. in which the glycerol alone accounts for 10% of total emission.

The other major reason for this assessment is to account for all the impacts in the process because the LCA for the pilot scale plant results are not coherent, and only GWP is estimated. And the contributors contributing less than 5% are neglected from the assessment calculation. The comparison study infers the situation by which the biomass waste produced alongside the IPA could end up in the environment y two different ways. First, the biomass waste is considered to be incinerated and the other way is to consider a treatment procedure to use it as an alternative to the soybean composition in the fish meal. The impact values for the fish meal are lower as the multifunctionality system expansion is applied to deduct the impact value of biomass waste as it could be considered as the co-product. The midpoint indicator impact value for GWP of biomass fish feed is 0.7 kgCO_2 eq. which is deducted as the base case scenario of 27.656 kg CO_2 eq. However, the EU has mandated laws to ban the use of GMOs in the region. Even though considering the lower impact value the incineration procedure appears to be the ideal situation and estimated that the BOF gas fermentation procedure would satisfy the 0.945% of global soybean demand.

To identify the process parameter scenario with the minimum impact value for all the impact categories, the base case along with the sensitivity cases were compared across the impact category values, and the process parameters with the lower value in each midpoint indicator were chosen to provide suggestions for the further optimization of the process. On an interesting note, the lowering of the Dilution rate process parameter value by -30% results in minimal impact values across all the midpoint indicators. The major suggestion is to optimize this process further by which the steam and glycerol usage could be lowered further to reduce the values. The human health indicator of carcinogenic toxicity is within the limits but high considering the normal values. The most contributional component glycerol used for the impact assessment study accessed from the ecoinvent database, is derived from the process of esterification of rapeseed oil, whereas the previous work suggests glycerol production through the fermentation method. This could result in an increase in impact values for the impact categories of SOD, ME, and LU. To conclude the impact assessment values for this BOF gas fermentation process are extremely treated when compared with the conventional IPA production method of 2.02 kg CO_2 eq. and further optimizing the overall process could lead to further lower in values. From the interpretation, it can be observed that by modifying the base case process model by lowering the dilution rate by -30% and glycerol mole fraction by -30%, -30% decrease in glycerol purge fraction and increasing volumetric mass transfer rate CO by 30% considering the base case values could result in lower overall impact value for the process across all the impact categories. This identification of process parameters was based on the impact assessment perspective, but if the modification is performed in the process a complete new impact assessment and interpretation study has to be performed and compared with the existing results. But the percentage study for the major contributors on the glycerol and steam utilization reveals that zero percent usage of steam and glycerol for the base case scenario results in the GWP impact category value of 6.16 kg CO_2 eq. which is still a 204.05% increase compared with the base case scenario. So, other components like NH_3, $NaOH$, and compressed air, etc., account for the impact category value. Reducing the utilization of steam and glycerol to less than 25% could yield a break-even impact value for the freshwater eutrophication (0.006761 kg P eq.) and a negative value (-0.0002 kg N eq.) for the impact category of marine eutrophication. A new process model should be modeled in terms of lowering the environmental impact values, as the lower impact values less than the base case values for the impact categories cannot be attained as the major product of IPA is the only product for the process. So, the impact values cannot be deducted for the co-products, leading to higher impact values. It also implies that the process model should be optimized so that an optimal value that will be higher than the conventional method will be obtained with the same process model unit process steps. However, the CO_2 emissions from the process can be sequestrated to lower the impact value of GWP by 43% in impact value. The impact category of water consumption should be added to the list of existing seven impact categories because the biotechnological process has high usage of water even though the impact category does not have an indicator for the direct effect on the ecosystem. Because this accounts for the resource usage and not the direct effects on the water bodies.

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A

Appendix A

A.1. BOF gas flaring in Steel mill

For the heat/electricity replacement in the steel for redirecting IPA and Preventing the CO_2 from emitting to the environment by preventing the flaring.

The BOF gas leaves the furnace at nearly $1100°C$ and the heat recovery and electricity generation for the internal supply. Since the BOF gas is flared after the generation process, it is flared for further heat generation as the major constituents of BOF gas like CO and H_2 combust with the presence of O_2 and emit CO_2 and water vapor. Since the BOF gas already has 20% of CO_2, it is not involved in the combustion reaction, and the amount of CO_2 gets added up during emission. This calculation is performed to assess the total amount of CO_2 is prevented by redirecting it to the IPA production instead of the flaring process

Calculated moles and kg of CO_2 and H_2O per mole and kg of BOF gas flared:

1 mole of BOF gas = 0.5 CO, 0.1 H_2, 0.2 CO_2, and 0.2 N_2

$$\mathrm{CO} + 0.5\mathrm{O_2} \rightarrow \mathrm{CO_2}$$
$$\mathrm{H_2} + 0.5\mathrm{O_2} \rightarrow \mathrm{H_2O}$$

Moles of $\mathrm{CO_2}$ produced from CO:

$$\text{Moles of } \mathrm{CO_2} = \text{mol conc. of CO} \times \text{molar ratio}(\mathrm{CO_2}/\mathrm{CO})$$
$$\text{Moles of } \mathrm{CO_2} = 0.5 \times (1/1) = 0.5 \text{ mol}$$

Moles of $\mathrm{CO_2}$ already present:

$$\text{Moles of } \mathrm{CO_2} = \text{mol conc. of } \mathrm{CO_2}$$
$$\text{Moles of } \mathrm{CO_2} = 0.2 \text{ mol}$$

Total moles of $\mathrm{CO_2}$ from 1 mole of BOF gas:

$$\text{1mole of } \mathrm{CO_2} = 0.5 + 0.2 = 0.7 \text{ moles } \mathrm{CO_2}$$

1 kg BOF gas contains:

$$\text{Mass of CO} = 0.5 \text{ mol} \times 28 \text{ g/mol} = 14.005 \text{ g} = 0.014 \text{ kg}$$
$$\text{Mass of } \mathrm{H_2} = 0.1 \text{ mol} \times 2 \text{ g/mol} = 0.2 \text{ g} = 0.0002 \text{ kg}$$
$$\text{Mass of } \mathrm{CO_2} = 0.2 \text{ mol} \times 44 \text{ g/mol} = 8.8 \text{ g} = 0.0088 \text{ kg}$$
$$\text{Mass of } \mathrm{N_2} = 0.2 \text{ mol} \times 28 \text{ g/mol} = 5.6 \text{ g} = 0.0056 \text{ kg}$$

$$\text{1 mole of BOF} = 0.0286 \text{ kg}$$
$$\text{34.965 moles of BOF} = \text{1 kg BOF gas}$$

1 mole of BOF gas:

$$\begin{aligned} &= 0.7 \text{ mol of } CO_2 \\ &= 0.7 \text{ mol} \times 44 \text{ g/mol} = 30.807 \text{ g} \end{aligned}$$

1 kg BOF gas:

$$\begin{aligned} &= 34.965 \text{ mol} = 24.4755 \text{ mol } CO_2 = 1.07716 \text{ kg } CO_2 \\ 1 \text{ kg BOF gas} &= 1.07716 \text{ kg } CO_2 \end{aligned}$$

Consuming 1 kg of BOF gas for IPA production instead of flaring them could save up to 1.07716 kg CO_2 from ending up in the environment. During the flaring process, two types of heat are liberated: Latent heat and Chemical heat during the conversion of BOF gas.

Latent heat:

$$\begin{aligned} &\Delta H = m \times C_p \times \Delta T \\ &\Delta T = (1100 - 169) + 273.15 \text{ K} = 1204.15 \text{ K} \\ &\Delta H_{\mathrm{CO}} = m_{\mathrm{CO}} \times C_p(\mathrm{CO}) \times \Delta T \\ &\Delta H_{\mathrm{CO}} = 0.014 \times 29.07 \times 1204.15 = 409.065 \text{ J} \\ &\Delta H_{\mathrm{H_2}} = m_{\mathrm{H_2}} \times C_p(\mathrm{H_2}) \times \Delta T \\ &\Delta H_{\mathrm{H_2}} = 0.0002 \times 28.82 \times 1204.15 = 6.9407 \text{ J} \\ &\Delta H_{\mathrm{CO_2}} = m_{\mathrm{CO_2}} \times C_p(\mathrm{CO_2}) \times \Delta T \\ &\Delta H_{\mathrm{CO_2}} = 0.0088 \times 37.13 \times 1205.15 = 393.498 \text{ J} \\ &\Delta H_{\mathrm{N_2}} = m_{\mathrm{N_2}} \times C_p(\mathrm{N_2}) \times \Delta T \\ &\Delta H_{\mathrm{N_2}} = 0.0056 \times 29.12 \times 1205.15 = 196.5262 \text{ J} \\ &\Delta H_{\mathrm{total}} = 409.065 + 6.9407 + 393.498 + 196.5262 = 1006.02 \text{ J} = 1.006 \text{ kJ} \end{aligned}$$

Total enthalpy change for 1 kg of BOF gas cooling from 1100°C to 25°C is 1.006 kJ of heat liberated.

Chemical heat during conversion:
Combustion of CO:

$$\begin{aligned} &CO + 0.5O_2 \rightarrow CO_2 \\ &\Delta G^\circ = \Sigma\Delta G^\circ \text{ of products} + \Sigma\Delta G^\circ \text{ of reactants} \\ &= (-394.36) - (-137.3 + [0.5 \times 0]) \\ &= -394.36 + 137.3 = -257.2 \text{ kJ/mol} \end{aligned}$$

At 169°C :

$$\begin{aligned} &\Delta G^\circ = \Delta G^\circ + RT/\ln(Q) \\ &\text{Equilibrium partial pressure (assuming gas behaves ideally) } P = 1 \text{ atm} \\ &\text{(Let us assume eq. conc. is directly proportional to stoichiometric Coeff)} \\ &\Pi \times V = n \\ &Q_p = \frac{P_{\mathrm{CO_2}}}{(P_{\mathrm{CO}} \times (P_{\mathrm{O_2}})^{0.5})} \\ &Q_p = \frac{(P_{\mathrm{CO_2}} \times 1.414)}{(0.5 \times P_{\mathrm{CO}} \times P_{\mathrm{O_2}})} \\ &Q_p = \frac{(101.325 \times 1.414)}{(0.5 \times 101.325 \times 101.325)} \\ &Q_p = 0.0279 \\ &\Delta G^\circ = -257200 + (8.314 \times 442 \times \ln(0.0279)) = -270.352 \text{ kJ/mol} \end{aligned}$$

Combustion of H_2:

$$\begin{aligned}
&H_2 + 0.5O_2 \rightarrow H_2O \\
&\Delta G^\circ = \Sigma\Delta G^\circ \text{ of products} + \Sigma\Delta G^\circ \text{ of reactants} \\
&= (-237.1) - (-0 + [-0]) \\
&= -237.1 \text{ kJ/mol}
\end{aligned}$$

At 1100°C:

$$\begin{aligned}
&\Delta G^\circ = \Delta G^\circ + RT/\ln(Q) \\
&\text{Equilibrium partial pressure (assuming gas behaves ideally) } P = 1 \text{ atm} \\
&\text{(Let's assume eq. conc. is directly proportional to stoichiometric coeff)} \\
&\Pi \times V = n \\
&Q_p = \frac{P_{H_2O}}{(P_{H_2} \times (P_{O_2})^{0.5})} \\
&Q_p = \frac{(P_{H_2O} \times 1.414)}{(0.1 \times P_{H_2} \times P_{O_2})} \\
&Q_p = \frac{(101.325 \times 1.414)}{(0.1 \times 101.325 \times 101.325)} \\
&Q_p = 0.1397 \\
&\Delta G^\circ = -237100 + (8.314 \times 442 \times \ln(0.1397)) = -244.333 \text{ kJ/mol}
\end{aligned}$$

For 1 mole of BOF gas, the molar composition is 50% CO, 10% H_2, 20% CO_2, and 20% N_2. and H_2 combustion For C_O combustion

$$\begin{aligned}
&\text{No. of moles of } CO = \Delta G \times \text{no. of mol of } CO \\
&\text{No. of moles of } CO = -270.352 \times 0.5 = -135.176kJ
\end{aligned}$$

For H_2 combustion

$$\begin{aligned}
&\text{No. of moles of } H_2 = \Delta G \times \text{no. of mol of } CO \\
&\text{No. of moles of } H_2 = -244.433 \times 0.1 = -24.4433kJ
\end{aligned}$$

$$\begin{aligned}
&\text{1 mole of BOF gas} = CO \text{ combustion} + H_2 \text{ combustion} \\
&\text{1 mole of BOF gas} = -135.176 - 24.4433 = -159.6093\text{kJ} \\
&\text{1 kg of BOF gas} = 34.965 \text{ mol BOF} \times 159.6093\text{kJ} = -5580.74\text{kJ} \\
&\text{1 kg of IPA} = 9.415716 \times 5580.74\text{kJ} = 52.74756\text{MJ}
\end{aligned}$$

The CO and H_2 after reaction with oxygen produce the energy of 52.74756 MJ for 9.415 kg BOF gas. This energy is considered a replacement for steel mills, as it is not utilized for heat/ electricity generation as it is used for IPA production.

A.2. Heat and Electricity replacement in Steel mill

The BOF gas enters the heat exchanger process after the emission from the Blast oxygen furnace. And the temperature of the BOF gas was reduced to 169°C from 1100°C (Brouwer, 2023). 100% BOF gas is considered in the Base case calculations,

$$\begin{aligned}
&\text{1 kg IPA} = 9.451716kgBOFgas \\
&\text{For most industrial gasses,} C_p = 1kJ/kgK \\
&\Delta T_{BOF} = (1100 - 169) + 273 = 1204\text{K} \\
&Q_{BOF} = m_{BOF} \times C_p \times \Delta T \\
&Q_{BOF} = 9.451716 \times 1 \times 1204 = 11379.004kJ
\end{aligned}$$

Considering the heat exchanger efficiency in the steel mill of Tata Steel (Keys, 2019). 38% efficiency is considered. And the heat-to-electricity ratio is 1.37.

$$\begin{aligned}&38\% \times 11379.004kJ = 4324.02152kJ = 4.3241MJ\\&\text{Electricity generated} = \text{Energy from heat / heat to electricity ratio}\\&\text{Electricity generated} = 4324.02152/1.37 = 3156.22kJ = 0.87672\text{kWh}\end{aligned}$$

Considering 1 kg of IPA production, nearly 9.45 kg of BOF is required. Suppose the BOF gas from the steel mill is redirected for IPA production. In that case, the steel mill has to look for the replacement of heat and electricity generated for internal use. Nearly, 0.876 kWh if 9.45 kg of BOF gas is redirected.

A.3. Biomass waste incineration

The biomass waste that is generated during the IPA process, $CH_{1.75}O_{0.5}N_{0.25}$ was incinerated with the presence of oxygen and CO_2, water and N_2 were emitted from the process.

$$CH_{1.75}O_{0.5}N_{0.25} + 1.5\text{O}_2 \rightarrow 1.75\text{CO}_2 + 0.25\text{H}_2\text{O} + \text{N}_2$$

$$\begin{aligned}\Delta G^\circ &= \Sigma\Delta G^\circ \text{ of products} + \Sigma\Delta G^\circ \text{ of reactants}\\&= (-698.173 - 60.498 - 4.95636) - (-71.956 - 7.4545)\\&= -763.61836 - (-79.39054)\\&= -684.22782 \text{ kJ/mol}\end{aligned}$$

The biomass comes out of the process at 37°C

$$\begin{aligned}\Delta G^\circ &= \Delta G^\circ + R(T1 - T2)/\ln(P1/P2)\\\Delta G^\circ &= \Delta G^\circ + (8.314 \times -12 \times \ln(1.380))\\\Delta G^\circ &= -684.267 \text{ kJ/mol}\end{aligned}$$

1 mol of $CH_{1.75}O_{0.5}N_{0.25}$ liberates -684.267 KJ/mol.

Molarmass of $CH_{1.75}O_{0.5}N_{0.25}$= 25.2705 g/mol 1 kg of this biomass waste generation has 39.5712 moles which generates about 26.8052 MJ of energy as heat.

When considering the treated biomass waste as fish feed, there are no losses during the treatment.

A.4. Replacing the world demand for Soybean meal

The reports from World Steel (WSA, 2021) indicate that the annual production of steel is about 1.4 billion tonnes and each ton of steel production involves the emission of CO2 of about 1.8 tons of CO2. So, the total emission would be 2.5×10^9 ton of CO_2. If the total emission of carbon dioxide can be captured for our BOF gas fermentation process.

$$\begin{aligned}&\text{1kg of IPA requires} = 10.18\text{kg of CO}_2\\&\text{So,}2.5 \times 10^9\text{CO}_2\text{produces} = 247.91 \times 10^3 ton\text{IPA}\\&\text{1kg of IPA Co-produces} = 0.07957\text{kg Biomass waste}\\&\text{So,}247.91 \times 10^3 ton\text{IPA produces} = 19.7124 \times 10^3\text{ton Biomass out}\end{aligned}$$

Through the BOF gas fermentation method, 19712.4 tons of Biomass waste can be generated, which will be treated with a waste treatment procedure and can be utilized as a replacement for the Soybean meal. As already described in the previous part about the procedure and research study. The total demand for the soybean meal was identified. And a calculation is performed to know, whether the soybean meal demand can be satisfied with the treated biomass waste. Soybean meal production is one of the huge productions that is carried out throughout the world to satisfy all the needs of living beings. Global soy production is used widely in three different sectors namely, as direct human feed, as animal feed, and industry for the production of bio-diesel, lubricants, and other essential products. The World soybean usage according to 2021 is 372.85 million tons (Ritchie & Roser, 2024). Of these nearly 5.6% of the soy production is consumed only for the aquaculture sector (Ritchie & Roser, 2024).

$$5.6\% of 372.85 million\ ton = 20.8465 \times 10^6 ton$$

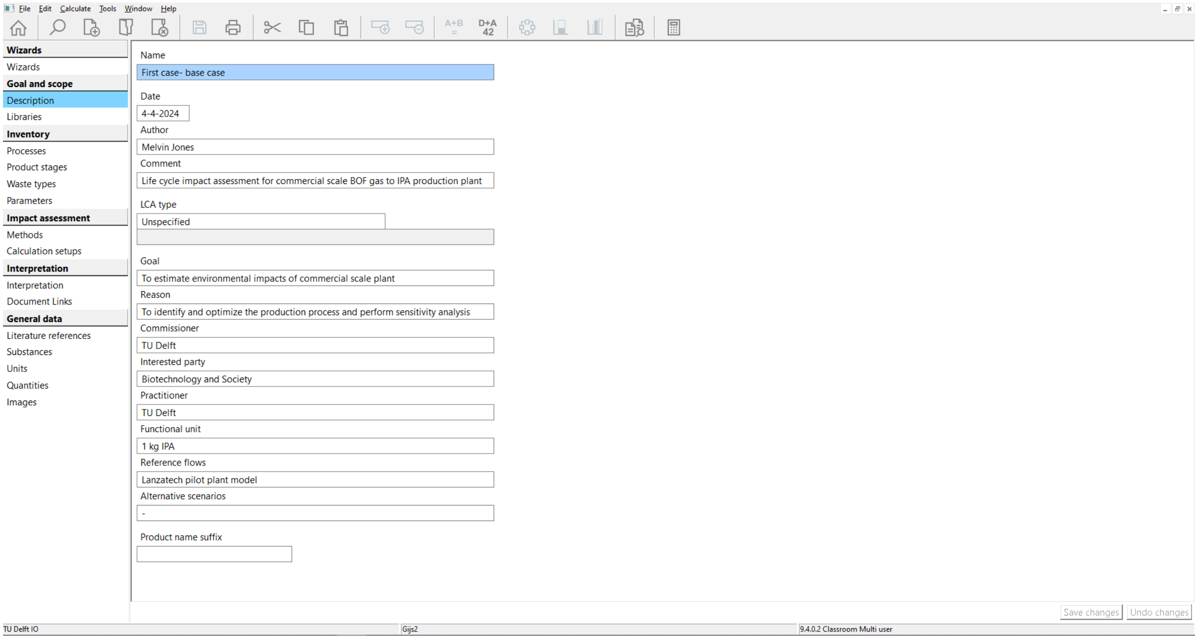
The treated biomass waste as a replacement for the soybean meal aquaculture feed demand could only be able to replace **0.0945%.** This replacement value is very low. But by considering this method, the biomass waste could be treated and sent to other industries rather than incinerated, accounting for the carbon dioxide and nitrogen emissions.

B

Appendix B

B.1. LCA using SimaPro software

The main goal of this LCA work using this software is to estimate the environmental impacts of the commercial scale model, and the reason for this project work is to identify and optimize the production process and perform different sensitivity analysis scenarios. Then the functional unit "1 kg IPA" was defined. The Lanzatech pilot scale plant model is considered the reference flow for this project. No scenarios were considered as alternative scenarios for this system. This tool has certain stages listed on the left side. These are the order of the stages in which the LCA work has to be performed. Isopropyl alcohol is produced through this route because it is considered biogenic as it is derived from living organisms.



Name: First case- base case

Date: 4-4-2024

Author: Melvin Jones

Comment: Life cycle impact assessment for commercial scale BOF gas to IPA production plant

LCA type: Unspecified

Goal: To estimate environmental impacts of commercial scale plant

Reason: To identify and optimize the production process and perform sensitivity analysis

Commissioner: TU Delft

Interested party: Biotechnology and Society

Practitioner: TU Delft

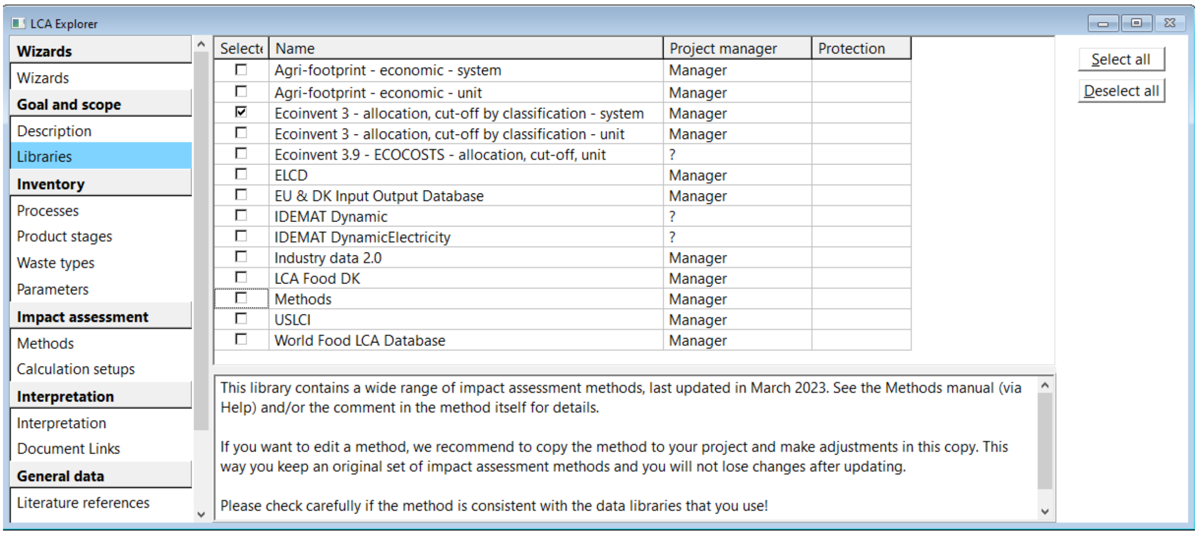
Functional unit: 1 kg IPA

Reference flows: Lanzatech pilot plant model

Alternative scenarios: -

Product name suffix:

Figure B.1: Defining the scope and purpose of LCA work



Selecte	Name	Project manager	Protection
☐	Agri-footprint - economic - system	Manager	
☐	Agri-footprint - economic - unit	Manager	
☑	Ecoinvent 3 - allocation, cut-off by classification - system	Manager	
☐	Ecoinvent 3 - allocation, cut-off by classification - unit	Manager	
☐	Ecoinvent 3.9 - ECOCOSTS - allocation, cut-off, unit	?	
☐	ELCD	Manager	
☐	EU & DK Input Output Database	Manager	
☐	IDEMAT Dynamic	?	
☐	IDEMAT DynamicElectricity	?	
☐	Industry data 2.0	Manager	
☐	LCA Food DK	Manager	
☐	Methods	Manager	
☐	USLCI	Manager	
☐	World Food LCA Database	Manager	

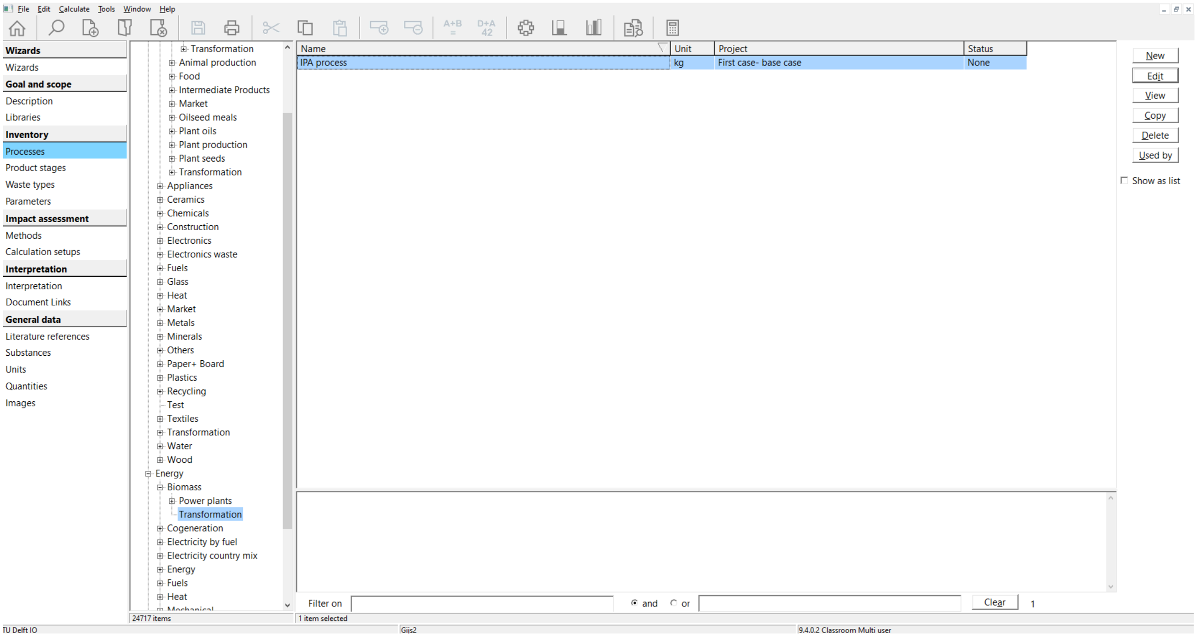
This library contains a wide range of impact assessment methods, last updated in March 2023. See the Methods manual (via Help) and/or the comment in the method itself for details.

If you want to edit a method, we recommend to copy the method to your project and make adjustments in this copy. This way you keep an original set of impact assessment methods and you will not lose changes after updating.

Please check carefully if the method is consistent with the data libraries that you use!

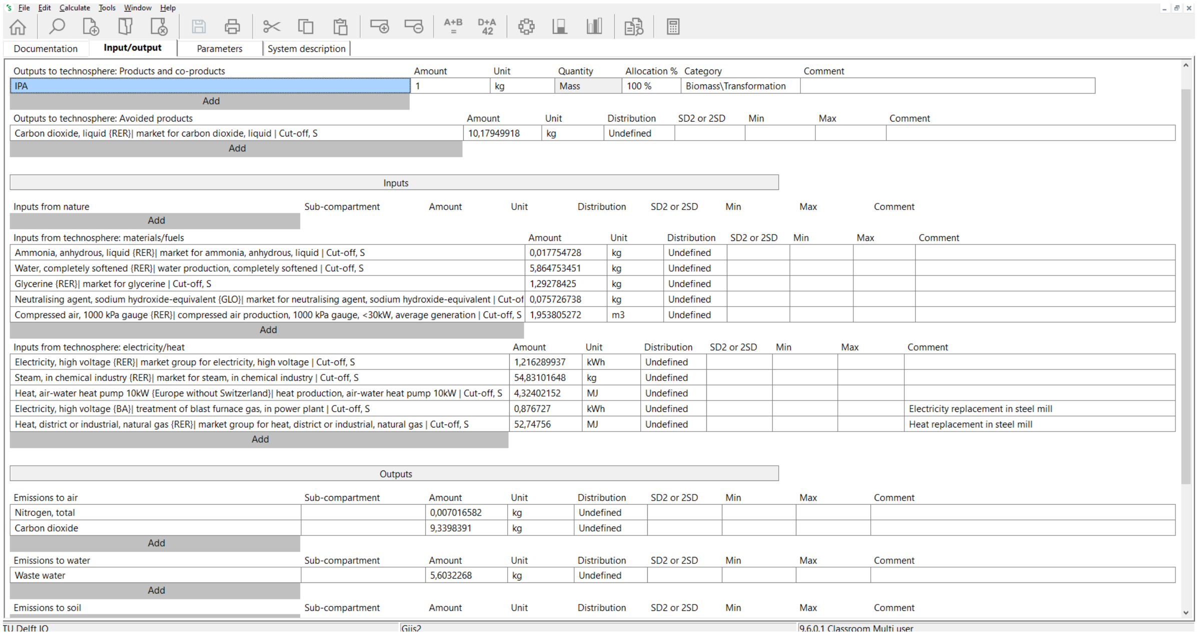
Figure B.2: Defining the database in SimaPro

Next, the process is created in the process area of the inventory stages. The process named IPA process is created in the Biomass transformation section in the tab. The process is created by inputting all the inputs and outputs for the particular IPA process.



Name	Unit	Project	Status
IPA process	kg	First case- base case	None

Figure B.3: Creating the process in Inventory stage



Outputs to technosphere: Products and co-products	Amount	Unit	Quantity	Allocation %	Category	Comment
IPA	1	kg	Mass	100 %	Biomass\Transformation	

Outputs to technosphere: Avoided products	Amount	Unit	Distribution	SD2 or 2SD	Min	Max	Comment
Carbon dioxide, liquid {RER}| market for carbon dioxide, liquid | Cut-off, S	10,17949918	kg	Undefined				

Inputs

Inputs from nature	Sub-compartment	Amount	Unit	Distribution	SD2 or 2SD	Min	Max	Comment

Inputs from technosphere: materials/fuels	Amount	Unit	Distribution	SD2 or 2SD	Min	Max	Comment
Ammonia, anhydrous, liquid {RER}| market for ammonia, anhydrous, liquid | Cut-off, S	0,017754728	kg	Undefined				
Water, completely softened {RER}| water production, completely softened | Cut-off, S	5,864753451	kg	Undefined				
Glycerine {RER}| market for glycerine | Cut-off, S	1,29278425	kg	Undefined				
Neutralising agent, sodium hydroxide-equivalent {GLO}| market for neutralising agent, sodium hydroxide-equivalent | Cut-of	0,075726738	kg	Undefined				
Compressed air, 1000 kPa gauge {RER}| compressed air production, 1000 kPa gauge, <30kW, average generation | Cut-off, S	1,953805272	m3	Undefined				

Inputs from technosphere: electricity/heat	Amount	Unit	Distribution	SD2 or 2SD	Min	Max	Comment
Electricity, high voltage {RER}| market group for electricity, high voltage | Cut-off, S	1,216289937	kWh	Undefined				
Steam, in chemical industry {RER}| market for steam, in chemical industry | Cut-off, S	54,83101648	kg	Undefined				
Heat, air-water heat pump 10kW {Europe without Switzerland}| heat production, air-water heat pump 10kW | Cut-off, S	4,32402152	MJ	Undefined				
Electricity, high voltage {BA}| treatment of blast furnace gas, in power plant | Cut-off, S	0,876727	kWh	Undefined				Electricity replacement in steel mill
Heat, district or industrial, natural gas {RER}| market group for heat, district or industrial, natural gas | Cut-off, S	52,74756	MJ	Undefined				Heat replacement in steel mill

Outputs

Emissions to air	Sub-compartment	Amount	Unit	Distribution	SD2 or 2SD	Min	Max	Comment
Nitrogen, total		0,007016582	kg	Undefined				
Carbon dioxide		9,3398391	kg	Undefined				

Emissions to water	Sub-compartment	Amount	Unit	Distribution	SD2 or 2SD	Min	Max	Comment
Waste water		5,6032268	kg	Undefined				

Emissions to soil	Sub-compartment	Amount	Unit	Distribution	SD2 or 2SD	Min	Max	Comment

Figure B.4: Defining the process input and output

In this step all the required inputs for the Input to technosphere, emissions from the process and the outputs to technosphere were entered and further calculations steps and the methods to perform the impact assessment were chosen. In this case, the requirement of the midpoint category was compensated by choosing the ReCiPe 2016 Midpoint (H) method for the calculation. Then the impact assessment for 1 kg IPA is performed and the midpoint category results can be viewed.

C

Appendix C

C.1. Verification methodology

C.1.1. Verification methodology: KPI of CO conversion

The verification methodology of the KPI of CO conversion, the % change in the values for the impact categories when comparing the predicted values and the calculated values are in the range of 2E-06 % to 1E-05. These minor changes in the value can be neglected and the methodology can be applied for the impact assessment where the base case scenario and the sensitivity case scenario components are the same. Applying this methodology tends to reduce the complexity of the SimaPro tool by which only the base case can be altered and all the sensitivity cases can be performed with negligible errors in the range of 1E-06 %. The impact category of the KPI compares the change for both the lowerbound and upperbound cases. Only the components that vary when the KPIs are altered are alone performed verification methodology for this study. The rest of the components like heat replacement, electricity replacement, and the BOF gas prevented from flaring do not vary, as they remain constant due to the calculations per kg of IPA. And the emission of nitrogen stays inert. For the case of wastewater, the particular impact category of water consumption is not considered for the impact assessment study, so it is neglected. The graphs represented below represent the percentage change for the lower bound and upper bound for each midpoint category.

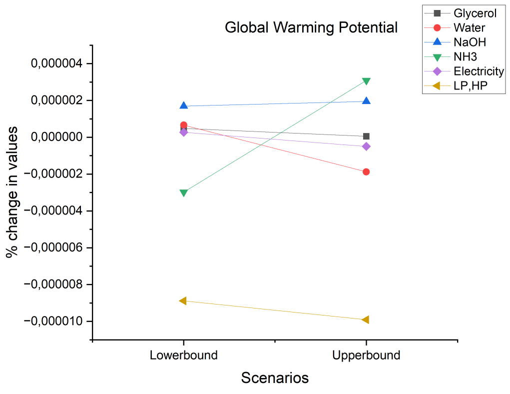


Figure C.1: GWP: CO conversion KPI

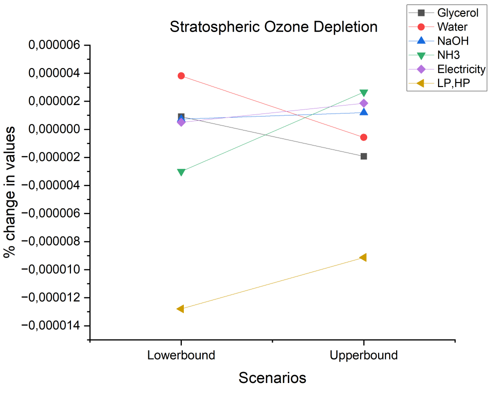


Figure C.2: SOD: CO conversion KPI

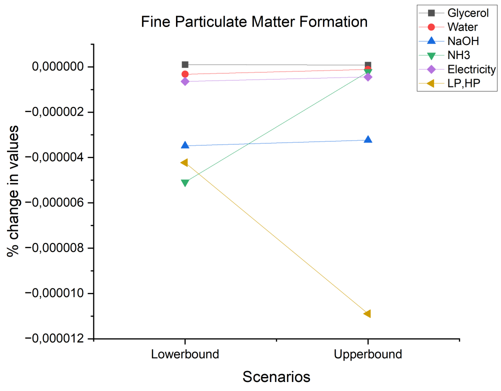


Figure C.3: FPMF: CO conversion KPI

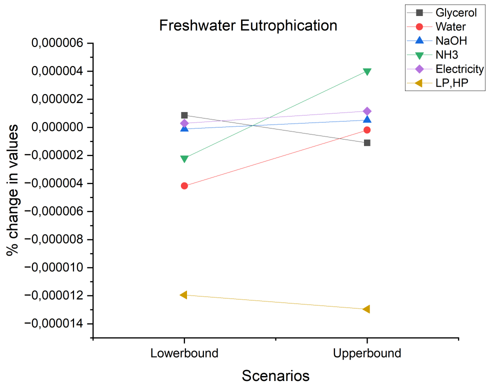


Figure C.4: FE: CO conversion KPI

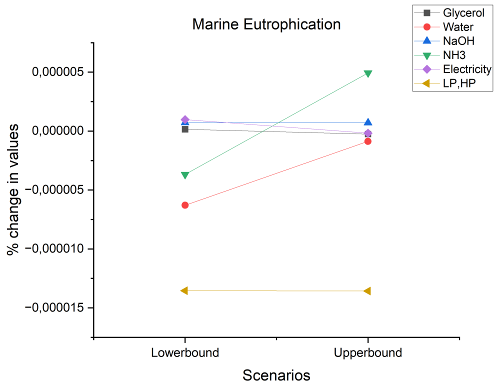


Figure C.5: ME: CO conversion KPI

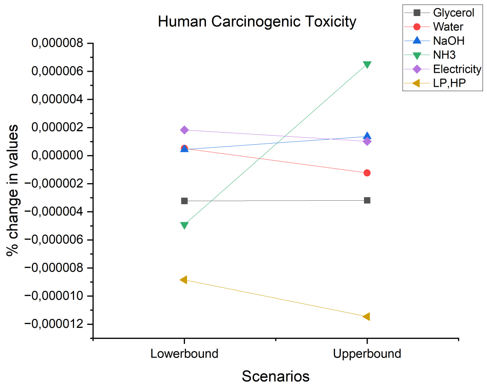


Figure C.6: HCT: CO conversion KPI

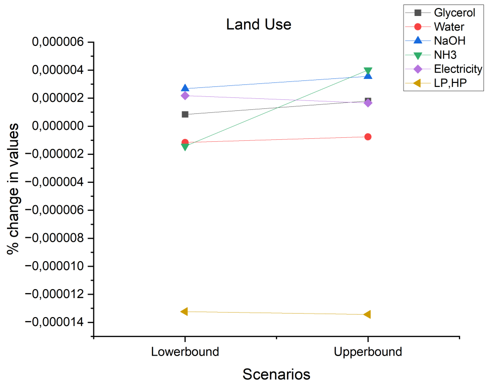


Figure C.7: LU: CO conversion KPI

C.1.2. Verification methodology: KPI of Volumetric Mass transfer rate of CO

When comparing the predicted values with the calculated values, the % change in the category values for the Volumetric mass transfer rate of the CO KPI verification methodology falls between the range of 3E-06 and 1.2E-05 for both lower bound and upper bound sensitivity cases.

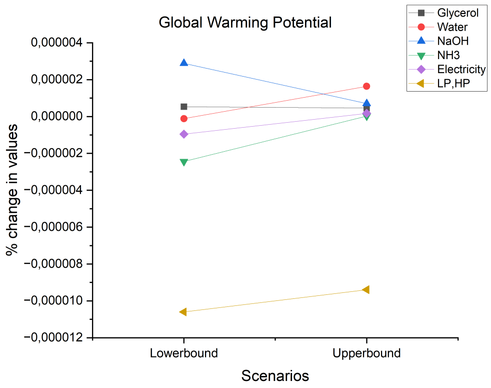


Figure C.8: GWP: Volumetric Mass transfer rate of CO

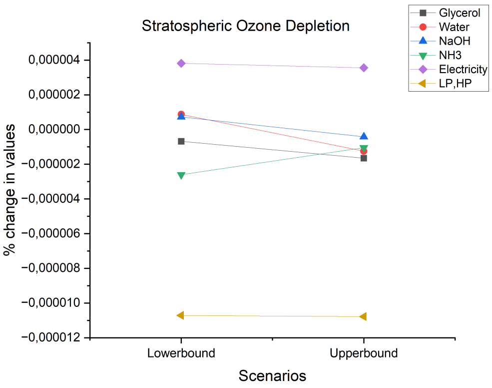


Figure C.9: SOD: Volumetric Mass transfer rate of CO

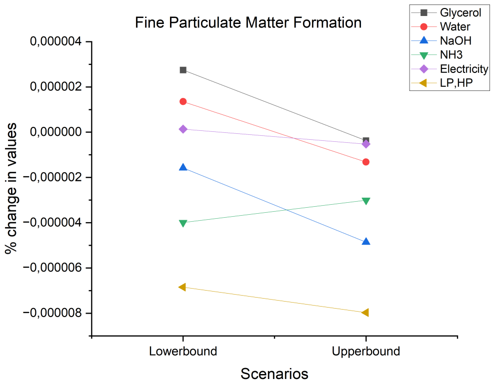


Figure C.10: FPMF: Volumetric Mass transfer rate of CO

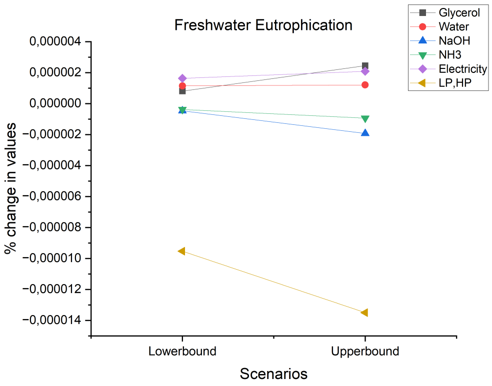


Figure C.11: FE: Volumetric Mass transfer rate of CO

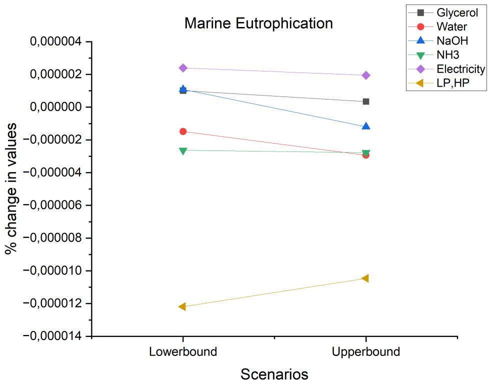


Figure C.12: ME: Volumetric Mass transfer rate of CO

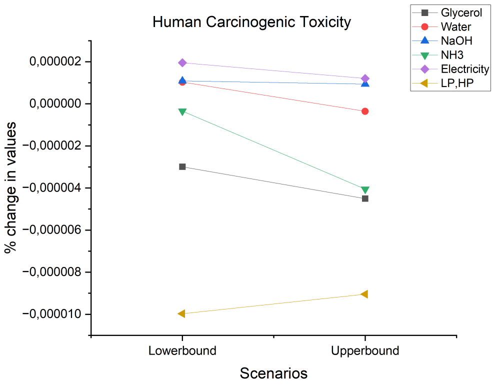


Figure C.13: HCT: Volumetric Mass transfer rate of CO

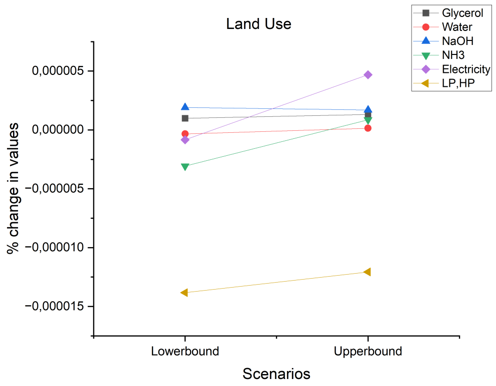


Figure C.14: LU: Volumetric Mass transfer rate of CO

C.1.3. Verification methodology: KPI of Product Selectivity

The verification methodology of the KPI of Product selectivity, the % change in the values for the impact categories when comparing the predicted values and the calculated values are in the range of 2E-06 % to 1E-05. The graph below represents the comparison for both the lowerbound and upperbound.

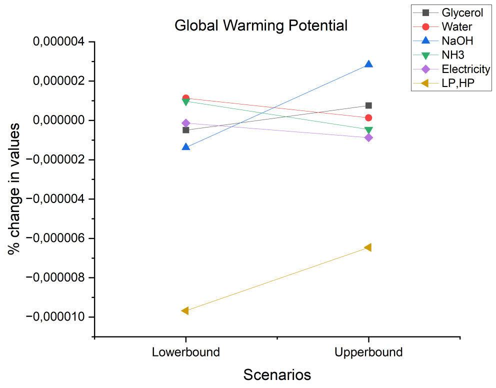


Figure C.15: GWP: Product Selectivity

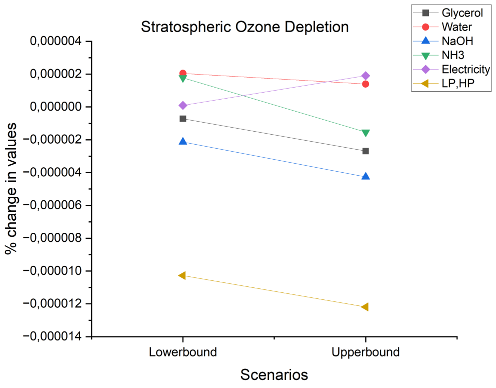


Figure C.16: SOD: Product Selectivity

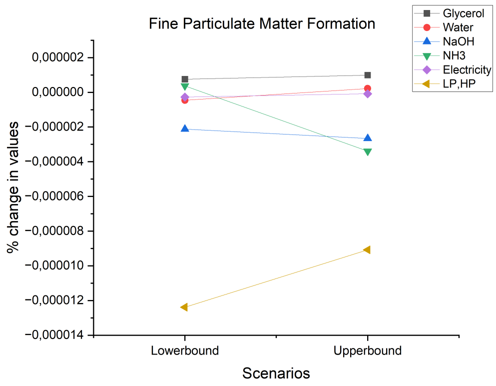


Figure C.17: FPMF: Product Selectivity

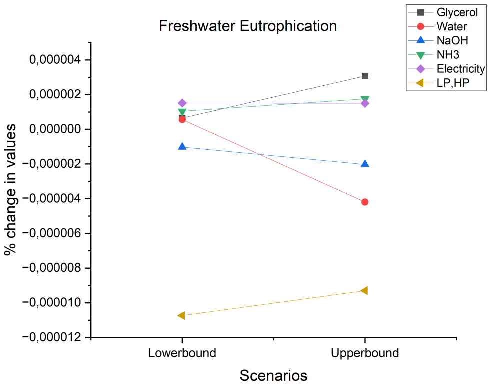


Figure C.18: FE: Product Selectivity

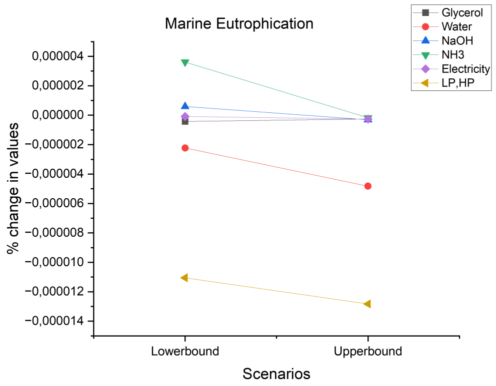


Figure C.19: ME: Product Selectivity

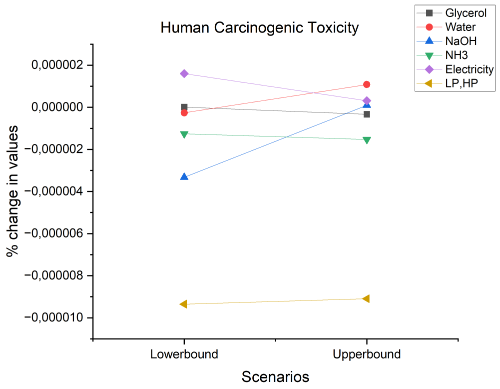


Figure C.20: HCT: Product Selectivity

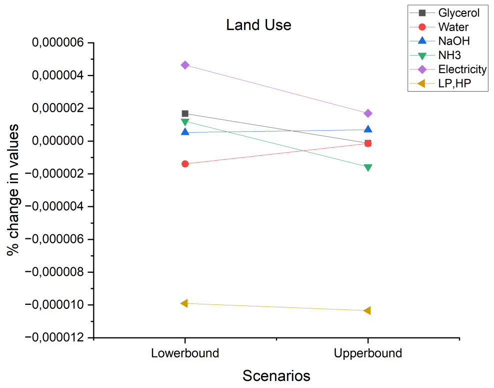


Figure C.21: LU: Product Selectivity

C.1.4. Verification methodology: KPI of Dilution Rate

The graphs below represent the comparison of the predicted values with the calculated values. the % change in the effect category values for the Dilution rate KPI verification method falls between 1E-06 and 1E-05.

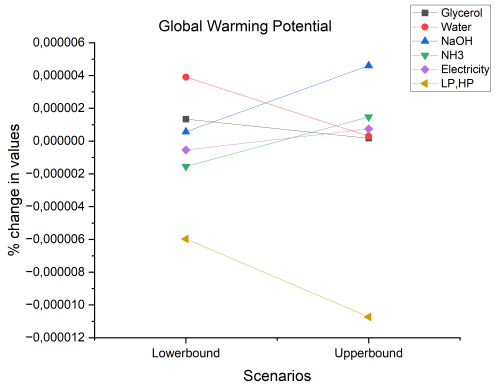


Figure C.22: GWP: Dilution Rate

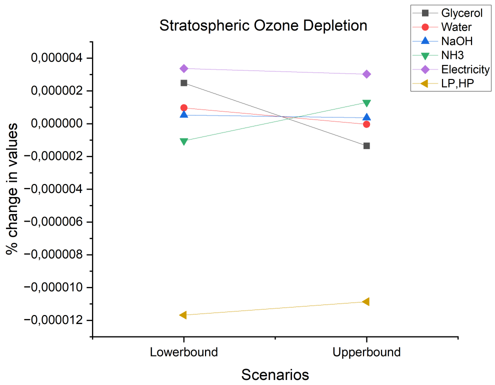


Figure C.23: SOD: Dilution Rate

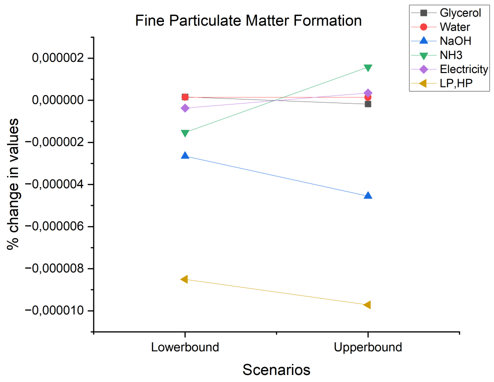


Figure C.24: FPMF: Dilution Rate

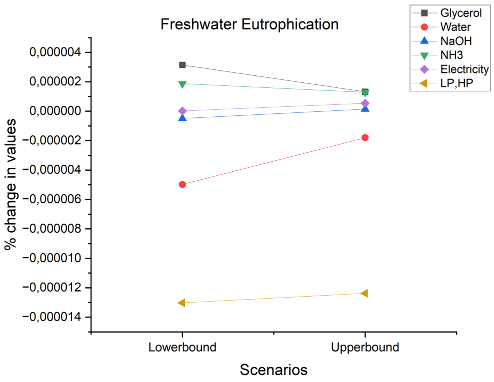


Figure C.25: FE: Dilution Rate

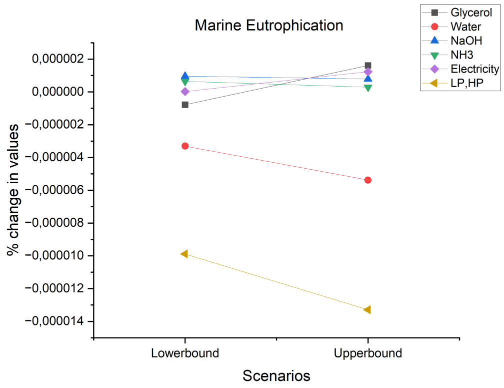


Figure C.26: ME: Dilution Rate

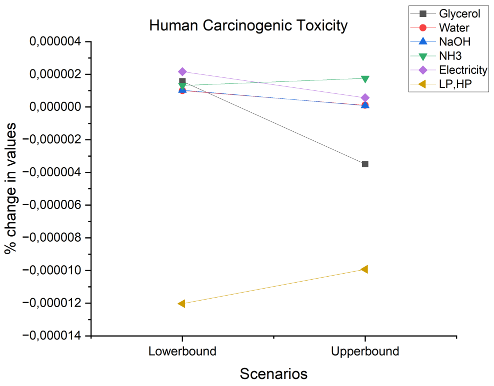


Figure C.27: HCT: Dilution Rate

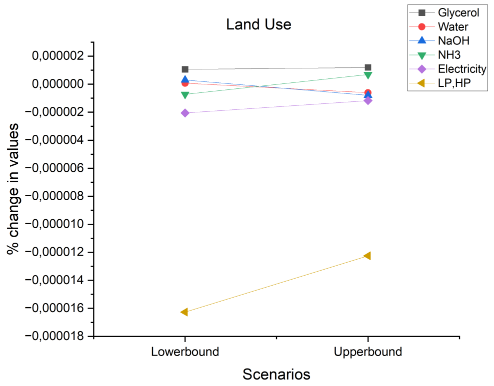


Figure C.28: LU: Dilution Rate

C.1.5. Verification methodology: Glycerol mole fraction

When comparing the predicted values with the calculated values, the % change in the effect category values for the Glycerol mole fraction KPI, the verification methodology ranges between 1E-06 and 1E-05 for both the lower and upper bounds.

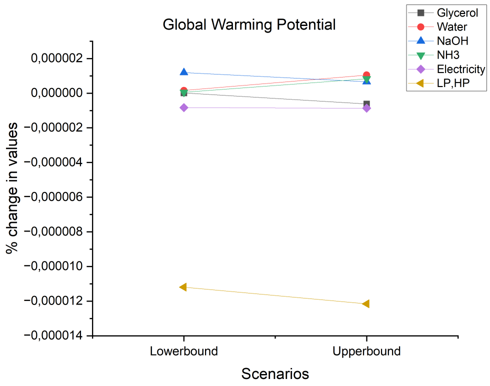


Figure C.29: GWP: Glycerol mole fraction

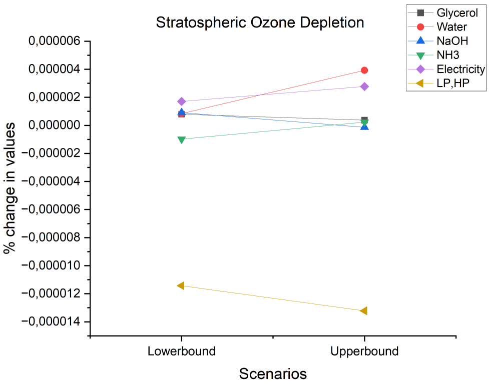


Figure C.30: SOD: Glycerol mole fraction

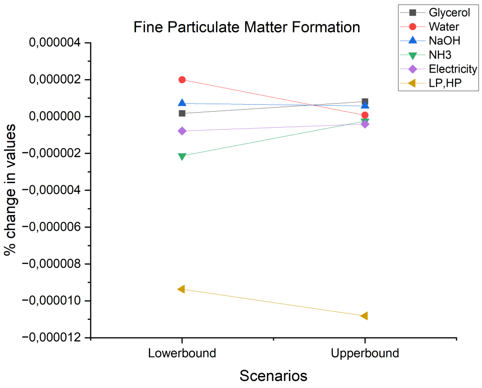


Figure C.31: FPMF: Glycerol mole fraction

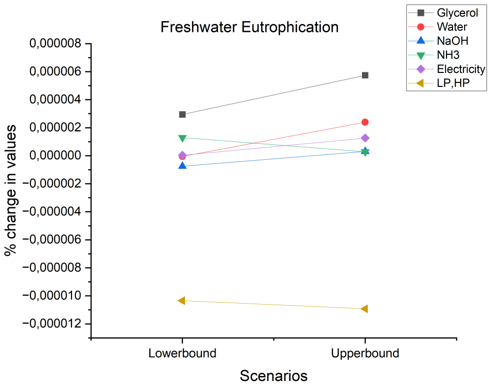


Figure C.32: FE: Glycerol mole fraction

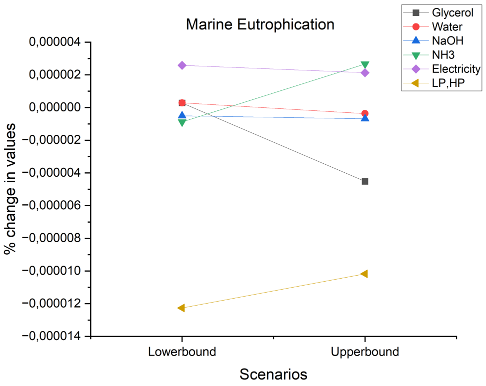


Figure C.33: ME: Glycerol mole fraction

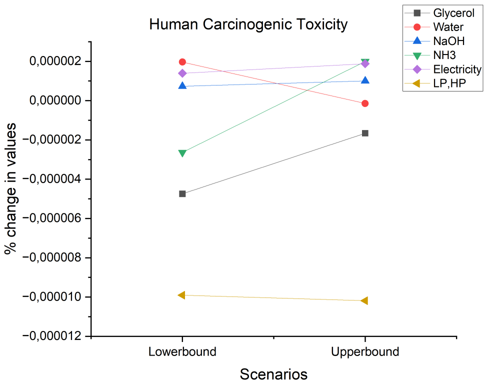


Figure C.34: HCT: Glycerol mole fraction

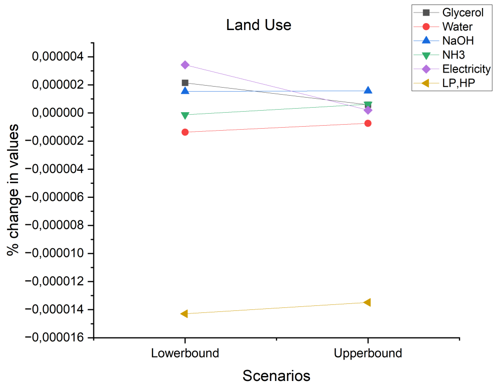


Figure C.35: LU: Glycerol mole fraction

C.1.6. Verification methodology: Temperature Offgas condenser

When comparing the predicted values with the calculated values, the % change in the effect category values for the Temperature offgas condenser KPI, the verification method ranges between 1E-06.

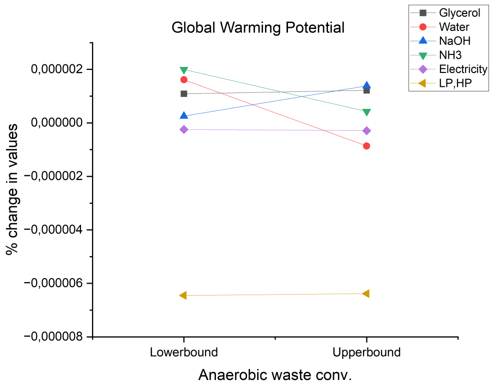


Figure C.36: GWP: Temperature Offgas condenser

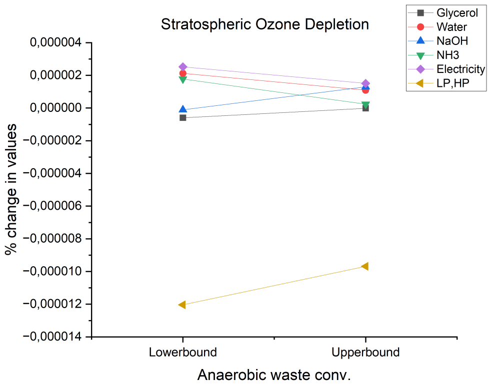


Figure C.37: SOD: Temperature Offgas condenser

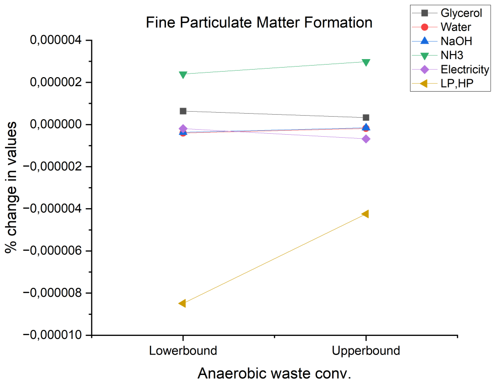


Figure C.38: FPMF: Temperature Offgas condenser

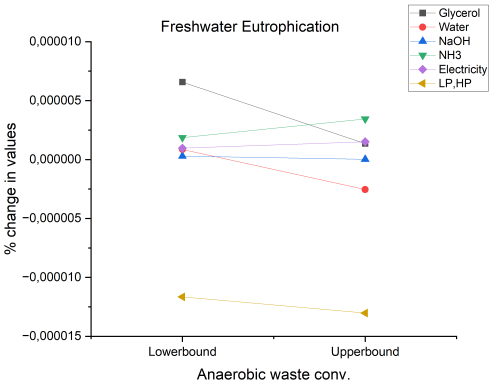


Figure C.39: FE: Temperature Offgas condenser

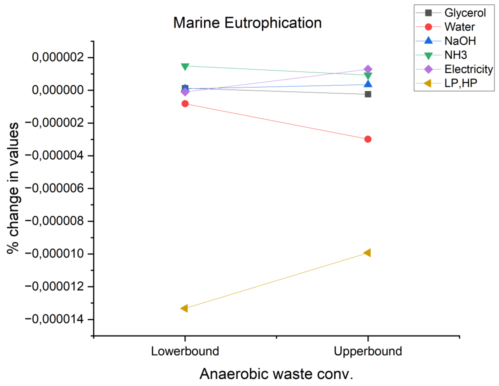


Figure C.40: ME: Temperature Offgas condenser

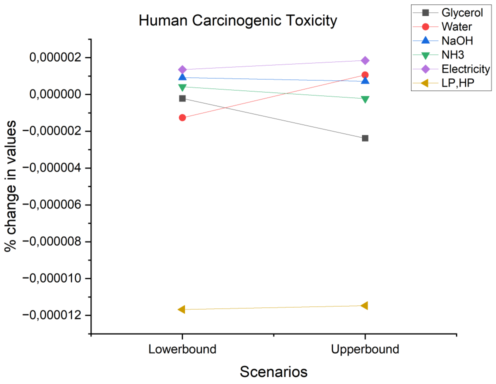


Figure C.41: HCT: Temperature Offgas condenser

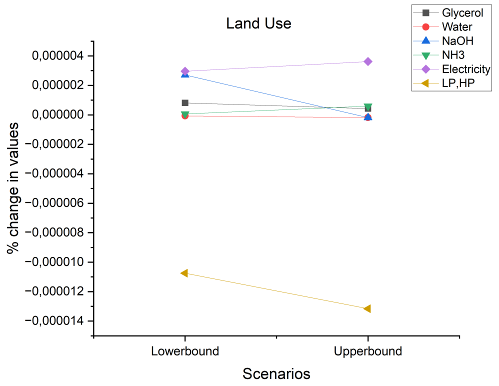


Figure C.42: LU: Temperature Offgas condenser

C.1.7. Verification methodology: Anaerobic waste conversion

When comparing the predicted values with the calculated values, the % change in the effect category values for the anaerobic waste conversion KPI, the verification method ranges between 1E-06 and 1E-05 for both the lower and upper bound case scenarios.

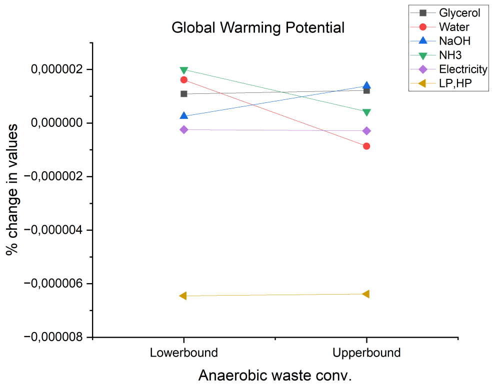


Figure C.43: GWP: Anaerobic waste conversion

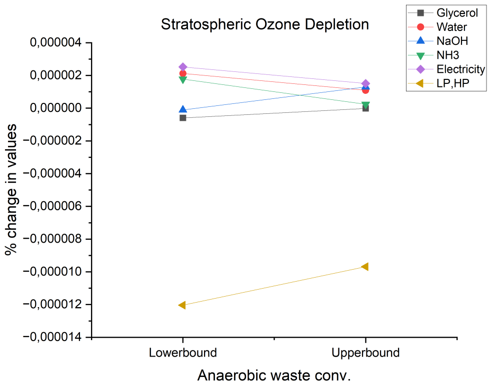


Figure C.44: SOD: Anaerobic waste conversion

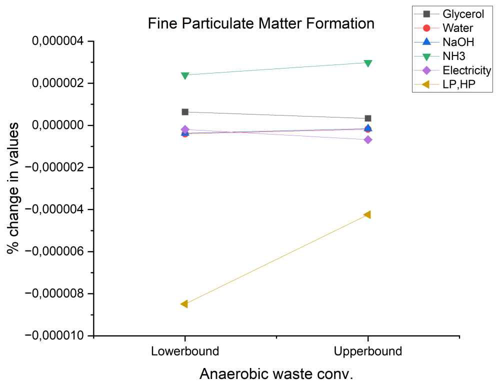


Figure C.45: FPMF: Anaerobic waste conversion

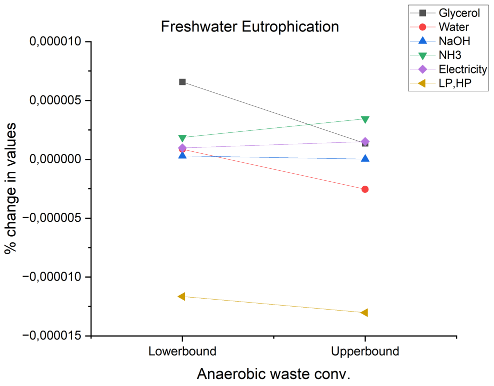


Figure C.46: FE: Anaerobic waste conversion

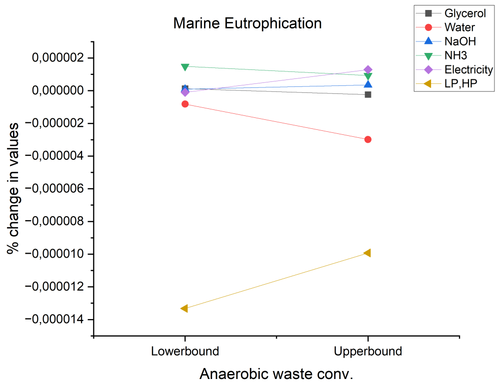


Figure C.47: ME: Anaerobic waste conversion

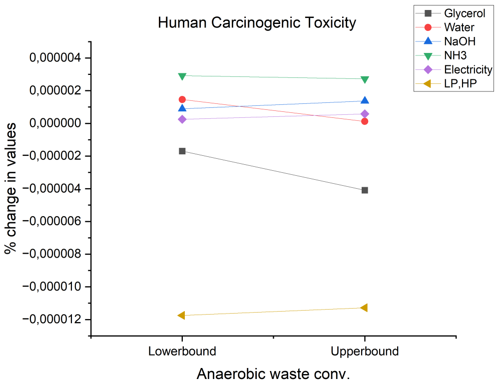


Figure C.48: HCT: Anaerobic waste conversion

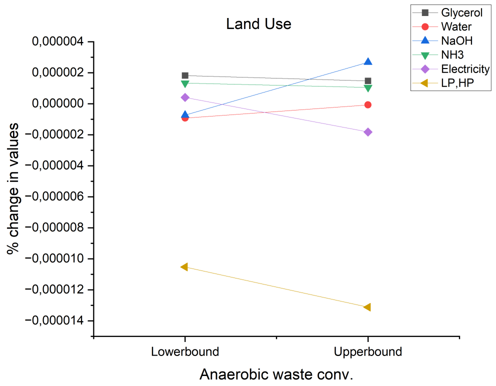


Figure C.49: LU: Anaerobic waste conversion

C.1.8. Verification methodology: Extractive distillation molar reflux ratio

When comparing the predicted values with the calculated values, the % change in the effect category values for the Extractive distillation molar reflux ratio KPI, the verification method ranges between 1E-06 and 1E-05 for both the lower and upper bound case scenarios.

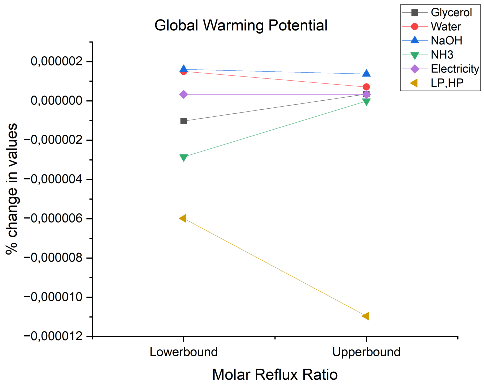


Figure C.50: GWP: Extractive distillation molar reflux ratio

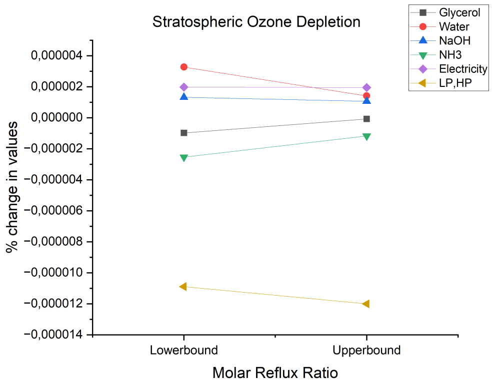


Figure C.51: SOD: Extractive distillation molar reflux ratio

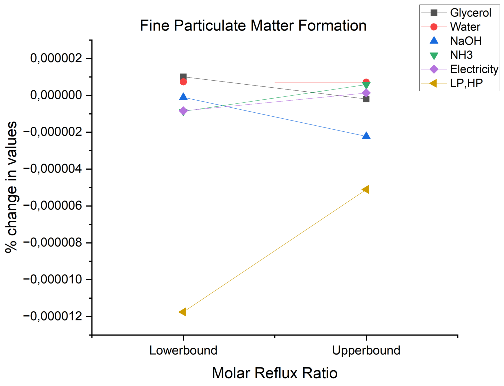


Figure C.52: FPMF: Extractive distillation molar reflux ratio

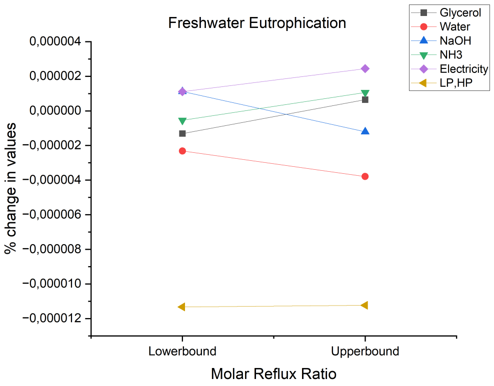


Figure C.53: FE: Extractive distillation molar reflux ratio

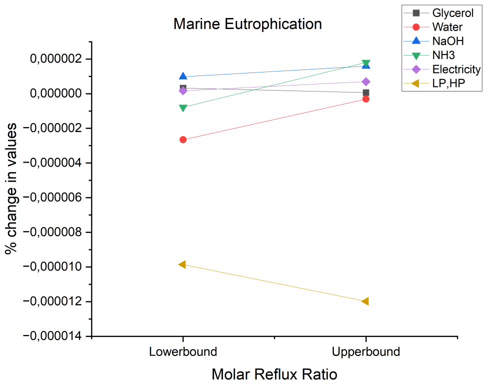


Figure C.54: ME: Extractive distillation molar reflux ratio

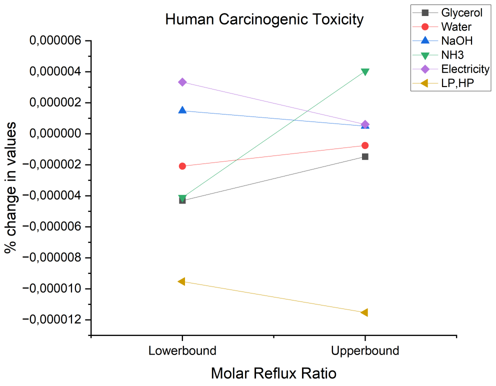


Figure C.55: HCT: Extractive distillation molar reflux ratio

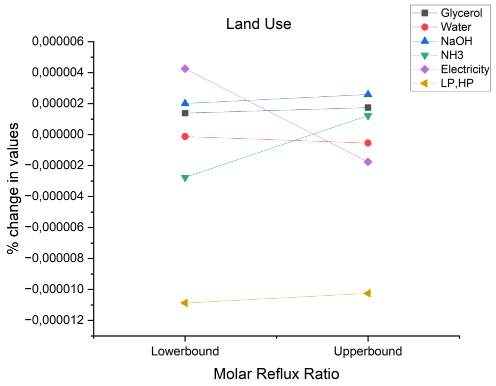


Figure C.56: LU: Extractive distillation molar reflux ratio

C.1.9. Verification methodology: Biomass filtration liq-liq mole fraction

When comparing the predicted values with the calculated values, the % change in the effect category values for the Biomass filtration liq-liq mole fraction KPI, the verification method ranges between 1E-06 and 1E-05 for both the lower and upper bound case scenarios.

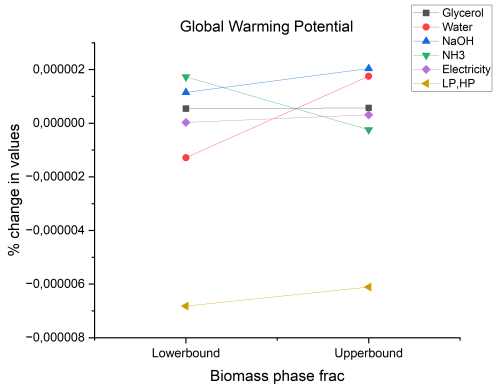


Figure C.57: GWP: Biomass filtration liq-liq mole fraction

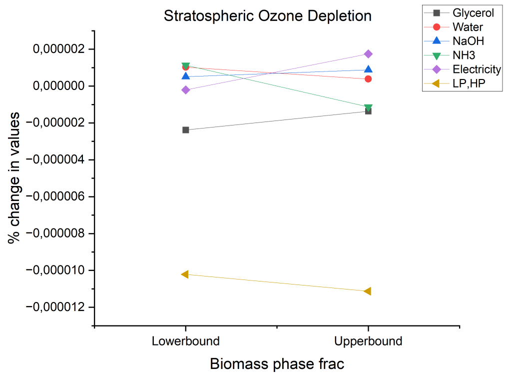


Figure C.58: SOD: Biomass filtration liq-liq mole fraction

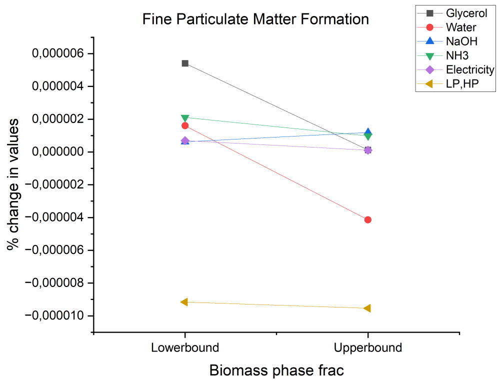


Figure C.59: FPMF: Biomass filtration liq-liq mole fraction

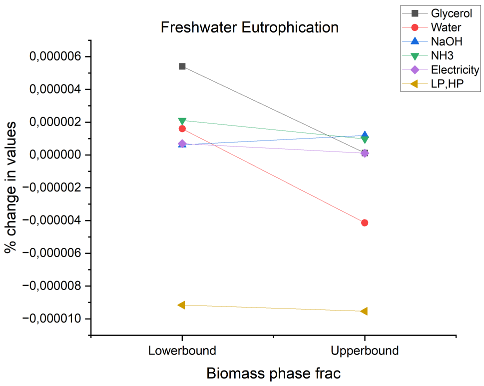


Figure C.60: FE: Biomass filtration liq-liq mole fraction

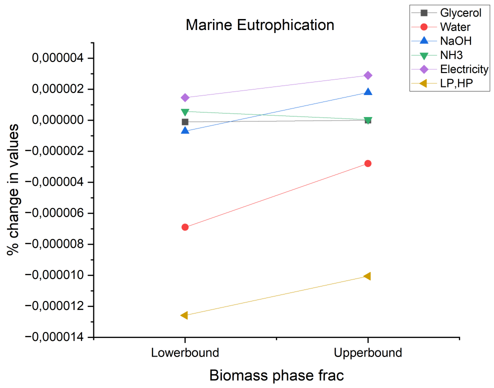


Figure C.61: ME: Biomass filtration liq-liq mole fraction

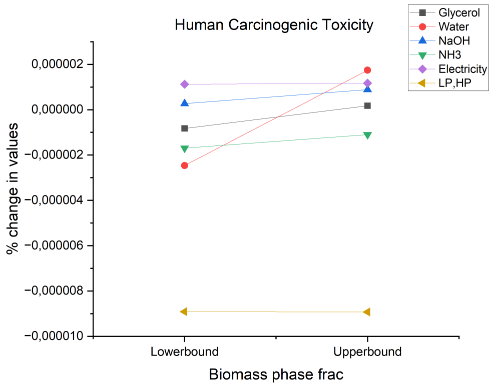


Figure C.62: HCT: Biomass filtration liq-liq mole fraction

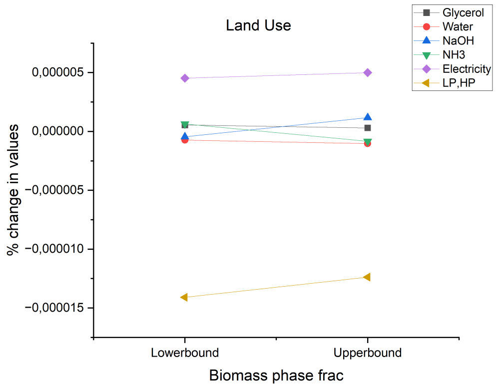


Figure C.63: LU: Biomass filtration liq-liq mole fraction

C.1.10. Verification methodology: Broth purge

When comparing the predicted values with the calculated values, the % change in the effect category values for the Broth purge KPI, the verification method ranges between 1E-06 and 1E-05 for both the lower and upper bound case scenarios.

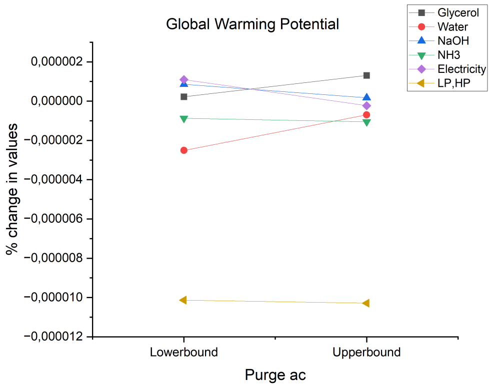


Figure C.64: GWP: Broth purge

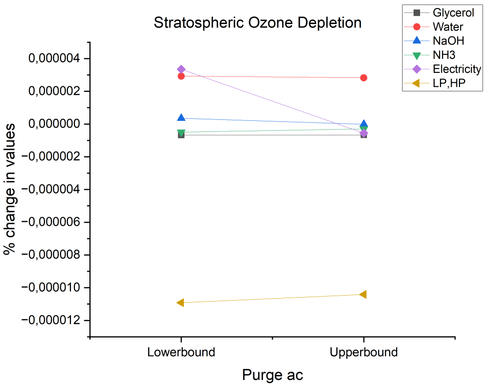


Figure C.65: SOD: Broth purge

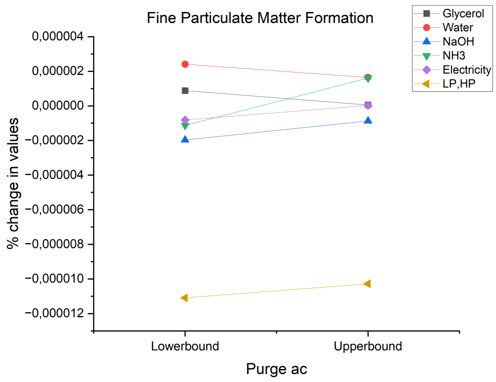


Figure C.66: FPMF: Broth purge

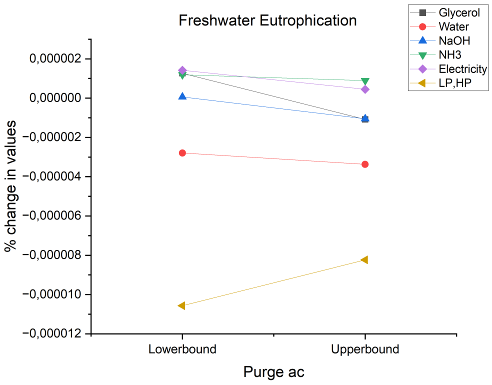


Figure C.67: FE: Broth purge

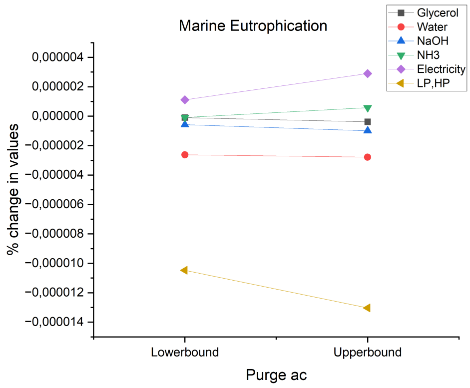


Figure C.68: ME: Broth purge

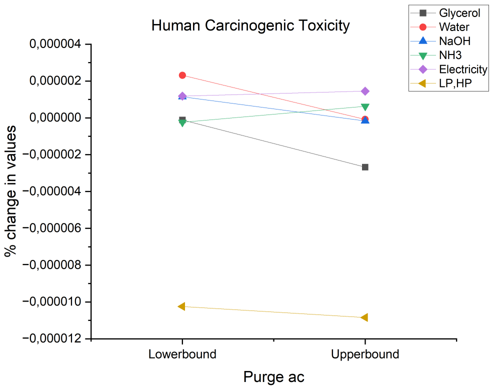


Figure C.69: HCT: Broth purge

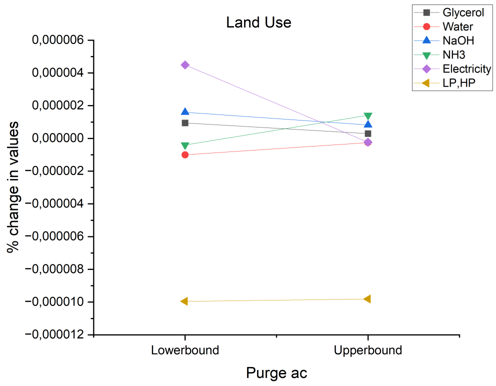


Figure C.70: LU: Broth purge

C.1.11. Verification methodology: Glycerol purge

When comparing the predicted values with the calculated values, the % change in the effect category values for the Glycerol purge KPI, the the verification method ranges between 1E-06 and 1E-05 for both the lower and upper bound case scenarios.

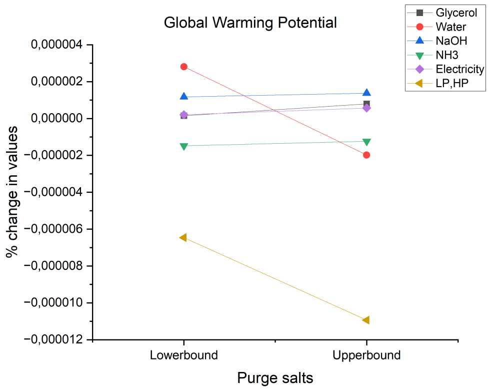


Figure C.71: GWP: Glycerol purge

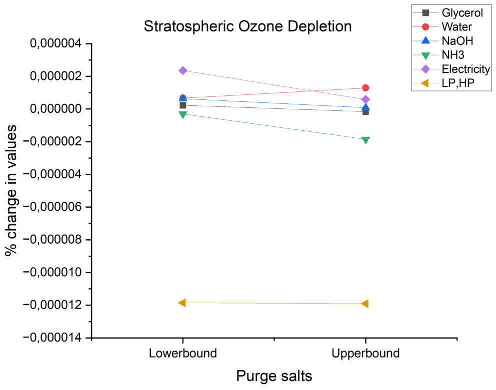


Figure C.72: SOD: Glycerol purge

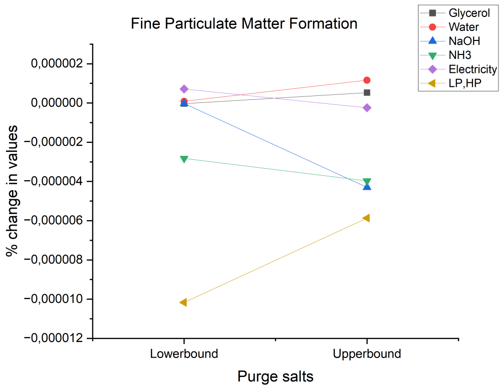


Figure C.73: FPMF: Glycerol purge

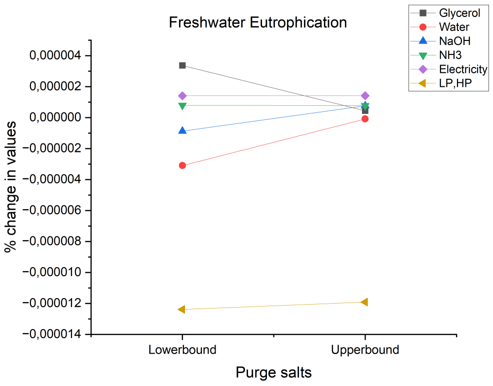


Figure C.74: FE: Glycerol purge

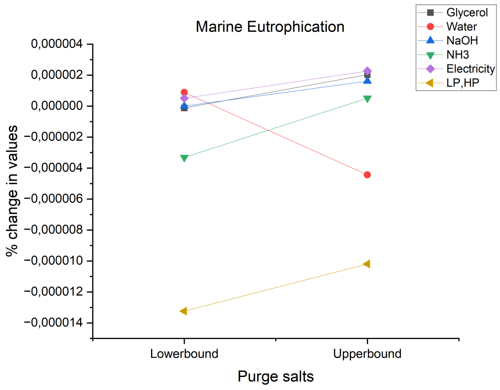


Figure C.75: ME: Glycerol purge

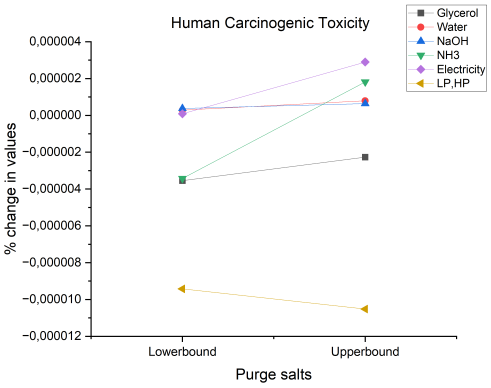


Figure C.76: HCT: Glycerol purge

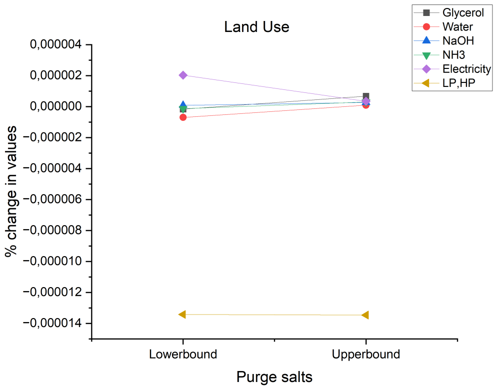


Figure C.77: LU: Glycerol purge