Assessing marginal abatement cost of bioplastics with an integrated assessment model

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Abstract of the master's thesis

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Abstract

This thesis studies the climate change mitigation potential of replacing conventional plastics production with bio-based plastics. The approach covers primarily the economic potential with varied climate policies. To achieve this system-level conception, an integrated assessment tool (IAM) called SuCCESs developed by the Finnish Meteorological Institute (FMI) is used. Such system-level modelling allows to consider the dynamics of decisions and changes in the system or in the climate policy. The results show that bioplastics are not economically beneficial alone, but with climate policies following the Paris Agreement, bioplastics become both an economically attractive and viable method of climate change mitigation. Bio-based production processes also enhance the flexibility of commodity production, which slightly decreases the system costs even without considering the environmental impact. However, the choice of bio-feedstocks is substantial in determining the climate and sustainability impact since the production of some bio-feedstocks can result in major negative outcomes, such as deforestation and increased world hunger. The limitations of the study include assumptions and approximations required to model bioplastics production. Although a simple sensitivity analysis suggests that the result is relatively insensitive to variability in techno-economic parameters, the role of uncertainty in future development and competing technologies remains a question for future studies. However, the results provide an example scenario showing how bioplastics could be utilized in the future.

Keywords Bioplastics, fossil-based commodities, integrated assessment model, marginal abatement cost

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Tiivistelmä

Tämä työ tutkii biopohjaisten muovien tarjoamaa ilmastonmuutoksen hillitäpotentiaalia. Hillintäpotentiaalia analysoidaan hyödyntäen Ilmatieteen laitoksella kehitettyä SuCCESs-nimistä integroitua arviointimallia (eng. integrated assessment model, IAM). Biomuovituotanto mallinnetaan osaksi SuCCESs-mallia ja sen avulla arvioidaan biomuovien systeemistason vaikutuksia sekä talouspoliittisten ohjureiden ja päätösten vaikutuksia biomuovituotantoon. Tulokset osoittavat, että biomuovit eivät ole taloudellisesti kannattava hyödyke ilman kannustimia, mutta Pariisin ilmastosopimuksen mukaisilla ilmastopolitiikkaohjureilla ne ovat taloudellisesti kannattava ja kustannustehokas päästönhillintäkeino. Lisäksi biohyödykeprosessit tekevät hyödyketuotannosta joustavampaa, mikä parantaa järjestelmän kustannustehokkuutta. Bioraaka-aineen valinnalla on suuri rooli biomuovien ilmasto- sekä yleisimmissä kestävyysvaikutuksissa, sillä tiettyjen bioraaka-aineiden tuotannosta voi koitua merkittäviä haittoja, kuten metsäkatoa ja globaalin nälänhädän kasvua. Työn merkittävimmät rajoitteet johtuvat mallinnuksen vaatimista yksinkertaistuksista sekä oletuksista. Vaikka teknoekonomiset lukuarvot on työn herkkyystarkastelussa todettu tulosten kannalta suhteellisen epäherkiksi, tulevaisuuden epävarmuus tekonologisessa kehityksessä sekä kilpailevissa teknologioissa korostaa tarvetta lisätutkimukselle. Työn tuloksia tulee tulkita huomioiden se, että ne esittävät mahdollista kehityspolkua eivätkä yhdestä päätöksestä juontuvaa lopputulosta.

Avainsanat Biomuovit, fossiiliset hyödykkeet, talous-ilmastoyhteismalli, rajavähennyskustannus

Preface

I want to thank all those being part of and helping out in the process of making this thesis. Especial thanks go to Tommi Ekholm, who provided me with great support and guidance both through the modelling phase as well as the writing phase.

Tuukka Mattlar
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Contents

Abbreviations

Abbreviations

BAU	Business as usual, a scenario of no changes
BIO	Bioplastics scenario, a scenario with the opportunity of producing bioplastics
BTP	Butylene to propylene process
BTX	Mixture of benzene, toluene, and xylene isomers
CFC	Chlorofluorocarbon, a halogenated hydrocarbon
COTC	Crude oil to chemicals, a petrochemical process with a major output of non-energy commodities
ETP	Ethanol to propylene process
GHG	Green house gas
IAM	Integrated Assessment Model
MAC	Marginal abatement cost
MACC	MAC curve
MTP	Methanol to propylene process

Central terms

Bioplastics	Plastics produced using bio-based feedstocks
Upstream production	The early phase of the chemical production processes where primary resources are explored and extracted.
Downstream production	The final phases of the chemical production processes where extracted chemicals are turned into marketable products.
Drop-in bioplastics	Bio-based plastics with a chemical structure identical to conventional RIC #1 - #6 plastics.
Climate policy	Refers to policies regarding emissions either by introducing costs or a cap for temperature increase.

1 Introduction

1.1 Problem description

Climate change is a significant and rising concern for the future of ecosystems and human society. The increase of greenhouse gas (GHG) concentration in the atmosphere strengthens the greenhouse effect, which results in a global mean temperature increase. Carbon dioxide (CO_2) is considered the major GHG, which is why much of the mitigation discussion focuses on CO_2 emissions.

There have been multiple attempts of forming global agreements to reduce GHG emissions. The most well-known and influential climate agreement relevant today is the Paris Agreement, which aims at limiting temperature increase preferably to 1.5 °C, but well below 2 °C above pre-industrial times (UNFCCC, 2016). Despite almost all UN countries being part of the agreement, the actions required for meeting the agreement have been insufficient. The main reason for the lack of action are the costs and investments required to change routines from business-as-usual (BAU), which in many cases are not or have not been economically viable until the last few years. Moreover, uncertain techno-economic development and unknown future political decisions give rise to risks related to the profitability and timing of investments in new technologies (Rosen and Guenther, 2015).

The most substantial source of GHG emissions is the use of fossil resources in e.g. the electricity, heat and transportation sectors. In 2018, these sectors corresponded to a 48 %-CO_2eq share of all GHG emissions. Moreover, other industries and land-based emissions and removals covered 24 %-CO_2eq and 21 %-CO_2eq respectively, of all GHG emissions in 2018. (Lamb et al., 2021)

Emission reductions in the heat, electricity and transportation sectors have been studied actively in recent years. This has also resulted in new and emerging innovations and technological breakthroughs, as well as reductions in emissions in some areas. Since these industries are primarily utilizing fossil resources as energy sources, a rough division is often made between the energy and the non-energy sector. The non-energy sector has been less studied in terms of emissions and mitigation possibilities.

Plastics form a particularly interesting and central topic in the non-energy use of fossil fuels. While new technologies are decarbonizing the energy sectors, the plastics industry remains heavily fossil-dependent. Plastics are currently responsible for approximately 4.5 % of global GHG emissions and with the expected demand development, the emission share is expected to double by 2050 if no action is taken (Stegmann et al., 2022b; Manabe, 2019). However, the majority of the emissions related to plastics originate from the production phase (Rosenboom et al., 2022). Therefore, the question regarding the emissions of plastics is not straightforward. Other concerns related to plastics, such as the plastic waste problem, recycling challenges and microplastics are not modelled, although also these topics matter too.

Since plastics are on average 93% (Geyer et al., 2017) polymerized hydrocarbons with various combinations of e.g. chemical bonds and other compounds, the main building materials are carbon (C) and hydrogen (H). In addition to oil, gas and coal, also biomass is essentially constructed of hydrocarbon chains. This makes biomass a possible alternative feedstock for plastics production. Today, almost all common plastics can be produced from bio-based feedstocks (Rosenboom et al., 2022). In this thesis, plastics produced with bio-based feedstocks are referred to as bioplastics. The term bioplastics is sometimes used to describe, and often confused with, biodegradable plastics but the topic of biodegradability is not included in this thesis.

Changing the main feedstock for plastics production from fossils to bio-based feedstocks comes with new challenges and questions. The main technological challenges include e.g. changes required in existing production processes to utilize the new feedstocks efficiently. Another key question is the economic viability of the feedstock change and therefore the attractivity for investors, which is required for the development of the technologies. Moreover, bio-feedstock production creates a potentially problematic setting for overall sustainability in terms of agricultural resources, food production and land use. Biomass and first-generation feedstock production can be seen as a competitor to food production (Calvin et al., 2021). In addition to the competition for land-use in food production, also deforestation and other land-use-related problems are expected to cause harm to overall sustainability (Bishop et al., 2022). These questions on technological development, economic viability and sustainability issues are relatively recent and lack comprehensive analysis with a system-level approach combining all three aspects.

Assessing climate change mitigation and the future techno-economic potential of bioplastics involves large uncertainties in the future techno-economic development. The development and commission of bioplastics production has been rather rapid and therefore also more innovations are constantly emerging. Therefore, it may be expected that in the future, production costs and process efficiencies will become more favourable, and new competitive alternatives will be introduced. Since this thesis is limited to modelling bioplastic production under the current technological knowledge, the results can be seen as the worst-case scenario if no further techno-economic development is assumed.

Integrated assessment models (IAMs) refer to the types of models that have been developed to comprehensively assess both natural as well as socioeconomic and industrial inter-linkages. These models are especially suitable for mitigation studies, since the impact of selected actions, policies or larger strategies can be modelled and studied as a part of a broader system. Such system-level modelling allows for a comprehensive overview of the estimated impacts.

This thesis studies the system-level impact and economic viability of bioplastics production with an IAM called SuCCESs. The IAM considers competing technologies, feedstocks, land-use and energy for determining a cost-wise optimal solution under mitigation policy constraints. Bioplastics are studied as a potential mitigation method and compared to the business-as-usual (BAU) scenario while altering mitigation strategies, i.e. the maximum allowed mean temperature increase. The economic viability of bioplastics as a possible emission reduction method is then measured by marginal abatement cost (MAC) under a temperature-based policy and difference in global temperature increase under a corresponding price-based policy.

1.2 Problem framing

Bioplastics form a highly complex industry. The set of bioplastics contains alternatives to conventional plastics that can be either identical to the current materials but also materials that are not yet utilized. Therefore, the range of possibilities is vast. Deciding on what technologies to concentrate on is hard and calls for approximation. The discussion on which plastics to include is presented in Chapters 2 and 4. In brief, the study focuses on drop-in bioplastics but the approach utilized can be seen covering a more broad approach to replacing feedstocks with bio-based materials.

Assessing the mitigation potential of bioplastics quickly leads to high levels of complexity as feedstock processes and the connections related to these are considered. In general, when studying emission reductions, the list of possible changes is vast and to reach optimum, changes in multiple processes and industries are likely to be required. However, in this thesis, only bioplastics are considered and the rest of the model is left untouched. This allows to assess bioplastics but does not describe the whole spectrum of possibilities.

1.3 Thesis structure

Chapter 2 describes the background of plastics and bioplastics and introduces the topics relevant to understand the problem setting and analyzing the results. Chapter 3 introduces the purpose and general designs of IAMs, as well as the SuCCESs IAM both on the general level and also how the plastics-related aspects are included in the model. The analysis required for modelling, such as framing and discussion, as well as the modelling methodology, including approximations and economic approach, is introduced in Chapter 4. Finally, the results are presented and assessed in Chapter 6. Discussion and conclusions are presented in Chapter 7.

2 Plastics and bioplastics

Plastics are a very practical and suitable material for multiple purposes, especially as a packaging material. Thus, a major reason for the popularity of plastics is their superiority as a durable, flexible and light material that is easy to manufacture and dispose. (Brizga et al., 2020; Rosenboom et al., 2022)

This Chapter first describes in more detail what plastics are. This is necessary for understanding what types of plastics exist and how are these used. After the basic concepts and categorization have been introduced then, the plastics industry's size and demand are presented. To help understand the magnitude of the plastics industry and the relevance for this thesis. Finally, the production of plastics is covered at required level.

2.1 Plastic types and categorization

Plastics can be categorized in multiple ways, but the most relevant taxonomy, for this thesis, is the division between fossil-based plastics and bio-based plastics, from now on referred to as bioplastics. Fossil-based plastics are also often called conventional plastics, although the term conventional is rather vague in the feedstock and biodegradability evaluation. (Rosenboom et al., 2022) Moreover, plastics can be produced with partially bio-based feedstocks, which means that the plastics are not 100% bio-based. No exact threshold for the share required to fulfill the definition of a bioplastic was found in the literature. However, this is not a critical problem due to the architecture used in modelling, as seen in Section 4,

Bioplastics can be easily confused with biodegradable plastics. In the literature, the term is sometimes used intentionally to refer to biodegradable plastics. Despite this contradiction and lack of coherence, the term bioplastics is only used to refer to plastics made from bio-based feedstocks in this thesis. Both fossil-based and bio-based plastics can be produced in biodegradable and non-biodegradable variants. However, a vast majority of plastics used today are non-biodegradable fossil-based plastics.(Rosenboom et al., 2022)

Most non-biodegradable bioplastics today are produced to be similar to conventional fossil-based plastics. These plastics are often called drop-in bioplastics, which refer to synthetically produced bioplastics that are chemically identical to their conventional counterparts. These plastics, also including conventional fossil-based plastics, are uniquely labeled by resin identification codes (RIC) ranging from 1 to 6 and an abbreviation of the chemical name of the plastic, such as #1 PET for polyethylene terephthalate (Rosenboom et al., 2022). In this thesis, the plastic abbreviations are utilized but the RICs are not discussed further.

One further distinction is the separation of thermoplastics and thermosets. Thermoplastics are solid in normal conditions and can be melted and molded when heated. Thermosets are plastics that can be liquid in normal temperatures but become solid after the molding process is completed. Thus, thermosets are a more temperature-resistant material.

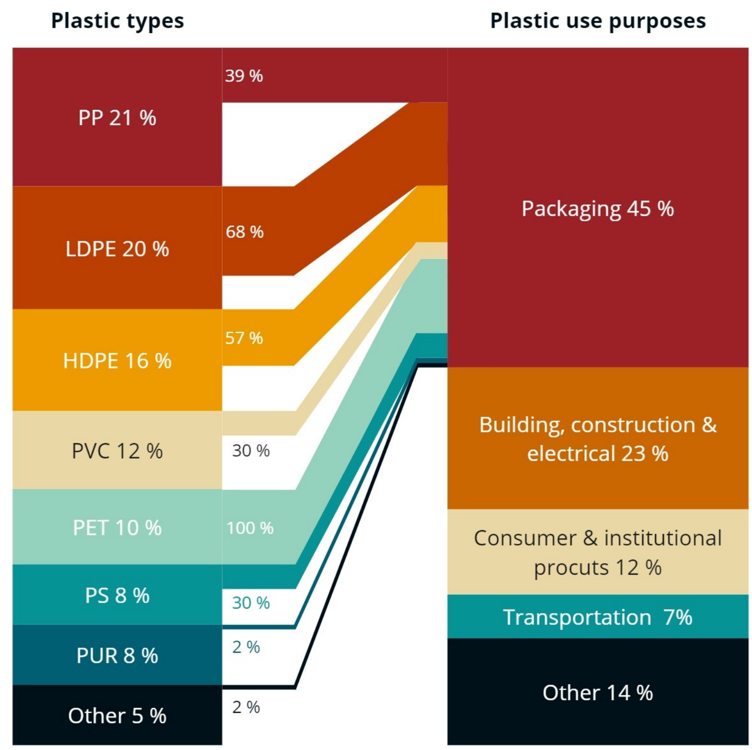

Figure 1: Central conventional plastic types and main plastics use purposes between 2002-2014 (Geyer et al., 2017). The Sankey paths indicate the share of each type used in packaging, the major plastic use purposes. Plastic type abbreviations are PP for polypropylene, LDPE and HDPE for low-density and high-density polyethylene, PVC for polyvinyl chloride, PET for polyethylene terephthalate, PS for polystyrene and PUR for polyurethane.

In Figure 1, the most common plastic types are polyethylenes (PEs), i.e. HDPE and LDPE, by an aggregated 36%, PP by 21% and PVC by 12% share of all plastics. The single major use purpose for plastics is the packaging sector which accounts for 45% of all plastics use, including also other plastic types outside the mentioned ones (Geyer et al., 2017). Although the data is relatively old, recent relevant and major studies refer to these values and consider the share values as descriptive while the plastics industry has grown since the data is gathered (Stegmann et al., 2022a).

The remaining plastics types, such as PET, PUR and PS, each account for less than 10% of plastics production. Major use cases for these plastics include drink bottles (mostly PET), building materials (especially PUR) and packaging (especially PS). (Geyer et al., 2017). The category for other plastics contains various materials but it is irrelevant in this thesis due to the small share of demand and high complexity among the class.

2.2 The market and the future of plastics and bioplastics

Reported estimated about the global annual plastics production vary depending on how plastics production is defined. However, the range for global annual plastics production is found between 360 and 440 Mt in recent years (Brizga et al., 2020; Rosenboom et al., 2022). The annual growth of approximately 3.5-4 % has been relatively constant and the future growth rate is assumed rather similar (Rosenboom et al., 2022; Shen et al., 2020). The production of plastics is therefore assumed to more than double of today's level by 2050, thus making today's plastics-related challenges possibly much more severe. Also, the emissions related to plastics production under the current development are expected to grow in a similar trend thus making emissions related to plastics an even more significant factor under the expectation of decarbonization of other industries. (Stegmann et al., 2022b). It is therefore estimated that under the remaining carbon budgets, plastics would account for 10 - 13 % of CO_2eq remaining in 2050 (Shen et al., 2020). In a broader picture, Levi and Cullen (2018) estimate that the non-energy use of fossil sources will become the largest source of growth in the fossils market by 2035.

The global production of bioplastics in 2019 was 2.4 Mt which accounts for less than 1% of global annual plastics production (Brizga et al., 2020). Plastics Europe (2022) estimates that total bioplastics production capacity would grow almost three-fold to 6.3 Mt/a by 2027.

Today, a significant share of the produced bioplastics are drop-in bioplastics, such as bio-PEs and bio-PP. Drop-in bioplastics offer an easy switch to bio-based plastics since the products are chemically identical to their fossil-based counterparts and can thus be used for exactly similar purposes. In 2019 drop-in bioplastics accounted for 42% of all bioplastics produced and Brizga et al. (2020) estimate the share to grow to 75% by 2021. However, Plastics Europe (2022) indicates that at least the production capacity share of drop-in bioplastics of all bioplastics remained at 49% in 2022. Plastics Europe (2022) also estimates that the share between biodegradable and non-biodegradable bioplastics would remain on approximately similar level by 2027. The large differences are likely to be caused by technological uncertainties and thus the future realized development path for bioplastics will depend heavily on the progress achieved in the years to come.

The non-drop-in bioplastic types, as categorized by Plastics Europe (2022) and discussed by Onen et al. (2020), are mostly biodegradable, such as variations of starch blends or polylactic acid (PLA). However, some of the included biodegradable bioplastics, such as PBAT which is used in biodegradable bags, is often produced from fossil resources (Rosenboom et al., 2022). This highlights the problematic nature of the vague and varying definition of the term bioplastics in the literature.

It is estimated that especially PLA-based plastics and polyhydroxyalkanoates (PHAs) are to take a more central role in the plastics industry of the future. However, the techno-economic development of these biodegradable plastics remains uncertain although a lot of research has been done and progress achieved. (Plastics Europe, 2022; Wellenreuther et al., 2022)

2.3 Emissions during the plastics life-cycle

Conventionally, plastics are produced from fossil resources such as oil and gas. The resources are refined, usually by a form of cracking, to monomers and aromatics that are then further polymerized to form hydrocarbon polymers (Levi and Cullen, 2018). This rough explanation provides a sufficient background for this Section. The production of plastics, in general, is described in more detail in Section 2.4. The plastics modelled are further discussed in Chapter 4.

During the life-cycle of plastics, on average approximately 61 % of plastic-related emissions occur during the material extraction and 30 % during the polymer production. The end-of-life stage accounts for only to 9% of all plastics-related emissions, most of which is related to incineration. (Rosenboom et al., 2022). It is thus clear that most emissions relate to the production phase, not the embedded carbon emissions that are released either fast via incineration or slowly during the long degrading time of plastic resins. Additionally, indirect impacts, such as decreased carbon absorption of oceans caused by microplastics, have been identified by e.g. Arkin et al. (2019). Although such aspects may matter in the future, these remain out of the scope.

The easy disposal and durability of plastics are coupled with problems related to plastic waste and a low rate of reuse. Although this thesis deals with the production of plastics, mostly ignoring the waste and disposal-related problems, it is worth mentioning that since plastics are not, at least yet, widely recycled, the production of plastics relies vastly on novel feedstocks. Geyer et al. (2017) estimate that out of 8.3 Gt of plastics and 6.3 Gt of plastic waste made in the whole history, 79% is assumed to be disposed in landfills, 12% incinerated and only 9% recycled. Additionally, Shen et al. (2020) estimate that plastic packaging waste is currently recycled at a share of 14% and Rosenboom et al. (2022) estimate that in the US 20 % and in the EU 40 % of plastic waste is incinerated. Despite the numbers by Geyer et al. (2017) summing up to 100%, Siracusa and Blanco (2020) estimate that 30% of the plastic waste in the US is unaccounted for therefore estimated to be either disposed by unaccounted burning or disposal in the nature. The low share of plastic recycling originates from the techno-economic limitations of cost-effective chemical recycling, which would be required for high-quality large-scale circularity of plastic olefins (Rosenboom et al., 2022; Shamsuyeva and Endres, 2021). If plastic material was better re-utilized, the emission-heavy feedstock extraction could potentially be replaced with less emitting methodologies since much of the processing-heavy extraction would not be required. Moreover, the high share of incineration means that much of the embedded carbon is released directly to the atmosphere at the end of the plastic life cycle.

Since recycling is not included in the scope, the extraction and production phases are studied under the assumption of a constant need for novel feedstocks. Multiple studies have been made on how emissions could be possibly reduced and how effective these could be. These means include e.g. bio-based feedstocks, change of production energy sources to renewable and the shift towards alternative materials, i.e., reduction of demand in growth (Zheng and Suh, 2019). Although this study focuses on bio-based feedstocks as a mitigation mean, at least Zheng and Suh (2019) have found a significant potential in changing the energy source to renewable sources. However, the change of energy source is complex due to the high heat required by the processes, which is often achieved most easily by industrial steam produced by utilizing natural gas as a fuel. Although this is a much longer topic beyond the scope, bio-based feedstocks are not the only possible approach in reducing the emissions of plastics. Moreover, the energy industry is included in the optimization model, thus energy-related emission reduction possibilities of plastics are handled by default.

Bioplastics are estimated to potentially cut plastic-related GHG emissions. The approaches to production methods differ and so do the results. Some studies have found good potential in GHG emission mitigation by bio-feedstocks, as reviewed by Spierling et al. (2018), whereas some studies have found bio-based feedstocks to cause even greater negative climate impact. An example of overall negative impact is a study by Chen et al. (2016) on bio-PET bottles. In this study, however, the feedstock choice and relatively detailed factors were found to have a significant role in the overall emission and sustainability impact. Moreover, the study accounts to a 100% bio-based material, whereas a minor fossil-based share could provide a less emitting alternative. This indicates the central role assumptions and approximations may have in studying bioplastics.

2.4 Foundations on the chemistry in producing plastics

There are multiple types of plastics. Each of the plastic types is produced with slightly different processes and extracted from slightly different feedstocks. To add complexity, some plastic types can be produced with several processes. Despite a high level of variation and possible paths to achieve similar results, conventional plastics production is still based on rather similar frames independent of the end product. (Arkin et al., 2019)

Common to all plastics production is polymerization, which is a process of bonding together multiple monomers to form polymers. Fossil-based conventional plastics and drop-in plastics are polymerized from olefins and usually additional materials, such as plasticizers. Other bioplastics, such as PHAs and PLAs, are polymerized from, e.g., esters, which are produced by utilizing microbiologic bacteria cultures to process feedstock materials (Arkin et al., 2019; Surendran et al., 2020; Murariu and Dubois, 2016; Serafim et al., 2008).

Especially fossil-based plastics production can be seen as having a relatively similar path of origin. After the fossil feedstocks, such as oil or gas, are extracted, the materials are broken down and separated, most commonly by a process of the form of cracking. After the smaller molecules are cracked and separated, the monomers are polymerized to form polymers, such as PE. At this point, the selection of input chemicals, enzymes and process conditions defines the end product plastic (Arkin et al., 2019).

The most crucial olefins include ethylene and propylene, which are central to producing PEs, namely polyethylenes, and PP, namely polypropylene. The conventional processes for cracking these olefins are straightforward and the input material can be either natural gas, crude oil or sometimes even coal. (Arkin et al., 2019) Conventionally, the main focus of the fossil extraction industry has been the production of transportation fuels, and the chemicals production has been heavily based on low-value side products of the fuel industry. However, this setting is changing since a new form of downstream fossil industry, crude oil to chemicals (COTC), has been recently developing. This set of technologies aims at producing chemical products more efficiently from fossil feedstocks with a special emphasis on improving propylene yield. (Corma et al., 2017)

Since drop-in bioplastics are chemically similar to their fossil-based counterparts, the changes required for the production processes are limited to the process before the polymerization. Therefore, the most common approach is to process and dehydrate the olefins from bio-ethanol, which is most often obtained by fermenting polysaccharides. (Siracusa and Blanco, 2020; Rosenboom et al., 2022)

Fermentable polysaccharides can be obtained from many sources. These can be categorized into two classes, first and second-generation biomass. First-generation biomass is considered to consist of edible crops and other sources with a direct producing purpose for the chemical sector, such as corn and sugarcane. Second-degree biomasses are considered to be agricultural and forestry residues as well as food waste and other inedible bio-based materials (Rosenboom et al., 2022). The production methods are further discussed in Chapter 4, where the processes are described for modelling purposes.

Other types of bioplastics are formed in more complex ways as shown by e.g. Siracusa and Blanco (2020) and Chen and Patel (2012). The processes of producing these plastics rely on microbiologic processes and specific bacteria cultures. However, almost any feedstock that is also eligible for drop-in bioplastics production can be used (Serafim et al., 2008; Murariu and Dubois, 2016). These bioplastics are not modelled in this thesis. Reasons are explained in Section 4.1.

2.5 Issues with plastics and bioplastics

Non-biodegradable plastics give rise to long-lived waste that is still not widely recycled (Rosenboom et al., 2022). Some waste ends up in oceans causing problems in the marine environment. Marine plastic waste is also a significant source of secondary microplastics. However, even biodegradable plastics are not a straight-forward solution to plastic waste. There have been concerns especially about the conditions required for biodegradability, i.e. some plastics that are considered biodegradable are found not to degrade well under normal conditions the plastics face when disposed or left in the environment. Additionally, biodegradable plastics are considered to produce microplastics. (Wang et al., 2021). The topic of biodegradability is not discussed in further detail.

The production of some chemicals is not yet either environmentally or economically beneficial. For example, it is found to be challenging to produce butylene, a key chemical in PET production, from bio-based feedstocks (Chen et al., 2016). In this thesis, the major feedstock chemicals are considered based on the recent literature. Thus the overall environmental and economic impact is studied and these topics are in the focus.

The challenges related to bio-based feedstocks also account for broader sustainability concerns. As with palm oil and bioethanol as fuels, bioplastics also come with similar ethical and sustainability questions and concerns. Utilizing some of the most efficient biomass materials in bioplastics production, such as corn or sugarcane, sets a competition between food and plastics production. The possible outcome is that such edible products are planted for plastic feedstock instead of feeding humans. While currently, only 0.02 % of the global agricultural land-use is dedicated to bioplastic feedstock production, the agricultural resources required for a complete bio-based packaging industry would be large in the case of first-generation bio-feedstocks. According to Brizga et al. (2020), such a shift would require 54 % of the global corn production and in EU, consume 60 % of the current fresh water usage. However, Bishop et al. (2022) find the choice of bio-feedstock plays a vital role in both overall sustainability as well as the impact on GHG emissions.

Additionally, utilizing crop residue, such as sugarcane bagasse, sets a different challenge for the agriculture industry as well as carbon cycles. At least in theory, more fertilizers are required for similar yields and less carbon is absorbed in the soil. Finally, an increase in bio-based feedstock production is feared to cause deforestation since more agricultural area is required. The SuCCESs model considers land-use, thus this topic is included by default.

Economically, a remarkable decrease in the non-energy use of fossils could increase the use of fossil-based resources in other industries. The petrochemistry sector is complex and contains processes that produce relevant commodities as byproducts. Therefore, some chemicals are automatically produced independent of demand alterations. This also means that if fossil fuel extraction was to decrease in the future, the supply market for chemicals would also be influenced under the changing market environment. Chemicals could become more expensive due to the decreased overall extraction and exploration. On the other hand, the decreased energy-related demand for fossils could, at least temporarily, decrease prices and make fossil-based chemical production more attractive an option. This also implies that studying bio-based feedstocks for the plastics industry is not only relevant in terms of emission mitigation but also in future possibilities. The SuCCESs optimization IAM makes economically optimal investments, which means that the approach can be seen to behave as a basic economic model. However, the model is not a comprehensive economic model thus the results in these terms must be considered with caution.

3 Integrated assessment models

3.1 General principles of IAMs

IAMs are most often considered as numerical models connecting economic and environmental factors in the long-term (Nikas et al., 2019). The focus of studies done using IAMs is usually on anthropogenic emissions. For the general level, this can mean e.g. combining a climate-emission model with a model simulating emission-heavy industries. The combination of the systems provides a coherent and broad view. Therefore, the IAMs are especially helpful in long-term climate change mitigation studies, since these analyses address questions involving complex interactions and feedback between systems. In addition to the mitigation analysis, IAMs also offer possibilities to assess long-term policy impacts on the system-level and can therefore be used in building techno-economically optimal mitigation strategies. (van Beek et al., 2020)

The first IAMs are considered to have been developed in the 1970s. One of the first-considered IAMs, the World3 model, represents topics such as population, some central industries and pollution. During the 80's, IAMs were utilized in especially acid rain assessment. In the 90's, IAMs started to focus on global climate change studies. The modern IAM development gained its latest boost in 2015, as the Paris Agreement put more emphasis on analyzing efficient responses to mitigate climate change, whereas the earlier studies had concentrated more on the causes of climate change. Today, IAMs have become a central assessment tool for climate change policy research. For example, the IPCC working group III (WGIII), which considers mitigation strategies, utilizes IAMs in their work extensively. (van Beek et al., 2020; Keppo et al., 2021)

3.2 Different types and use cases of IAMs

IAMs differ in structural factors and level of detail. Categorizing IAMs has proven hard but some categorization can be made. (Nikas et al., 2019)

One clear distinction is whether the purpose of the model is to provide detailed process-level representation or to assess the economically optimal level of mitigation in border terms. Of these, the first type is especially suitable for global assessment of overall climate change mitigation, such as the IMAGE model for the IPCC. The economic models are used e.g. in the national climate policies of the US. (van Beek et al., 2020). This thesis considers process-level IAMs.

Another approach to categorizing IAMs is based on the way the economic system is implemented. Nikas et al. (2019) identify six categories including partial equilibrium, general equilibrium and macroeconomic models. These three are are the most relevant in this thesis. The other categories are energy system, optimal growth and other models, including various types of models.

Macroeconomic and general equilibrium models seek to describe the economy in considerable detail and to cover all aspects of the economy even regionally. The macroeconomic models, in contrast to general equilibrium, do not assume perfect markets, exactly rational decisions nor base the market behavior on historical econometrics. This makes the macroeconomic models, in theory, more realistic, than historical knowledge, but more vulnerable to unexpected changes. Partial equilibrium models describe the interaction of environmental impacts and the economy thus focusing on e.g. the emission-heavy industries and describing these aspects in detail. Yet, as well as the general equilibrium models, the partial equilibrium models assume perfect and rational markets. (Nikas et al., 2019). The SuCCESs model is a partial equilibrium model.

In addition to the distinctions between the level of detail and the way of modelling economy, a more mathematically focused way of categorizing IAMs is the distinction between simulation and optimization-based IAMs. Simulation-based IAMs assume that future is not known since decisions cannot be based on inter-temporal knowledge. Therefore, simulation-based IAMs lean heavily on data and relationships, which are utilized to provide a possible development scenario or scenarios (Keppo et al., 2021). This thesis utilizes an optimization-based IAM.

Optimization IAMs determine the optimal strategy either for the whole period selected or for each time step though most models optimize the whole system intertemporally. Optimality can be achieved by e.g. minimizing total costs or maximizing total welfare. Each selected industry is therefore represented with constraints for processes and investments as well as costs or welfare utility. Moreover, with the optimization approach, it is possible to set long-term targets and constraints that can be assessed as policies and political targets. (Keppo et al., 2021). A more detailed discussion on the relevance and limitations of the optimization model approach is found in the following Section.

3.3 Critique and limitations of IAMs

Like all other models that simplify the real-world into a computable form, IAMs have limitations that need to be considered when interpreting and using the results. Keppo et al. (2021) discussed some general criticism and limitations of IAMs and different model designs and approaches, such as the issue of heterogeneous representation, technology diffusion and technological development relation to policies. Also the rough level of detail in e.g. process descriptions has gained criticism, especially by the experts of each corresponding industry. In this thesis, it is particularly crucial to consider the limitations relating to technological development and its relation to policy-making as well as energy-economy interrelationship, which in this case could also be considered with material production and economy since plastics have a substantial role in today's economy. Additionally, Weyant (2017) remarks that the models don't account for the risk averse behaviour of humans.

In addition to the critique above, a more specific optimization-IAM related topics include the limitations and features of optimization. Since the models are generally not accounting for the world after the considered time horizon, usually ending in 2100, the optimized paths are high likely to overshoot the selected temperature increase targets after the last time step of the model. This is important, since it states a clear limitation in the reliability of the results as a mitigation strategy. Since models under inter-temporal optimum can optimize the all-time costs or welfare in a way that is just enough to meet the target for 2100, the lifetime of emissions may set problems related to the practicality of the optimal path. For example, reinvesting into carbon-intensive technologies in 2090 can still keep the climate target met, would likely not be economically nor practically feasible solution over a longer time horizon. Moreover, some models involve carbon capture and storage (CCS) technologies, which are argued to be used too extensively to portray the current estimates on the real-world development (Vogt-Schilb and Hallegatte, 2014).

In studying climate goals, such as the 1.5°C Paris agreement goal, it is vital to understand the way an optimization-based IAM works. Under the assumptions that (i) reducing emissions in the model costs more or decreases overall welfare utility (at least temporarily) and (ii) that the desired temperature increase is low enough, the model is very likely to find the optimum in a point where the mean temperature increase constraint is active, i.e. the climate goal limitation is binding. This means that when studying alternative technologies or approaches under similar temperature-based climate goals, the impact on climate in 2100 remains the same, i.e., equal amount of CO_2eq emissions are emitted, however the portfolio of mitigation methods changes. While this is a limitation it is also a way of defining the problem. This aspect is also considered in this work, since the effectiveness of bioplastics cannot be directly measured through additional emission reductions. The approach is discussed in Chapter 4 in more detail.

3.4 Previous IAMs and the non-energy sector

Today, several IAMs are utilized for different and specialized purposes (Nikas et al., 2019). However, interesting in the context of this thesis, Stegmann et al. (2022a), among other authors, have found that models with non-energy modules are rather rare. In fact, Stegmann et al. (2022a) claim that Daioglou et al. (2014) is among the few, if not the only, IAM study and model extensions that contain the non-energy sector on a level adequate for the analysis of emissions. The model extension is a module called NEDE, which stands for non-energy demand and emissions. The IMAGE model, in which the NEDE module is included, is a simulation-based IAM.

When it comes to plastics and bioplastics specifically, the NEDE model is, according to Stegmann et al. (2022a), thought to be the first and possibly the only IAM module to consider (bio)plastics production. Moreover, Stegmann et al. (2022a) consider themselves the first to include plastics sector with circular economy in an

IAM with their plastics integrated assessment (PLAIA) model. Given this, Stegmann et al. (2022a) consider the PLAIA module one of the first models to allow global and regional assessment of plastics, and among the first ones to assess the long-term dynamics of the sector.

Based on the PLAIA model, Stegmann et al. (2022b) show that making the plastics industry carbon negative would be possible if the plastics production was shifted to utilize waste and bio-based feedstocks. Although this study on circular bio-economics indicated the potential, they and other authors such as Suh and Bardow (2022) identify a list of concerns, such as the great magnitude of required bio-based plastics production, which is heavily influenced by large taxation of conventional plastics in the study.

Based on Stegmann et al. (2022a), it seems that the non-energy use of fossil resources and especially plastics and bioplastics in IAMs is still nascent. Moreover, based on the recent conception by Stegmann et al. (2022a), it appears that there are no optimization-based IAMs with a bioplastics module. This adds motivation for this thesis.

3.5 The SuCCESs IAM

The SUCCESs model is a linear, inter-temporal optimization-based IAM developed at FMI. As an IAM, it provides an assessment tool for climate change studies with the environment of economics. SuCCESs is especially designed to portray sufficient system interactions on a level of detail that is both lightweight in terms of computational complexity, but provides general insights into different industries. The model covers the global partial economy from the year 2020 to 2100 with ten-year intervals. It also has an hourly-based electricity module. SuCCESs is implemented in GAMS, which is a language for mathematical programming problems, based on the OSEMOSYS modelling framework. (Ekholm et al., 2023)

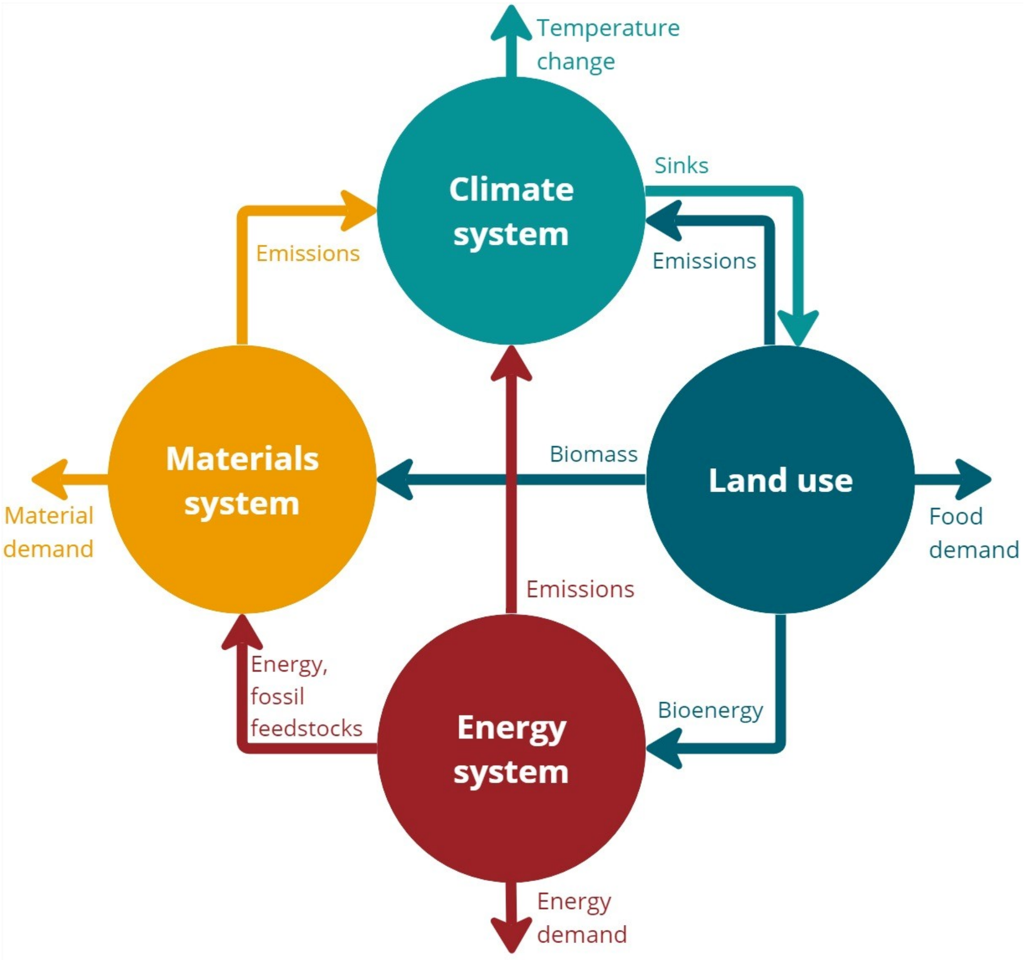

Figure 2: SuCCESs structure as described by Ekholm et al. (2023)

The SuCCESs model links energy, land-use, materials and climate systems, as seen in Figure 2. Each system, or module, has a different logic and structure, but the modules are connected to each other by data-exchanging interfaces. Each module is summarized, but the focus is set on the materials module in Section 3.6.

The material and energy modules model the use and investments in central material commodities and energy production. These modules consist purely of commodities and processes, where feedstocks and commodities are fed as an input for a process, which further produces commodities. Energy-related commodities are measured in energy units (PJ) and material-oriented commodities in mass units (Mt). The list of commodities and processes is long but, central to this thesis, the model contains e.g. electricity and natural gas as commodities and thermoplastic production and naphtha cracking as processes.

The land-use (LU) module, also referred to as the climate-responsive land allocation model with carbon storage and harvests (CLASH), models the land allocation to different uses, such as managed forests and croplands. The otherwise homogeneous global system is split into 10 biomes in the CLASH, consisting of e.g. boreal and dry tropical areas. The LU module essentially handles how much land-area is allocated to each biome, how much e.g. crops and wood are produced and how much carbon is sored in the terrestrial biopshere.

The climate module contains a simplified climate model which portrays atmospheric GHG concentrations, radiative forcing and the change in global mean temperature. The GHGs considered are CO_2, CH_4 and N_2O, the emissions for which are obtained from the other modules.

3.6 Conventional plastics in the SuCCESs model

Understanding the conventional plastics production is essential for building the bioplastics module. The conventional plastics production was already contained in the SuCCESs model prior to this thesis. The production follows the analysis of Levi and Cullen (2018). In comparison to the NEDE module of the IMAGE IAM, the non-energy module introduced in Section 3.4, which models feedstocks in energy units, the plastics are considered in mass units in the SuCCESs model.

Following the general structure within the materials and energy modules, plastics production modelling consists of processes that utilize and produce different commodities. Each process is associated with a value for lifetime, starting year capacity, availability factor and investment costs. Additionally, some processes involve variable costs which account for the expenses beyond those noted already in the input commodities. However, many processes for the production of plastics do not include variable costs since those are assumed marginal. (Ekholm et al., 2023)

The conventional plastics production is introduced here from downstream production (final products) to upstream production (refining and extraction). Generally, feedstock sources, such as natural gas and oil, are extracted from the ground and processed through processes into commodities required to build the end-products.

3.6.1 Downstream production

In the downstream part of the chemical production module, plastic types are aggregated into two final products, thermoplastics and thermosets. In terms of magnitudes, thermoplastics are produced on 222 Mt/a level and thermosets on 107 Mt/a based on data from 2013 (Levi and Cullen, 2018). However, the thermoset category provided by Levi and Cullen (2018) contains just a few of the previously discussed plastics, although the annual production of the two types combined, 329 Mt/a, is aligned with the plastics market as discussed in Chapter 2. Despite the contradiction between plastic-related literature and the study by Levi and Cullen (2018), the categorization is rather irrelevant for this thesis. However, more emphasis is given to the thermoplastic category.

When producing the end-products, thermoplastics and thermosets, the feedstock quantities are provided as an aggregate estimate of the whole industry. Therefore, the share of each plastic type is already considered in the share of input commodities, thus changes over time in use shares are not accounted for. The main inputs for the plastic end-products are therefore ethylene, propylene and BTX. Additionally, electricity and industrial steam are required for production. The required amount of each input for the production of plastics is described in Table 1.

Table 1: Input commodities required for producing 1 Mt of each plastic type in the end-product process of the SuCCESs model.

	Thermoplastics	**Thermosets**
Ethylene (kt)	436	58
Propylene (kt)	232	105
C4 olefins (kt)	11	52
BTX (kt)	104	223
Ammonia (kt)	6	52
Methanol (kt)	9	75
Other chemicals (kt)	202	435
Electricity (PJ)	4 000	600
Steam (PJ)	8 600	11 300

Table 1 shows the required feedstocks and energy sources for producing one Mt of plastics in the SuCCESs model. The input called other chemicals, a major input for especially thermosets, contains commodities that are not considered in detail. Other chemicals are not considered in detail, since this would increase the complexity of the model.

In some literature, plastic moulding and finished end-products, such as bottles, are part of the downstream process. However, in the SuCCESs model, these phases are not discussed since all upstream production processes are contained in the process of producing the end-products.

3.6.2 Upstream production

The fossil-based production processes are depicted in Figure 3. The figure contains all processes that produce commodities listed in the red box on the right side. In addition, many processes produce a variety of other outputs, which are beyond the current focus is on upstream plastic production commodities.

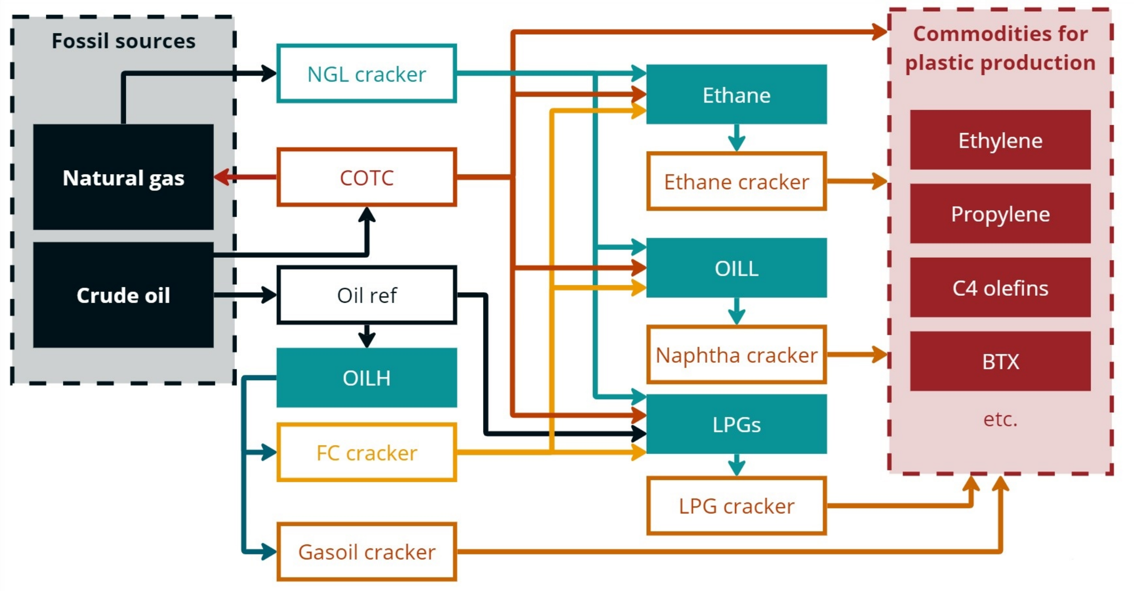

Figure 3: The upstream processes of the SuCCESs model for plastics production. The boxes with only outlines represent processes and the boxes with full colouring represent commodities.

The other feedstocks and resources needed for the plastics production, seen in Table 1, are ammonia, methanol and other chemicals as well as the energy requirements. Ammonia and methanol are not considered, since these only cover a small share of inputs required for the overall plastics production.

4 Modelling and assessing the mitigation potential of bioplastics

4.1 Framing and approximations in the modelling of bioplastics

Since bioplastics form a growing, vast and diverse industry, there is need for careful framing and approximation to set the suitable level of modelling detail. To better frame the problem, the structure of SuCCESs model and its conventional plastics module is first analyzed and considered in terms of the bioplastics production. After the model setting is understood, the required approximations are considered. The approach starts from the end-product, i.e. plastics, and continues towards the first production steps, i.e. feedstocks.

4.1.1 Demand and aggragate production

The SuCCESs model considers thermoplastics and thermosets as the end products and demand-driving commodities in the plastics production pipeline. The demand of the aggregated plastics classes is based on model input data, and is therefore not dynamically dependent on any model factors. To retain the current demand architecture, bioplastics are considered as a part of the current thermoplastic and thermoset categories. However, if the model is later augmented with a recycling or other end-of-life module for plastics, this categorization should be reconsidered, especially if biodegradable plastics are to be introduced.

The end product types are constructed from fixed shares of input feedstocks required to produce one unit of each type, thermoplastics and thermosets. This means that the model assumes that the demand profile remains the same although the total production levels increase over time. Changing the input profile is considered to be outside of the scope, since the current share is based on literature and changing these would require a more detailed analysis and estimates on the future of the plastics market. Moreover, as the future market development is uncertain, historical shares are a reasonable assumption. Re-considering the demand modelling is a topic for a further study.

The first approximation is that bioplastics are considered part of the total demand for all plastics in the model, i.e. the thermoplastic and thermoset commodities. Moreover, since the production process of the end products, thermoplastics and thermosets, is not changed, the demand profile of different plastic types is considered to remain similar when the demand is increased. This approximation decision is made under the suitable level of detail in comparison to other parts of the SuCCESs model and future uncertainty.

4.1.2 Bioplastic types

Since the bioplastics production has to be in line with the existing thermoplastic and thermoset categories, it is vital to decide how this is achieved. Roughly speaking, the bioplastics are categorized into drop-in plastics and other bioplastics that include e.g. PHAs and PLAs. As described in Chapter 2, the drop-in bioplastics are constructed of the same chemicals as conventional plastics, but other bioplastics are formed through more specific processes, although relying on rather similar feedstocks as the drop-in bioplastics.

Given the rather simple production process of drop-in bioplastics, one possible approximation approach is to simply alter the feedstock origins for plastic production from fossil-based resources to bio-based ones. In practice, this means offering alternative ways to produce the feedstock inputs seen in Table 1, such as ethylene, propylene and BTX.This approach describes the drop-in bioplastics production on a similar level of detail to the already modelled conventional plastics in the model.

In terms of approximation level, this approach therefore represents drop-in bioplastics on a suitable level but does not directly represent other bioplastic types. The approach is very similar to that of the NEDE model by Daioglou et al. (2014). Given the uncertainties related to the new bioplastics production processes, and especially the uncertain demand of these plastics, merely including drop-in bioplastics in the model seems justified. Additionally, with the supply possibility of bio-based feedstocks for the aggregated plastic end-products, the model approximates the overall picture of the chemical industry quite well and makes it possible to manufacture bio-based feedstocks for plastics production.

The approach only adds new paths for plastic end-product inputs and keeps the model simple. Since thermoplastics are the main focus, given that the thermoset commodity includes a vast list of commodities not generally considered as plastics, the input commodities to consider should be based on the thermoplastic input. In Table 1, ethylene, propylene and BTX form the vast majority of the input commodities. Therefore, these commodities are central and included in the model. The other chemicals input is an arbitrary category, thus the further commodities could be C_4-olefins, methanol and ammonia. For now, these commodities are left outside the focus of the thesis for simplicity and focus.

4.1.3 Other approximations and assumptions

Several further approximations need to be described and justified. These are mostly related to the way the SuCCESs model works, such as emissions, but also how the current approximations of the SuCCESs model influence the model extension work. Additionally, the parameters are assumed to remain the same until 2100, since no better data is available. This assumption is rather coarse since it is likely that the technologies would become more efficient or less expensive during the following decades. Thus, the results constitute a worst-case-scenario. To assess the robustness of the technologies, a sensitivity analysis is, however, carried out.

Emissions are central in the SuCCESs model. It is therefore vital to discuss how emissions from the use of fossil-based and bio-based resources and processes are considered. The SuCCESs model accounts for emissions from the origin of each feedstock. This way emissions are always released at the time of extraction of each feedstock, such as oil. Also, the emission impact related to land-use changes is accounted the same way. In the real-world, a significant origin of emissions form bioplastics is the fermentation to bio-ethanol. Following the chemical reaction, this process releases approximately the same mass amount of CO_2 as it produces ethanol. However, this is not accounted as an emission, since the carbon balance accounting is already handled when the feedstocks are extracted in the land-use module. The same idea applies to all other processes and commodities in downstream production, such as electricity and other energy sources. Therefore, the formation of emissions is not considered in the bioplastics module, as it is already considered elsewhere.

Process parameter values for the chemical sector have not been much discussed or studied in the literature (Levi and Cullen, 2018; Burman et al., 2020; Stegmann et al., 2022b). Therefore, approximations are required across the modelling of this sector. To find values for e.g. conversion processes, energy use or economic values, the data sources are usually limited or correspond to small-scale production. These values are linearly scaled up to represent the likely magnitude of each value. The rough approximations are considered valid under the level of detail used in the model. It is therefore more crucial to utilize values that represent the magnitude and are inter-comparable when such values are highly approximated for other similar processes.

The economic values for conventional plastics as well as the upstream chemical industry lack detail. Most costs of the processes are only considered in terms of investments but variable costs are not included apart from the required inputs. This is justified by the small scale of costs related to production outside the factors already considered as inputs. Therefore, in constructing the bioplastics module, variable costs are not considered other than significant maintenance or external input costs. The decision makes conventional and bio-based plastic feedstocks comparable as including costs, not considered in the conventional processes, would automatically reduce the competitiveness of bioplastics.

4.2 Defining required production processes for the selected commodities

This Section discusses how the real production processes function and how these should be captured in the model. With this approach, the required process paths can be identified and linked before considering the parametrization of the processes.

4.2.1 Bio-ethylene production

Ethylene, C_2H_4, is the simplest possible alkene, and more commonly known by its polymerized form, polyethylene (PE). By its chemical structure, ethylene is close to ethanol C_2H_6O, which is known to be an easily producible bio-commodity. The common path to achieve bio-ethylene in the real-world is therefore considered to be through bio-ethanol. (Siracusa and Blanco, 2020) The process of achieving bio-ethylene is shown in Figure 4.

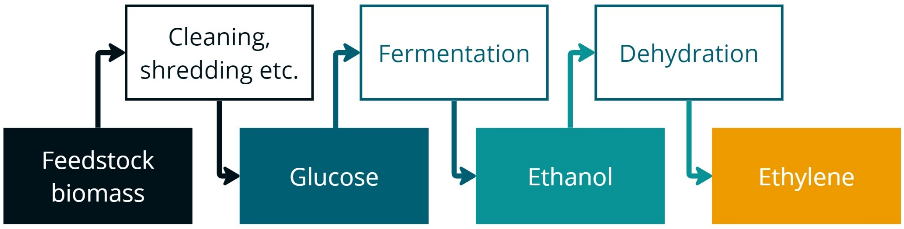

Figure 4: The most common bio-PE production process as described by Siracusa and Blanco (2020).

The process of producing bio-ethylene consists of two parts, the production of bio-ethanol and the dehydration of bio-ethanol to ethylene. This separation is made since bio-ethanol can be additionally be utilized in other purposes in the model or in the bioplastic module. Additionally, the process of producing bio-ethanol is fairly well-studied and well-established, which should allow for a better reliance on the literature. In addition to the inputs for each process, biomass and ethanol, both processes also require energy. Additionally, the processes utilize enzymes and catalysts, which, if significant, are accounted as costs but not feedstock streams.

4.2.2 Bio-propylene production

Propylene, C_3H_6, is the second most simple alkene commonly known by its polymerized form, polypropylene (PP). Producing bio-based propylene has turned out being more difficult than producing bio-ethylene. According to Siracusa and Blanco (2020), by 2020 only Braskem is known to produce bio-propylene on the industrial scale. However, the process details are not publicly available because the process is confidential and owned by the company. Central approaches to producing bio-propylene are illustrated in Figure 5

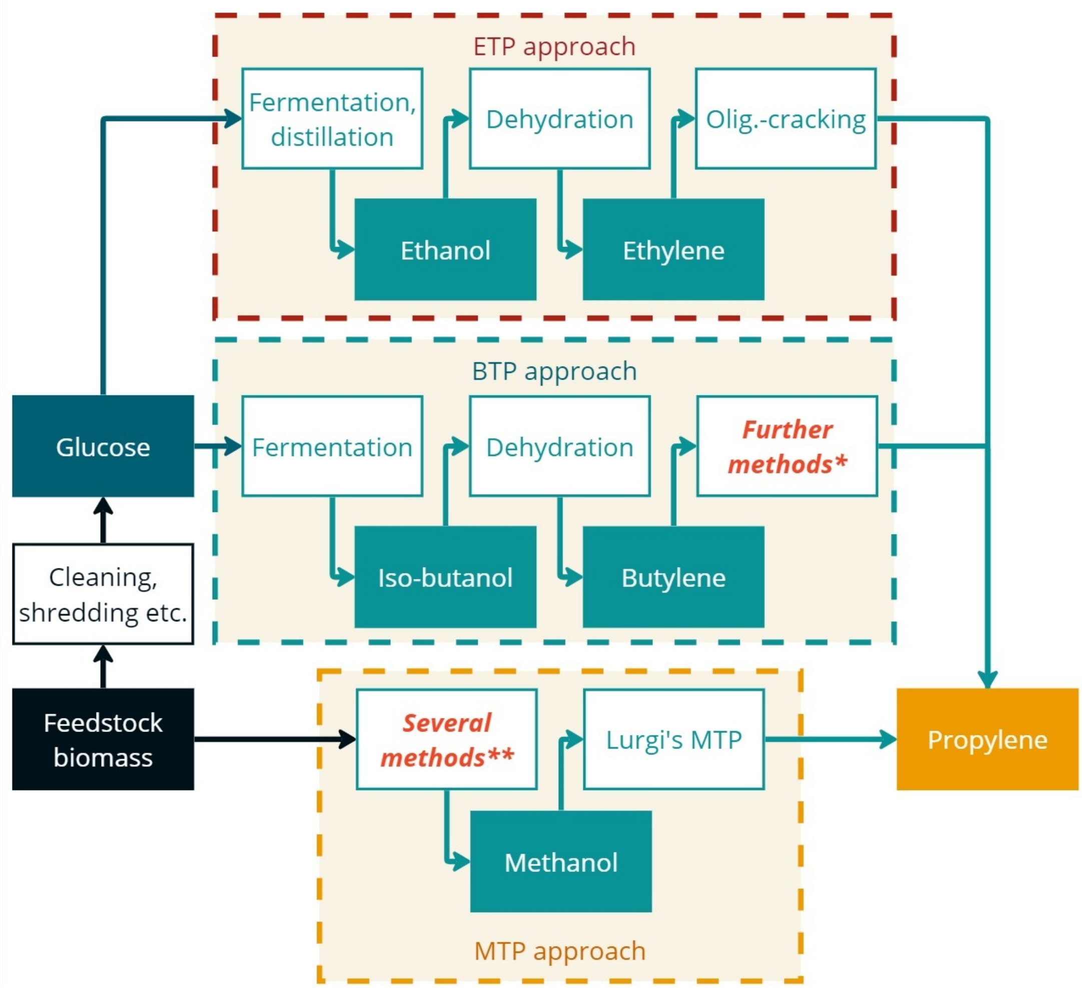

Figure 5: Three approaches to producing bio-propylene: (i) ethanol-to-propylene (ETP) (Xue et al., 2017), (ii) butylene-to-propylene (BTP) and (iii) methanol-to-propylene (MTP) approac Siracusa and Blanco (2020). The further methods for converting butylene to propylene (*) as well as producing methanol in the MTP approach (**), are more complex and described in required detail in the text.

Although otherwise recent and comprehensive, the review by Siracusa and Blanco (2020) does not mention the ETP approach even though it is seen as the most promising way of producing bio-based propylene. For example, Braskem is believed to produce propylene through this process (Phung et al., 2021). The two other approaches, BTB and MTP, are slightly more complex and come with more uncertainties during the stages indicated in Figure 5. Despite the shortage of public details on the processes, all three approaches are discussed below and the decision on the selected processes is based on the further details.

In the ETP approach, the previous definition of the bio-ethylene production can be utilized as a starting point. Given this, only the oligomerization cracking step from ethylene to propylene is required to model bio-propylene production. However, despite the discussion by Xue et al. (2017), further details on this process are not found. Thus the process is left out of the scope under the assumption that it is currently too far from industrial scale.

The further methods in BTP approach consist of isomerization and metathesis (Chen and Patel, 2012). However, finding further details on this process on the required level has turned out being very challenging. This suggests that the remark by Onen et al. (2020), on the bio-propylene development being still in progress remains relevant. Given the challenges, the BTP approach is not further discussed nor included in the model since defining it in more detail and finding parameters appropriately is not possible under the scope.

In the MTP approach, bio-methanol can be produced based on various methods, including gasification of biomass, bio-synthesis and pyrolysis. The paths are seen very similar to conventional production paths (Ajdari, 2020; Shamsul et al., 2014). The SuCCESs model already comes with a process for bio-methanol production thus this part of the process does not require additional processes. However, the MTP conversion process is not yet included in the model. This is a conventional process already utilized in the industry. The process requires methanol and energy while the further requirements are left out of the scope (Jasper and El-Halwagi, 2015).

Based on the above, the methanol-to-propylene process is required to be added in the model. The process is parametrized in Section 4.3.

4.2.3 Bio-BTX production

BTX refers to a combined consideration, i.e. stoichiometry, of benzene C_6H_6, toluene $C_6H_5CH_3$ and xylene $C_6H_4(CH_3)_2$ (Dagle et al., 2020). All of the chemicals are aromatic hydrocarbons, i.e. contain a benzene ring, but differ in what else is attached to the aromatic ring. Due to the relatively similar chemical structure, the chemicals are often considered together as BTX. The paths for producing bio-based BTX are shown in Figure 6. According to Li et al. (2017), the processes towards bio-based BTX are very limited in number and different approaches, apart from the ones introduced, have not yet been studied widely.

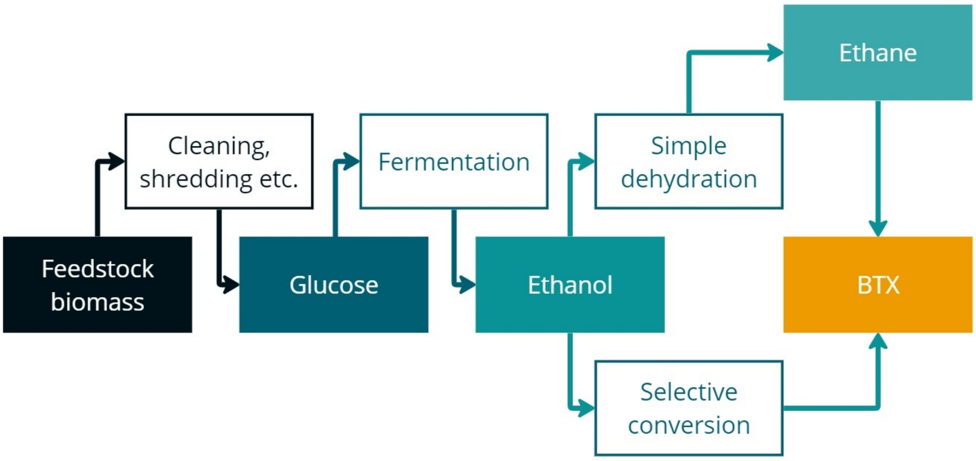

Figure 6: Two approaches to producing BTX from biomass. The route through ethane follows the work by Chen et al. (2015) and the route through selective conversion of ethanol is introduced by Li et al. (2017).

The most profoundly covered process, of the ones presented in Figure 6, is the ethane-to-BTX approach. In the study by Chen et al. (2015), a bio-BTX plant is designed and its profitability is studied yet found out not to have a positive return on investment under the studied circumstances. The approach utilizes ethane as input, which, however, is challenging since it has not been previously introduced by the bio-based processes. Yet, this process is considered to be worth implementing in the model. Moreover, since not much information is found on the process of producing ethane from ethanol, the production is assumed similar to that of ethylene, since ethane is only the less dehydrated version of this commodity.

Nor is the selective conversion, introduced by Li et al. (2017), considered to be economically profitable. According to the authors of both Li et al. (2017) and Dagle et al. (2020), the conventional processes for BTX production are well-established and thus remain economically superior to the bio-based process. Despite this statement, no economic figures were found for this process in the literature review. Therefore, the selective conversion process is left out of this thesis due to lack of overall process information and parameters.

4.3 Parametrization of the selected processes

In general, it is hard to find suitable parameters for the chemical sector. This remark is also widely shared by the modelling literature, such as Stegmann et al. (2022a), as well as the chemical reports, such as Mohsenzadeh et al. (2017). Despite this, alternative ways of defining some process parameters are utilized when possible and the parametrization is based on the discussion in this Section.

4.3.1 Bio-ethanol production

Bio-ethanol can be produced from a wide range of bio-feedstocks, including residues of forestry and agriculture, bio-based waste or any crop or other edible resource. The SuCCESs model provides agricultural and forestry residue as well as crop as biomass feedstock. For all of the feedstock, a shared path towards bio-ethanol is cleaning, shredding and distillation. However, the yields, energy need and economical figures of the processes differ. The three feedstocks are discussed under the following topics. The residue from the fermentation of the feedstocks is considered regular energy-biomass, therefore generating and additional output.

Crop biomass

Crop biomass contains first-generation biomass, such as edible crops and biomass especially grown for the purpose. In comparison to other feedstocks, the group of crop biomass sources is more studied. According to Mohsenzadeh et al. (2017), the output yield of ethanol from grains, such as corn or wheat, is approximately one third of the dry mass of the feedstock. This value is in line with other literature sources, such as the ranges from 0.29 to 0.41 $\mathrm{t_{ethanol}/t_{biomass}}$ based on Jeevan Kumar et al. (2020) and from 0.24 to 0.47 $\mathrm{t_{ethanol}/t_{biomass}}$ base on the analysis by Hattori and Morita (2010). Therefore, a value of 1/3 $\mathrm{t_{ethanol}/t_{biomass}}$, i.e. 3 $\mathrm{t_{biomass}/t_{ethanol}}$ as inverted, is used for the ethanol conversion yield from crop biomass.

Based on the data collected by Hattori and Morita (2010), the energy needed to produce one Mt of bio-ethanol from crop biomass ranges approximately between 0.7 and 18 PJ/Mt. Based on Manochio et al. (2017), the same values range between approximately 3.6 and 19 PJ/t, although it is not clearly stated if the energy used is compared to the input or the output of the industrial process phase. The variability is mainly considered to depend on thermal processing aspects which are further dependent on the type of the biomass used. A rough approximation is done based on an expectation of above average efficiency. Thus, the value of 5 PJ/Mt, is selected, since it is assumed to be presentable for crop biomass while the higher energy needs are associated with materials that contain less sugar and starch content, most likely the reason for the high-end values.

Manochio et al. (2017) find that electricity covers approximately 5 % of the energy consumption whereas natural gas is used as the main energy source. This indicates the use of industrial steam to achieve higher temperatures. Therefore, of the 5 PJ/Mt, 0.25 PJ/Mt is assumed from electricity and 4.75 PJ/Mt from industrial steam under the approximation of Manochio et al. (2017). Utilization of the process residue is not considered, although it could be used in producing energy, thus considerably reducing the need for external energy.

Data on economic figures is limited. Humbird et al. (2002) have determined an approximate investment cost of 1 300 M$/Mt for a rather basic design of a plant. Given that the applicable literature is limited, this value is utilized. The variable costs are, by default, not included in the model. All found parameter values are aggregated and contain factors that should not be included in the comparison. The energy-biomass output of crop-like fermentation residue is found to be approximately 6100 kWh per ton of bioethanol (Chen et al., 2021). Thus, the value used in the model is 22 PJ/Mt.

The other parameters usually defined in SuCCESs model, such as availability and capacity factors are not relevant for this process. The life-time of the capacity is assumed 30 years, since this value is also commonly used in all other industrial processes. An existing capacity, i.e. base year output, of approximately 90 Mt/a is found in the literature by Hoang and Nghiem (2021). The value covers global bio-ethanol fuel production for 2020, thus indicating the approximate existing capacity. Most of all bio-ethanol production originates from feedstocks most close to crop biomass, thus all of the base year output in the model is associated with crop biomass.

Agricultural residue

In comparison with the direct crop usage, agricultural residue or waste requires more pre-processing and energy (Jeevan Kumar et al., 2020). The conversion yields of different corn stovers, grain straws and e.g. sugarcane bagasse range between 0.18 and 0.2 $t_{\text{ethanol}}/t_{\text{biomass}}$ (Chen et al., 2021). Additionally, according to Hoang and Nghiem (2021), the theoretical maximum conversion yield from agricultural residue biomasses is approximately 0.4 $t_{\text{ethanol}}/t_{\text{biomass}}$, thus the real values should be considerably lower than this. Based on these sources, a value of 0.2, i.e. 5 $t_{\text{biomass}}/t_{\text{ethanol}}$ by its inverse, is selected for the model usage.

The energy need for producing bio-ethanol from agricultural residue is not widely studied. However, based on the conversion yield values, the energy need of agricultural residue is assumed higher than that of the crop biomass. Therefore, since the output ratios between crop and agricultural residue is $\frac{5}{3} \approx 1.7$, the energy need of crop biomass is multiplied with this value. Thus, the total energy consumption is approximated to 8.3 PJ/Mt, which with the similar share between electricity and steam, accounts to 0.4 PJ/Mt of electricity and 7.9 steam.

The energy-biomass output of fermentation residue of agricultural residue is approxmately 4200 kWh/t of bioethanol (Chen et al., 2021). Thus, the value used in the model is 15 PJ/Mt.

There is not much literature on the economic figures. Thus, the values are assumed similar to the values of crop biomass. However, the conversion by the output ratios between agricultural residue and crop biomass is made, which results in investment cost of 2 100 M$/Mt.

Forestry residue

The conversion yield of different forestry and wood processing residues ranges between 0.16 and 0.23 $t_{ethanol}/t_{biomass}$ (Chen et al., 2021; Frankó et al., 2016). Additionally, Hoang and Nghiem (2021), again, estimate a theoretical maximum of approximately 0.4, thus similar to that of agricultural residue. Therefore, a value of 0.2 $t_{ethanol}/t_{biomass}$, i.e. 5 $t_{biomass}/t_{ethanol}$ as inverse, is assumed as the yield factor of forestry residue.

The energy need for producing bio-ethanol from forestry residues is assumed to be greater than that the previously discussed since wood residues require more processing towards a good glucose yield. No exact values were found for this process during the literature review. Therefore, a value of 10 PJ/Mt is selected, since this represents the mid-high-end of the found literature values. Again, 5 % is accounted to electricity and 95 % to industrial steam, thus the amount of electricity required is 0.5 PJ/Mt and steam 9.5 PJ/Mt.

The energy-biomass output of fermentation residue of forestry residue is approximately 2000 kWh/t of bioethanol (Chen et al., 2021). Thus, the value used in the model is 7 PJ/Mt. The economic values are assumed similar to that of crop biomass with a similar scaling operation than in the case of agricultural residue. Therefore, the monetary values are the same as for the agricultural residue.

4.3.2 Ethanol to ethylene dehydration

The literature provides fairly limited information on process conversion, selectivity and energy requirements as most attention has been given to process optimization under specific conditions and catalysts. According to Mohsenzadeh et al. (2017), technological details of many industry-scale technologies are not publicly available. Cameron et al. (2012) stated that an ethylene stream of approximately 50% in comparison to input ethanol stream can be achieved. Thus, a value of 0.5 $t_{ethylene}/t_{ethanol}$, i.e. 2 $t_{ethanol}/t_{ethylene}$ as inverse, is used.

Finding the required energy has turned out being very challenging. According to Mohsenzadeh et al. (2017), the theoretical endothermic value of producing one gram of ethylene is 1632 J, thus 1.6 PJ/Mt. However, according to Cameron et al. (2012), the same value is 401 BTU/lb thus 0.19 PJ/Mt. The difference of the values is significant and is likely due to a different stage of the process, that is not made clear. Since the sources are contradictory, alternative sources need to be utilized. According to Poppick et al. (2015), a publicly available university group work, a process of converting 1 Mt ethylene from ethylene requires 0.17 Mt of natural gas, which in terms of energy means approximately 8.5 PJ/Mt. Although the source is a work by a student group, this value is used since no better alternatives seem to be available. The energy is considered to be in the form of steam, worth 8.5 PJ/Mt.

In terms of costs, Mohsenzadeh et al. (2017) discusses a plant producing 180 kt of ethylene annually for which the aggregated investment costs are estimated at 11.2 M$, thus 62 m$/Mt. Approximately a third of the price is accounted to storage which is discussed to be easily made less expensive. Based on the study by Cameron et al. (2012), the investment of a 1 Mt/a capacity plant is between 40 to 65 M$. Finally, Poppick et al. (2015) report a capital cost of 16.4 M$ for a 0.46 Mt/a plant, thus 35 M$/Mt. Therefore it can be concluded that a slightly over average investment cost of approximately 40 M$/Mt is worth considering under the assumption of decreasing costs.

As for the ethylene production, other parameters, such as availability and capacity factors are irrelevant for this process. The life-time of the capacity is, again, assumed 30 years. The existing capacity is hard to define under the vast amount of different processes towards bio-ethylene. However, an approximation over the annual production of plastics, share of bioplastics and drop-in bioplastics, as discussed in Chapter 2, an existing capacity of approximately 0.7 Mt/a is assumed.

4.3.3 Methanol to propylene

Based on Syah et al. (2021), the Lurgi's MTP requires approximately 3.5 t of methanol feed to produce 1 t of propylene. This is considered a fairly standard process, in comparison to the previously introduced processes, since the Lurgi's MTP is an existing process already utilized today. Based on this, the inverse conversion rate is set to 3.5.

The energy need of the MTP is not found in an exactly specified form. However, it is noted that the utility costs of the study by Syah et al. (2021) mainly consist of water and energy. If all of the energy was originating from electricity with a price of 0.05 $/kWh, the energy consumption would be 1.0 PJ/Mt. However, a rough estimate is done that only half of the cost is associated with energy, meaning 0.5 PJ/Mt, and that all of the energy is required in the form of steam. This is a rough estimate, but it is considered to cover a suitable level of detail.

The economics of producing MTP are based on Syah et al. (2021). In the case of 0.45 Mt/a capacity, investment costs are found to be approximately 280 M$, which means investment costs of 622 M$/Mt.

4.3.4 Ethane to BTX

The first step of the process, production of ethane, is assumed similar to ethylene. Thus, a process of ethanol to ethane is also implemented with parameters similar to those of ethylene production. These parameters are considered a conservative estimate since forming the double bond of ethylene is assumed more energy-requiring than replacing the hydroxyl group with simply hydrogen.

According to Chen et al. (2015), to produce 1 lb of BTX requires 1.6 lb of ethane, thus the inversed conversion rate is 1.3 Mt/Mt. The energy use is discussed in the same paper and found that the process of converting 1 Mt of ethane to BTX requires 3.1 PJ. Since the required temperatures are high, use of industrial steam is assumed as major input. In terms of economics, an investment cost of 702 M$/Mt.

5 Assessment methodology and metrics

5.1 Mitigation of climate change

Assessing the mitigation potential can be interpreted in many ways. Therefore it is essential to discuss and define the aim of this part of this thesis in more detail.

In economics, policy measures are used to shape the economic environment in a desired way. In terms of climate change mitigation, agreements on emission targets, emission taxes and cap-and-trade systems have been introduced. Additionally, total bans and technical limitations can be set on certain actions or substances, such as was set for the ozone-depleting CFCs in the late 1980's. These policy measures are commonly considered mandatory for effective climate change mitigation actions. Without incentives, industries would not have incentives to change existing procedures into anything new unless the new procedures were economically attractive. By introducing policy measures, industries are incentivised towards desired choices by making them relatively more economically attractive.

In the literature, bioplastics are generally not considered economically viable when compared to the conventional plastics (Rosenboom et al., 2022). This lack of viability is mainly due to the long history of fossil based production, during which the technology has been developed, i.e. the costly R&D and investments have already been done and processes have been optimized for efficient production. Therefore, many of the fossil technologies have become favourable in terms of costs. Additionally, the field of environmental economics is based on the argument that the harm on environment should be internalized by pricing emissions. Thus, if no emission prices are set, the price of fossils use is too low in comparison to its real impact. Therefore, it is assumed that policies are required to change the business-as-usual (BAU) setting, if the price of oil is not expected to increase considerably.

Since the literature on the overall sustainability impact of bioplastics is contradictory, it is not yet known if bioplastics offer a more climate friendly alternative than conventional plastics. Moreover, if bioplastics are found less emission-intensive, it is not clear how the investments in them could be enhanced and how large the incentives needed to be. This creates a need to model general emission policies that reduce overall emissions and assess the impact these policies have on the deployment of bioplastics production.

5.2 Marginal abatement cost

Marginal abatement cost (MAC) is a common way for policymakers to assess feasible mitigation strategies under emission reduction goals. The idea is, namely, to assess the marginal cost, i.e. the cost of reducing one more unit of e.g. emissions, in the context of emission mitigation. MAC curves (MACC) are used to visualize the behaviour of the MAC values but the term MAC is often also used to refer to the curves. (Huang et al., 2016; Kesicki and Ekins, 2012; Mckitrick, 1999)

In the literature, MAC analyses are generally considered to be the whole modelling and system setting. Therefore, e.g. IAMs are seen as a tool for assessing and quantifying MACCs. In this thesis, the approach differs from this by mainly utilizing MAC as a metric to assess a model augmentation.

The criticism of MAC analysis focuses on the modelling aspects, not the MAC metric itself. However, as a general remark, MAC should only be considered as one indicator and that overly relying on the MAC results may cause overconfidence. (Kesicki and Ekins, 2012) Thus, general awareness of model results must be taken when assessing the model results.

5.3 Prices vs. quantities

Weitzman (1974) introduces a theory of prices vs. quantities. The idea of this theory is to define two approaches in policy making and note the indifference between them under certain conditions. If policies seek to impact prices directly, commonly making a certain action or commodity more expensive, the market is artificially shaped, desirably, so that leads to the intended changes as outcomes, such as reduced output of certain commodities. With quantities, a cap can be set to forbid exceeding a certain quota of output. Under the theory, the mechanisms of the market lead to the possibility of finding the same outcome independent of the choice of the policy. In fact, both measures can be used to achieve the same outcome if no uncertainty is accounted for, but the real-world implementation and adaptation of businesses depending on the approaches may differ.

Directly following the theory by Weitzman (1974), a common approach in the recent climate change mitigation literature has been to implement emission caps derived from the Paris agreement or assess emission taxing and its impact. In optimization models, in which utility is maximized or total costs minimized, it is both possible to set an emission cap or to set an emission tax. Making such changes is not possible with the simulation-based IAMs, since the optimization cannot be ran intertemporally.

The SuCCESs model contains a simple climate module, which allows to estimate the most likely global mean temperature increase for each considered time step until 2100. This feature allows to set temperature targets as the climate policy, thus making a temperature-based climate policy possible. Alternatively, emission prices can be added to the objective function thus allowing a price-based climate policy. Following the theory by Weitzman (1974), for a quota-based policy, such as an emission cap, there exists a price-based policy forming an identical development scenario and identical emissions, as long as the system description remains the same in terms of other factors and no uncertainty is included. Therefore, there exist emission penalties $p^*_{e,y}$ for emissions e and years y, with which, the system is identical to its counterpart with emission cap-based policy in terms of outcome. An analysis by Williams (2002) suggests that at least in a slightly different system, the emission penalty prices $p^*_{e,y}$ are proven to be the shadow prices, i.e. marginal costs for emission reductions, of the quantity-based optimum in a deterministic system. Thus, it is possible to utilize the theory of of prices vs. quantities in the analysis and get helpful insight by considering both approaches together.

5.4 Policy approaches and metrics

The idea of prices vs. quantities is utilized to assess the mitigation potential of bioplastics. As seen in Section 5.3, the SuCCESs model can be used with both temperature-based policy resulting in a change in MACs and with a price-based policy resulting in different mean temperature increases. The climate impact of bioplastics can therefore be assessed in comparison to a business-as-usual (BAU) scenario by comparing the two measures with a scenario with bioplastics (BIO). The opportunity of utilizing both approaches is exploited, which allows for comprehensive understanding on the system.

As seen in Section 5.3, literature shows that price-based and temperature-based policies can be used to obtain a similar outcomes. Based on this, this thesis assumes that utilizing quantity-based, i.e. temperature-based, marginal costs for the price-based problem yields identical results in terms of investments and global temperature increase. This assumption is validated in the results.

To obtain the desired metrics of both MACC as well as the difference in temperature development between a scenario with (BIO as bioplastics) and without (BAU as business-as-usual) bioplastics, the model is ran under two configurations. First, the model is run with temperature-based policy, i.e., by setting a T_{lim} acting as the maximum allowed global temperature increase during the time period. The value of T_{lim} is varied between the 1.5°C and 2.2°C in approximately 0.1°C intervals for both BIO and BAU technology scenario to form MACC. The range is based on the Paris Agreement although it is extended to 2.2°C for a clearer examination on the model behaviour at 2.0°C. If bioplastics are an economically viable climate change mitigation method, the MACs of the BIO scenario should be lower than that of the BAU scenario, since meeting the same temperature target is found to be cheaper with the possibility of producing bioplastics.

After the MACs have been computed based on the temperature-based policies, the marginal costs $p^*_{e,y}$ for all applicable emissions e and years y of the BAU scenario are declared as the emission prices for the price-based model. For this, temperature caps of 1.5, 1.75, 2.0 and 2.2 °C are selected, since more detailed values do not provide additional value. The corresponding global mean temperature increase is therefore obtained for both technology scenarios BAU and BIO based on the price-based policy of the corresponding temperature-based BAU run. Thus, if bioplastics are an economically viable climate change mitigation method, the global temperature increase of BIO under the emission prices should be lower than that of the BAU scenario. This is because under the same emission costs, the system is found at an optimal equilibrium with a decreased amount of emissions produced.

6 Results

6.1 MACC and emission cost impact

Two scenarios are introduced to illustrate the impact of bioplastics: one without the possibility of producing bioplastics, i.e. business-as-usual (BAU), and one with the possibility of producing bioplastics (BIO). In Figure 7, the MACCs, following the temperature-based problem, as well as the price-based problem, as introduced in Section 5.4, of the two scenarios are visualized. The temperature limit range spans form 1.5°C to 2.2°C which approximately follows the Paris Agreement's below 2.0°C and preferably 1.5°C.

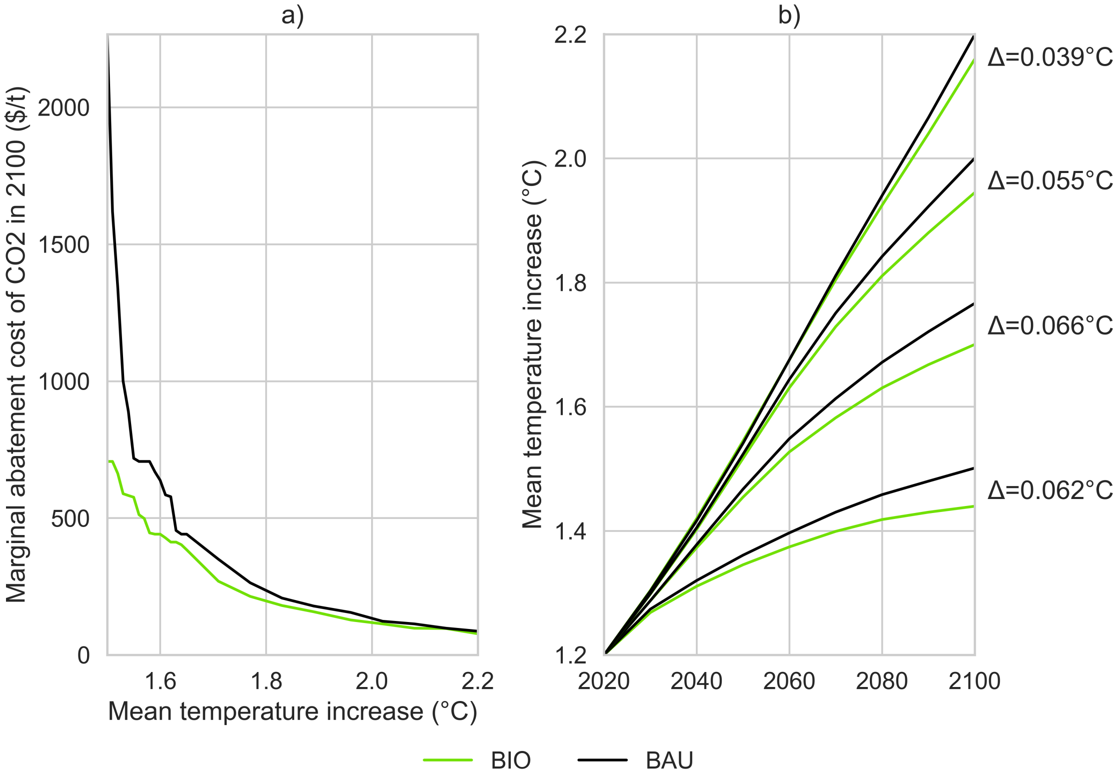

Figure 7: The a-panel illustrates the MACC of CO_2 for both scenarios under a temperature-based policy. The b-panel shows the temperature change under price-based policy for temperatures 1.5, 1.75, 2.0 and 2.2 °C. The values for each temperature scenario indicate the difference between the BIO and BAU values for 2100.

Figure 7 a) illustrates that the MAC value of CO_2 in the BIO scenario with bioplastics is clearly lower than in the BAU scenario. The difference is greater with stricter temperature limits, and in the proximity of the 1.5°C temperature limit, the MAC of BAU is up to 3 times larger than that of BIO. The result indicates that achieving the temperature increase target of 1.5°C is significantly cheaper if the production of bioplastics is possible.

Figure 7 b) shows that the same temperature increase can be achieved with price-based control, if the prices for GHG emissions are set according to the temperature-constrained case. This validates the assumption that there exist prices $p^*_{e,y}$ for which a similar T_{lim} is achieved with both price and temperature based policy, as described in Section 5.4 . The Figure also shows temperatures in 2100 are lower for the BIO scenario than the BAU scenario, i.e., with similar emission pricing, bioplastics would result in a lower increase in global mean temperature. The reduced mean temperature increase under the same constraints for 1.5°C is 0.062°C meaning that instead of 1.5°C the global temperature increase in 2100 would be approximately 1.44°C. The differences between the BAU and BIO scenarios in the global temperature increase are seen decreasing when the global warming target is increased. This result is aligned with the difference in the MAC curve of panel a), since it indicates that the marginal benefits the existence of bioplastics in the system offer decrease as the maximum allowed temperature rise is increased. Based on the results, bioplastics can be considered as a relevant emission mitigation mean in comparison to other mitigation means utilized in the model. Additionally, under a tightening climate policy, bioplastics are increasingly viable in terms of economical factors.

6.2 Impact of bioplastics on emissions

The result seen in Figure 7 indicate that in the price-based policy, the total emissions between the BIO and BAU scenarios differ, as expected. To better understand the change in emissions, Figure 8 illustrates emissions produced in both technology scenarios with a price-based policy obtained from a temperature-based run on the corresponding mean temperature cap.

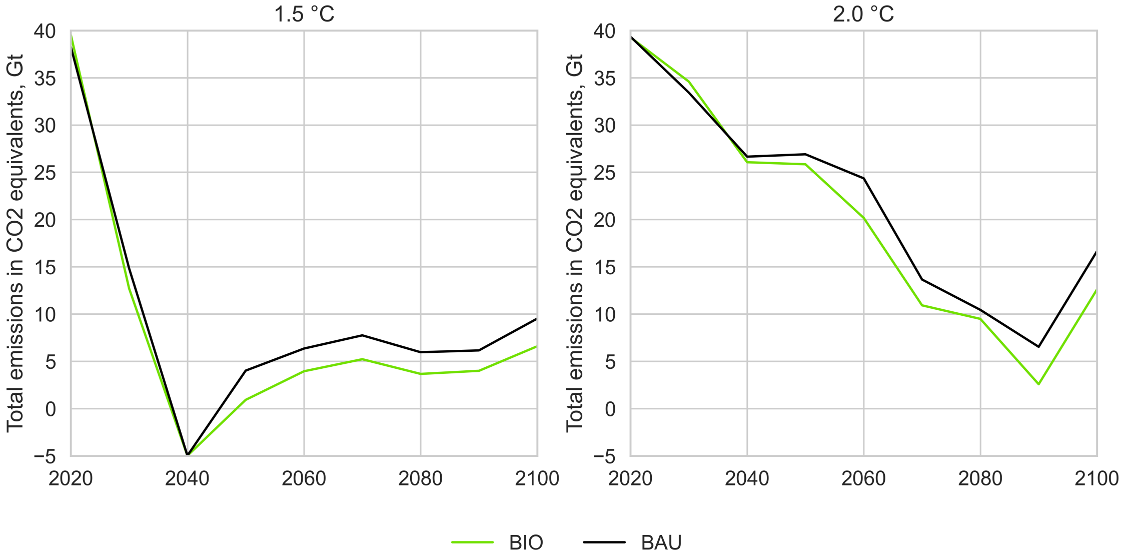

Figure 8: Total emissions of all GHG origins as converted to CO_2eq for both technology scenarios BIO and BAU as well as temperature cap scenarios 1.5°C and 2.0°C.

Figure 8 shows that for both temperature scenarios, the total emissions of a system with bioplastics are smaller than without bioplastics. The result is aligned with the previous findings. The figure additionally shows a fast decrease in total emissions in the 1.5 temperature scenario between years 2020 and 2040 which is assumed to be mainly caused by rapid decarbonization of the energy sector. The difference in emissions between the technology scenarios in the 1.5°C scenario is at a relatively constant value of 3 Gt/a of CO_2eq after the year 2050. In the 2.0°C scenario, the difference is generally smaller but on a similar level in 2100. To better see the main reasons for the difference, Table 2 represents processes, in which the rate of emission differs the most between BIO and BAU scenarios.

Table 2: The most significant differences in CO_2 emissions between BIO and BAU for 2050 and 2100 under 1.5°C and 2.0°C price-based policies. Negative values indicate that BIO scenario produces less emissions than BAU and vice versa.

	Difference in emissions (Mt)			
	1.5°C		**2.0°C**	
Process	**2050**	**2100**	**2050**	**2100**
COTC process	-2 320	-3 280	-530	-1 180
Naphta cracker	-440	-1 340	-470	-1 350
Terrestrial CO2-Sinks	-1 590	-370	60	60
Gasoline, transportation	0	0	-270	-1 170
Gasoil cracker	0	0	-510	-830
Oil refineries	190	280	-140	-440
Steam from natural gas	380	650	0	780
Methanol Gas Existing	710	1 180	0	0
Total	-3080	-2940	-1 790	-4 000

Table 2 shows that the most significant emission reductions caused by the introduction of bioplastics relate to the reduced emissions from the COTC and naphta cracker processes. COTC is an significant source of emission reductions in the 1.5°C scenario, which is because it is a major competitor for the bio-commodity processes. Additionally, a significant reduction is caused by carbon stored in terrestrial sinks in 2050 under the 1.5°C scenario, meaning that more carbon in stored in sinks in the BIO than in the BAU scenario. In the 2.0°C scenario, sinks are decreased in BIO in comparison to BAU. For positive values, the results show that emissions caused by methanol production and production of industrial steam increase in the 1.5°C scenario, especially significantly in 2100. In 2.0°C, the only remarkably large source of emission increase by BIO is the increased production of industrial steam using natural gas.

What is especially interesting in Table 2, is that in the 1.5°C scenario, terrestrial carbon sinks are increased by the introduction of bioplastics but decreased in the 2.0°C scenario. The increase in carbon sinks in the 1.5°C scenario is likely explained by a decreased production of crop-based biomass, since the production of bio-ethanol yields biomass that can be used to replace such need.

6.3 Bio-commodity production

The main raw materials for plastics production, as discussed earlier, are ethylene, propylene and BTX. Of these, the production of ethylene and BTX are presented below in Figures 9 and 10. Ethylene and BTX are presented primarily since ethylene is the major commodity in plastics production and BTX is found to have an interesting role as a bio-commodity. Additionally, propylene production is presented in Appendix

A and the upstream production of bio-ethanol is presented in the following Section 6.4.

The results are visualized for three temperature limit scenarios and two technology scenarios. For temperature, 1.5°C and 2.0°C are used as maximum allowed temperature increase following the Paris Agreement. In addition, a scenario with no climate policy is presented for comparison. The technology scenarios considered are, again, one with (BIO) and one without (BAU) the possibility of bioplastic production.

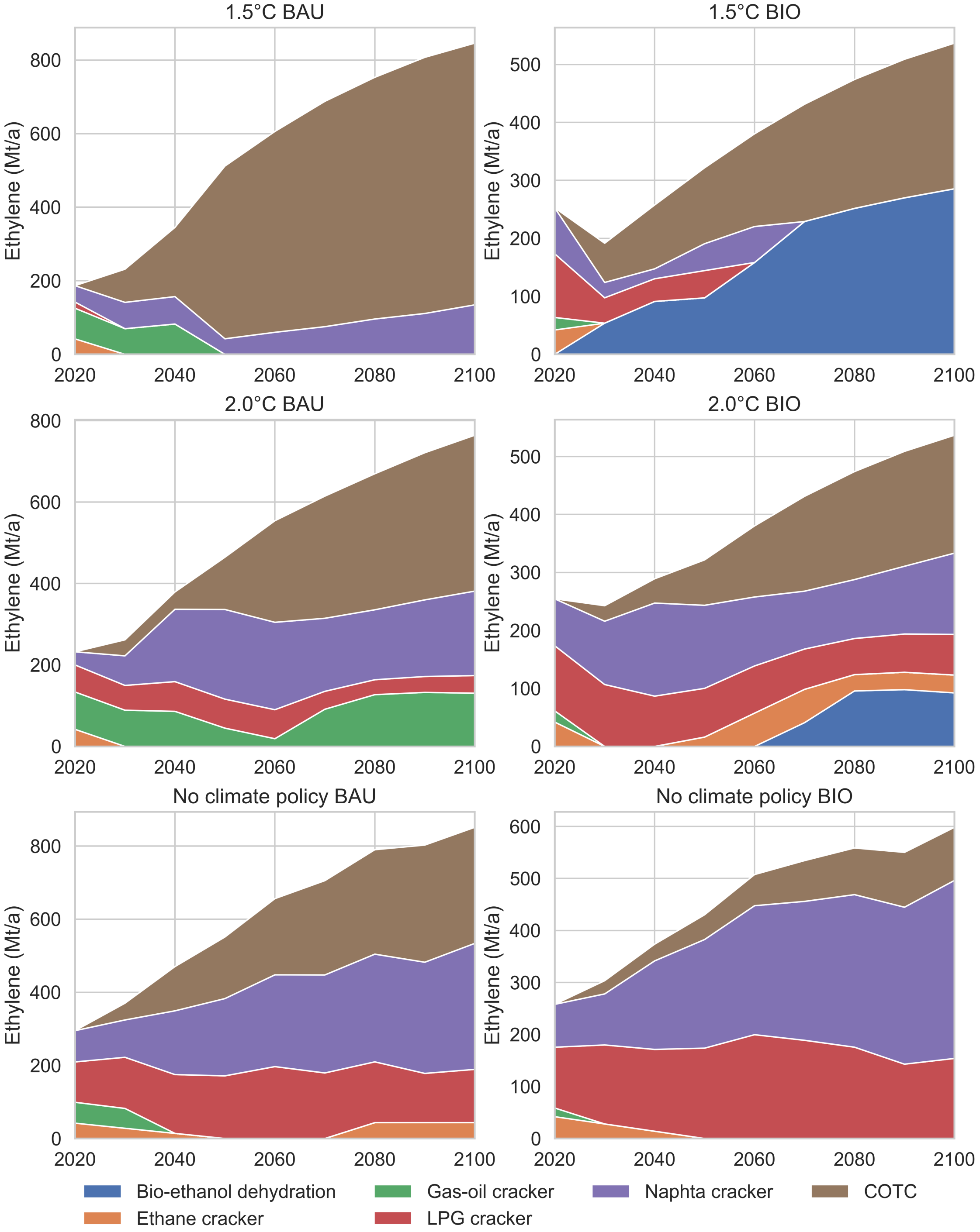

Figure 9: The production methods of ethylene for maximum mean temperature increases of 1.5°C, 2.0°C and a scenario with no climate policy; with (BIO) and without (BAU) the possibility of bioplastics production. The figures represent annual production that is linearly scaled between the ten-year intervals.

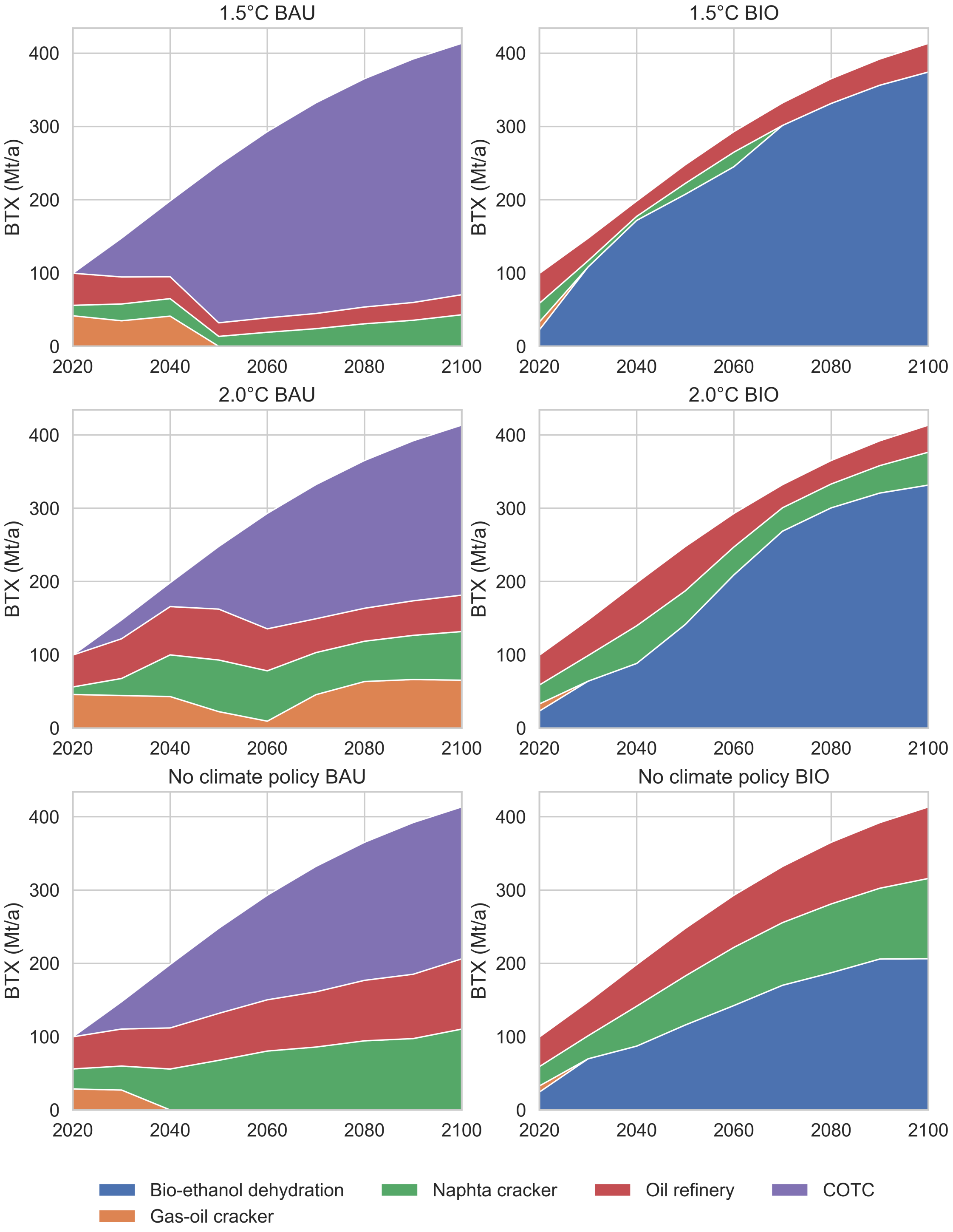

Figure 10: The production methods of BTX for maximum mean temperature increases of 1.5°C, 2.0°C and a scenario without a climate policy, in both BAU and BIO scenarios. The figures represent annual production that is linearly scaled between the ten-year intervals.

Figures 9 and 10 both show that stricter climate policies result in higher production of the two bio-commodities. Also, bio-propylene production behaves in the same way, as illustrated in Appendix A. This further proves that the bio-commodities studied are an economically viable mitigation method. However, the behaviour in relation to the climate policy differs especially between ethylene and BTX. In BAU scenarios, COTC production in BAU behaves in a similar way with the bio-based commodities, as its share in the total production grows in stricter climate policies.

Figure 9 indicates that in the absence of a climate policy, no bio-ethylene is produced. This means that producing bio-ethylene without a climate policy is not seen economically beneficial by the model. In contrast to ethylene, Figure 10 illustrates that bio-BTX production is also present in the absence of a climate policy. This indicates that producing bio-BTX is beneficial for the system even without policy incentives.

A closer look reveals that the total ethylene production between BIO and BAU differs in all policy scenarios as the total production levels in each BAU scenario are higher than in the corresponding BIO scenario. Since demand for each commodity is set to be constant across scenarios, the difference in total production indicates imbalance in ethylene production. Additionally, even though no bio-ethylene is produced in the absence of a climate policy, the portfolios of ethylene production differ between BAU and BIO. In BAU, COTC covers a large share of total production of ethylene whereas in BIO, the production of ethylene is dominated by naphtha cracker followed by LPG cracker. The reasons likely originate from the lack of flexibility in COTC production. These phenomena are further discussed in Chapter 7.

6.4 Bio-ethanol production and feedstock utilization

The results indicate that stricter climate policies imply more production of bio-ethylene, bio-propylene and bio-BTX. To produce these commodities, except for propylene the bio version of which is produced from methanol, bio-ethanol is required. The possible sources of bio-ethanol in the model are crop biomass as well as forestry and agricultural residues. In this Section, total production and the distribution between the biomass origins of bio-ethylene are presented in Figure 11. Additionally, the total production of biomass and selected fossil resources are presented in Figure 12.

For the source of bio-ethylene, only the BIO technology scenario is studied, but for the development of fossils and biomass, both technology scenarios, BIO and BAU, are analyzed. As for climate policies, 1.5°C and 2.0°C as well as a scenario with no climate policy is included.

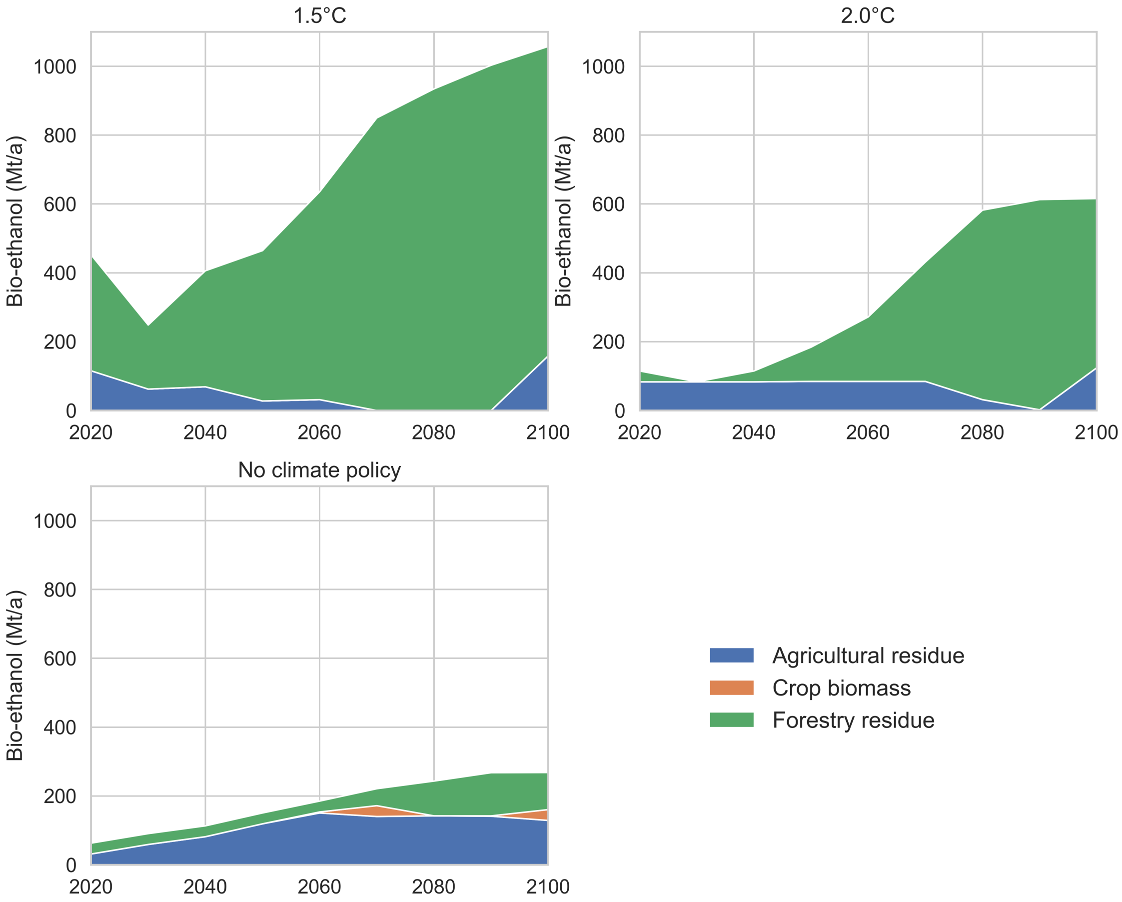

Figure 11: Feedstocks used in bio-ethanol production in 1.5°C, 2.0°C and no climate policy scenarios.

Figure 11 confirms the expectations based on the earlier results, i.e. the production of bio-ethylene is at its highest in the case of the strictest climate policy, 1.5°C. Since bio-BTX is still produced in the scenario with no climate policy, the production of bio-ethanol is seen also in this scenario. Forestry residue is the main source of bio-ethanol in the stricter climate policy scenarios. The use of agricultural residue is relatively small but increases slightly as climate policy loosens. The use of crop biomass as a feedstock is only seen in the scenario with no climate policy and even in this scenario, in very small amount in comparison to the other sources. This indicates that although the crop biomass process is efficient in terms of energy and raw material usage as well as investment costs, its environmental impact is not as positive as of the residues.

The changes in upstream feedstock production are in Figure 12. Since the overall demand for plastics, among many other commodities, is assumed to grow over time, also the use of both fossils and biomass increase during the century. However, the rate of increase in fossil feedstock production depends on the climate policy, with the strictest policy resulting in the slowest increase and vice versa. Moreover, the introduction of bioplastics has a discernible effect on overall fossil feedstock production, although majority of the fossil-based commodities are used for energy and transportation purposes and not for non-energy feedstocks.

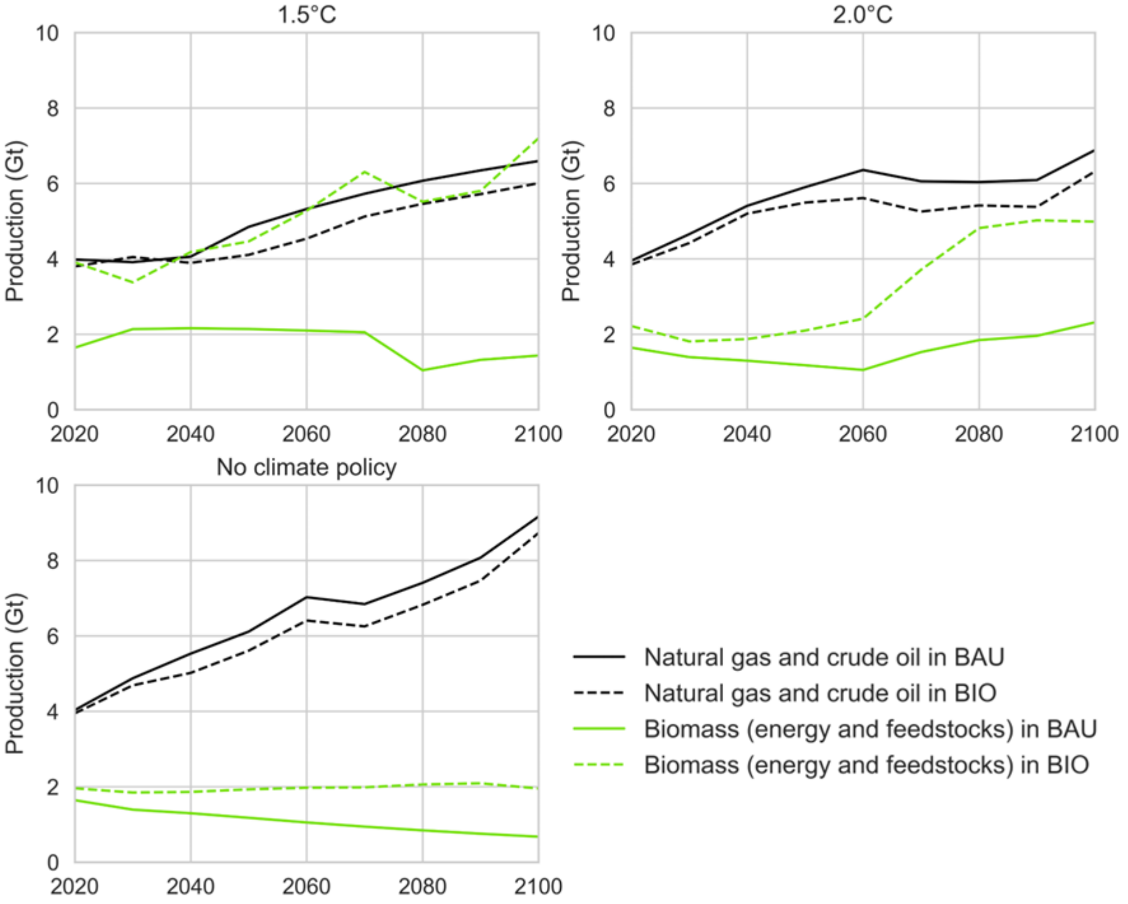

Figure 12: Aggregated production of crude oil and natural gas and all biomass types for 1.5°C and 2.0°C policies as well as no climate policy in both technology scenarios. Although some of the feedstocks are described by energy value, a conversion to mass units is carried out to make results more inter-comparable.

For biomass use, a clear distinction can be observed both between the technology scenarios as well as policy scenarios. In all BIO scenarios, the production level of biomass is higher than that of BAU and the production level of fossils is lower in BIO than in BAU. In terms of climate policies, the stricter the climate policy, the more biomass and less fossils are produced.

Stricter climate policies lead to reduced consumption of fossils since the production of conventional commodities is partially replaced with bio-based commodities and renewable energy substitutes fossil energy thus decreasing the demand. However, although there is a large difference between, e.g., the production of bio feedstocks in BIO between the 1.5°C and 2.0°C climate policy scenarios, the difference in the production of fossils is not equally drastic.

6.5 Sensitivity analysis

To assess the robustness of the results, a sensitivity analysis is carried out with cases describing the most plausible development scenarios regarding the future of plastics. Although external factors, such as demand, have a key role in shaping the future of bioplastics, analysis on such uncertainties would require more extensive scenario building and is thus left out of the scope. However, when it comes to aspects such as techno-economic development of the production processes of bioplastics, the analysis is both easily included in the scope of this thesis and central to the topic. Additionally, changes in the availability of feedstocks can be assessed based on the results obtained earlier. It can be assumed that there are generally two types of possible development scenarios in these terms: those that can be assumed advantageous and those that are expected to be disadvantageous for the techno-economic attractivity of the production processes of bioplastics. Since bioplastics have been developed quite recently and the research is constantly improving techno-economic factors, it can be assumed that majority of the future uncertainties lean towards the favour of bioplastics production and deployment. However, uncertainties considering the availability of feedstocks may cause challenges.

Techno-economic development is likely to affect the efficiency and costs of the processesses. Chemical boundaries, mainly theoretical conversion rates, are limiting the feedstock utilization efficiency thus this aspect is not considered. However, enhanced energy-efficiency, especially through catalyst research, and reduced costs have potential in achieving major advantages in terms of competitive edges in comparison to other technologies. This indicates that there is need to consider a reduced energy consumption as well as both investment and feedstock costs. The decrease in each aspect is assumed 50 %, which is only used to provide one example of reduction and is thus not based on detailed reasoning. Unfavourable changes for bioplastics production in these aspects are not expected, since the technologies already exist and it would be unlikely that the relative price to other processes would increase given the today's environmental policies and growing interest in carbon neutral technologies.

The model introduces both first and second generation feedstocks. The utilization of first generation feedstocks is negligible. However, the large-scale utilization of second generation feedstocks would require changes and investments. Additionally, the price of the second generation feedstocks is relatively low and forms an opportunity for only a small-margin business. Although much of literature studies the use of second generation feedstocks, it is assumed that much of the bioplastic production today relies on first generation feedstocks (Siracusa and Blanco, 2020). Given this, an additional case consisting of only first generation feedstock availability, i.e. the crop biomass, is introduced.

Thus, the cases used for the sensitivity analysis, in addition to the previously introduced BIO and BAU, are:

- A 50% reduction in biomass price, referring to the possibility of biomass becoming a more affordable future feedstock.
- A 50% reduction in investment costs into production processes aiming towards bioplastics. This includes both bio-ethylene production as well as the processes converting bio-ethylene to bio-commodities.
- A 50% reduction in energy demand of all bio-processes, referring to the potential of technological achievements in making the processes more efficient e.g. by utilizing catalysts.
- Exclusion of second-generation feedstocks, i.e. forestry and agricultural residues. This case is used to illustrate how the availability of feedstock can affect the outcome.

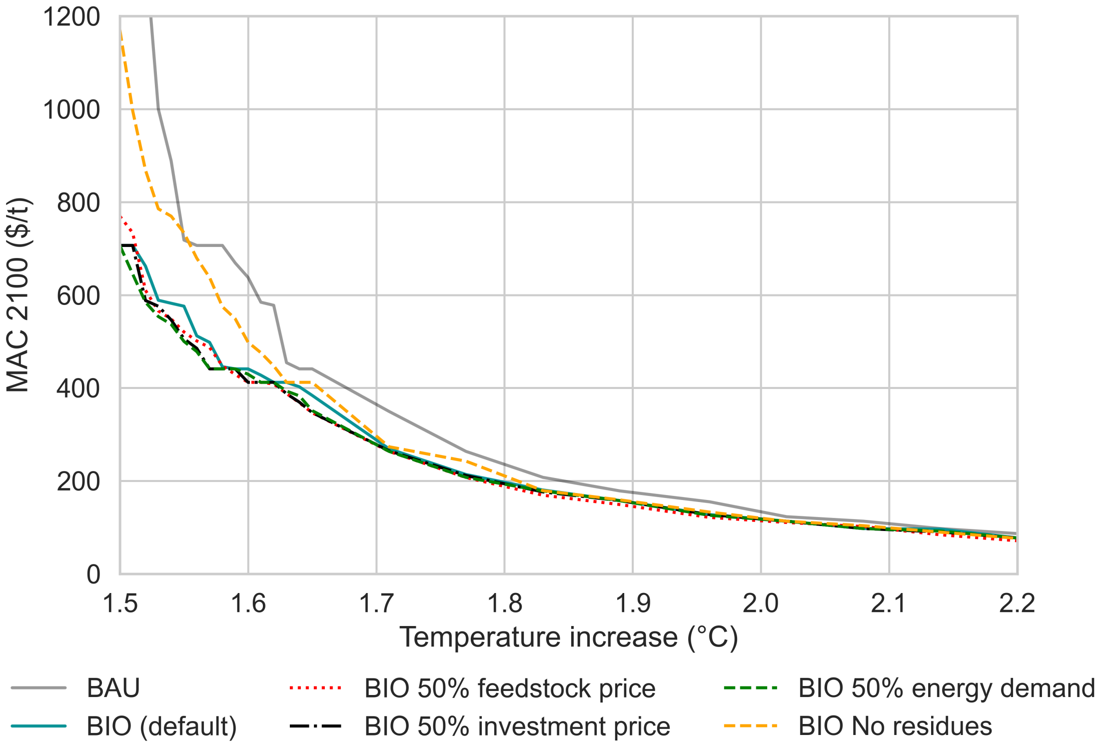

Figure 13: MAC sensitivity analysis with reductions in global biomass price, investment costs and energy demand of all bioplastic processes as well as an exclusion of second-generation feedstocks. Also the default BIO and BAU scenarios seen in the earlier results are included for comparison.

The sensitivity analysis in Figure 13 shows that MACC of the default BIO scenario is very similar to all of the introduced advantageous-assumed sensitivity variation cases, i.e. all other sensitivity scenarios but the exclusion of residues. This indicates that the mitigation potential of bioplastics production is relatively robust in terms of the given variations in feedstock price, investment cost and energy demand. In the absence of residues, the model shows a significant increase in MAC. This means that a significant decrease is seen in mitigation cost-effectiveness of the system in comparison to both the other varied cases as well as the default BIO case. A case without the possibility of using residues is still more efficient, in terms of MAC, than the BAU scenario.

From approximately 1.7°C towards more loose climate policies, MACCs of all sensitivity cases converge nearly to the default bioplastic scenario. In policies stricter than 1.7°C, there is a difference between the varied cases and the default bioplastic module, although the differences are still very minor. Despite the difference between the varied and the default case, all advantageous-assumed cases, i.e. all but the absence of residue feedstocks, seem to follow a fairly similar path together indicating that none of the cases is significantly better than the others. However, the reduction in the price of feedstocks seems to be the least beneficial option, especially when considering a temperature cap of 1.5°C, at which the MAC of the case with reduced feedstock price is higher than that of the default bioplastic case. This indicates that the low price of bio-feedstocks generates a system in which it is more expensive to mitigate emissions to reach the temperature goal of 1.5°C. It is likely that the land-use impact caused by the highly reduced bio-feedstock price is negative in terms of emissions since less carbon is left in the soil under the increased demand for biomass and thus other technologies are required to fulfill the climate target.

Additionally, in the absence of residue biomasses, the MAC values are seen to increase especially towards stricter climate policies. Additionally, the clear horizontal step around the MAC value of 700 $/t in the MAC curve seen in especially BAU but also other BIO scenarios, it not present in the case with no residues. These results indicate that disallowing the use of residues in bio-commodity production significantly reduces the benefit offered by bioplastics.

7 Discussion and conclusions

7.1 Mitigation potential of bioplastics

The results indicate that according to the model and the assumptions made in this thesis, drop-in bioplastics are an economically viable mitigation method, especially when considering stricter climate policies aiming at a maximum global warming of 2.0°C and below. The benefit of bioplastics, in terms of both lower global temperature increase but especially MAC, is however quickly decreased as the climate policy is loosened. It is therefore clear that, according to the modelling, bioplastics offer a cost-efficient way to mitigate emissions.

While bioplastics are beneficial in terms of climate change mitigation, this thesis has not yet discussed how the reductions in MACs or in emissions are caused and what is the magnitude in comparison to earlier studies. According to Zheng and Suh (2019), the most substantial method for emission reductions in the plastics industry by 50-75% would be a complete switch to renewable energy used in during the production phase of plastics. Additionally, an approximately 25% decrease in emissions could be achieved by changing the feedstocks from fossil-based to bio-based. In this thesis, corresponding values cannot be defined easily since the SuCCESs model is complex and industries, such as the plastic industry, cannot be isolated from the whole system. In terms of energy, the decarbonization of the energy used in the production of bioplastics is based on the system dynamics and the development of the energy sector under the prevalent temperature target or emission price scheme. Moreover, it is not possible to define exact emissions caused by the plastics sector since many of the processes along the path towards plastics produce other commodities as well. Thus, instead of the numerical and exact values provided by previous literature, a more central result of this thesis is the relative impact bioplastics have on MACCs and the difference in temperatures in the price-based scenario. However, some very general values can be defined to be compared to the previous literature to validate the results.

The results show that under the 1.5°C price-based policy, the scenario with bioplastics emits approximately 3 Gt/a less emissions than BAU after 2050. A major share of this emission reduction is caused by a decreased utilization of the COTC process, i.e. use of crude oil. The reduction of embedded fossil-based carbon in plastics, i.e. what is stored in the mass of the material, can be calculated with the given amount of bio-based commodities and carbon mass share of the chemical structure. This simplified calculation reveals that the savings on embedded carbon corresponds to approximately 920 Mt of CO_2 in 2050 and 2 Gt of CO_2 in 2100. Because these numbers only account to 31% in 2050 and 68 % in 2100 of the total CO_2 emission reductions seen in the results, embedded carbon does not alone account to the change seen in emissions.

In addition to the impact of the embedded carbon, the emissions of the whole plastics industry can be assessed on an approximate level. Based on Rosenboom et al. (2022), the CO_2 emissions of the conventional plastics industry today are approximately twice the mass of plastics produced. Thus, since the model assumes the production of plastics in 2050 to be approximately 700 Mt and 1.3 Gt in 2100, it can be concluded that in a BAU scenario, the CO_2 emissions based on the today's' technologies would be 1.4 Gt and 2.6 Gt in 2050 and 2100, respectively. Thus, the emission reductions seen in the results can be considered to contain also other reasons outside the simplified direct emissions caused by the production of bioplastics. This, together with the results of bio-ethylene and BTX production, indicates that the modelling of bioplastics in adition to providing a bio-based alternative, makes the system more efficient and less emitting beyond the direct impact of the reduced fossil-based embedded carbon in plastics. This topic is further discussed in Sections 7.2 and 7.3.

7.2 Other impacts caused by bioplastics

As seen in the literature review, e.g. collectively by Rosenboom et al. (2022), also land-use has potential of making environmental impact of bioplastics worse than that of fossils. The previous literature, e.g. Bishop et al. (2022), is especially concerned on the use of first-generation feedstocks, such as crops, while second-generation feedstocks, such as residues, are seen more sustainable. The results of this thesis show that no first-generation feedstocks, i.e. crop biomass, are utilized under a climate policy. In the absence of a climate policy, only small amount of crop-based bio-ethylene is produced. Although the production happens on an almost irrelevant scale, it indicates that crop biomass is not as beneficial in terms of climate change mitigation as residues, since it is not produced under a climate policy. However, the sensitivity analysis shows that by only introducing crop biomass as a bio-feedstock, the MACC still remains under the business-as-usual scenario indicating that at least moderate use of crop biomass still offers a better-than-nothing option for the bioplastics industry. Despite the positive impact on MAC, first-generation feedstocks may still have negative influence on the more general sustainability factors.

Forestry residues are used extensively in the case of a strict climate policy. Out of the bio-feedstock options used, forestry residue has the weakest properties as having the worst energy efficiency and producing the least heat biomass as side product. Given these parameters, the use of forestry residue has the best environmental impact. This is sensible, because forests store more carbon than crop fields, and under strict climate policies, the model, in addition to cutting emissions, also seeks to maximize carbon sinks thus preferring the conservation of forests over crop fields for land-use.

The broad sustainability challenges linked to bioplastics are often considered to be deforestation, fresh water usage, waste and microplastics. (Rosenboom et al., 2022; Bishop et al., 2022; Shen et al., 2020) While this thesis does not assess the impact of waste and microplastics, the other two aspects can be assessed indirectly. However, bioplastics yield microplastics as well as non-biodegradable waste similarly to conventional plastics, thus a business-as-usual impact can be assumed in these factors. Since crop biomass is not utilized under any of the climate policy scenarios, and very little even in the absence of a climate policy, no deforestation linked to bioplastics production occurs. Since the use of crop biomass is minimal even in the absence of a climate policy, using crop biomass is too expensive and requires too much land area, thus, based on the results of this study, bioplastics should not cause deforestation if the model assumption hold. However, this finding assumes that residues are available at a reasonable price, as motivated by the sensitivity analysis. Little water usage can be assumed, since by utilizing forestry residue no excess freshwater is required outside what is naturally directed to the forests. In terms of agricultural residue, the collection of the material should not cause additional water demand outside that what is already required for the first-generation production of the corresponding croplands. Again, the use of crop biomass should not be economically viable if alternatives exist, otherwise there is potential in an overly increased fresh water demand causing especially local problems.

Although the result shows a straightforward benefit from switching from fossil-based to bioplastics, the changes in, e.g., ethylene production between the two main technology scenarios and the significant reduction in emissions in Section 7.1 indicate that the supply-demand balance is also altered by the introduction of bioplastic processes. The results show that the total production of ethylene is decreased in the BIO scenario while demand in both scenarios remain the same and ethylene is not used as an input for other processes. Additionally, the production portfolio of ethylene in the absence of climate policies differs between the technology scenarios although no bio-ethylene is produced in neither technology scenario. A closer look at the conventional processes reveals that COTC, a heavily deployed technology for fossil based commodity production, produces a significant share of ethylene in comparison to other output commodities. This finding highlights that without the introduction of bioplastics, the commodity market is not at equilibrium since at least ethylene is overly produced. Since all bio-commodities are produced separately, the setting makes some bio-commodities, especially BTX, more attractive to the model even without a climate policy. Although the MACC shows a clear benefit in mitigation, the flexibility offered by bio-commodities enhances the use of them even without the consideration of a climate policy. This is a limitation of the current model version and is thus further discussed in Section 7.3.

Forecasting technologies into the future, 80 years onwards to 2100 in this case, involves large uncertainties in both external market factors as well as techno-economic development. Although the future can never be accurately predicted, the sensitivity analysis reveals that bioplastics behave in a relatively robust way in terms of MAC for reduced energy need, feedstock price and investment costs. This result can be interpreted as showing that development in the studied factors alone does not make bioplastics significantly more attractive in terms of climate change mitigation than the base case of bioplastic production. However, the sensitivity analysis is limited to altering some central parameters used in modelling thus it does not account for major technological development nor external factors, that are left out of the scope.

Accounting for these more major changes would require more extensive scenario building.

7.3 Limitations

A number of assumptions and approximations in modelling choices affect the results. Additionally, the optimization-based modelling approach comes with certain aspects that need to be acknowledged while reading the results. These limitations require reflection on the validity, robustness and generalizability of the conclusions made. In addition to modelling-related limitations discussed in this Section, there are uncertainties related to the future, e.g. demand and technological development.

The most substantial limitation in describing the bioplastics industry is the approximation of only considering drop-in bioplastics. As seen in the literature review, it is expected that drop-in bioplastics will only cover up to half of total bioplastics production. Thus, e.g. biodegradable bioplastics are left out of the scope. However, when considering the level of approximations required for the whole model and how the model describes e.g. the plastics industry, the approximation of only including drop-in bioplastics is very justifiable. Moreover, given the demand modelling of plastics, the approach used can be considered to approximate the production of other bio-based plastics as well, since these can originate from the same feedstocks and go through processes that are relatively similar, at least in the context of IAM modelling.

Another substantial limitation is the unintended efficiency gain in commodity markets caused by the introduction of bioprocesses. As noted earlier, the single-output bio-processes are more flexible than the conventional processes already included in the model prior to this thesis. This is a clear limitation when trying to assess the climate change mitigation potential. The enhanced flexibility of the bio-processes make the new processes seem superior to the conventional ones although in reality, all processes would adjust their output based on demand and market price to maximize profit. Thus, the results are overly in favour of bioplastics due to the efficiency gains which also result in cheaper mitigation in the temperature-based model and less emissions in the price-based model.

Variable costs outside input commodity prices are not mostly considered in the SuCCESs model. Although the costs are equally excluded between bio-processes and conventional processes, the costs can differ, e.g. due to labour costs under less automation in new processes. This could change the competitive balance between bio-processes and conventional processes. Yet, as seen in the literature review, majority of the costs related to bioplastics production originate from feedstock, energy and capital costs, which is further why this aspect is considered to be justified to exclude. Moreover, the values for commodity costs and investments are based on limited sources, since little economic figures are available. However, the sensitivity analysis showed that altering at least the central cost and investment cost parameters does not affect the system much. This means that this limitation is not severely affecting the results.

Model-specific limitations can be also identified when discussing the SuCCESs model and IAMs in general. These limitations include the low spatial resolution, as the model only considers the world as a single market area, overly perfect description under optimization and the uncertainty on what happens after 2100. Especially the lack of analysis beyond 2100 needs to be highlighted. It is likely that, in at least some temperature-based scenarios, the global mean temperature increase would overshoot the corresponding target after 2100, e.g. due to the model not facing full consequences of the actions during this century.

7.4 Conclusions

The results indicate that bioplastics may not be economically viable without incentives, but under stricter climate policies, bioplastics offer both climate change mitigation potential as well as become economically viable in comparison to more emitting technologies, at least under the approximations and assumptions made with this modelling setup. In other words, bioplastics can be an economically viable mitigation method to cut down fossil-dependency. Although the setting of this thesis illustrates a single optimal scenario that is unlikely to be exactly met in the real-world, the results should be considered as an illustration of what could happen. From a wider perspective, the results also show that although much of the mainstream discussion regarding climate change mitigation has focused on fossil fuel use in electricity and transportation, also plastics constitute a noteworthy topic, especially when considering the projected future demand development. Additionally, since the model contains land-use optimization, the question of how carbon sinks and storage are influenced by such increase in the need of biomass can be quantified with the modelling approach used in this thesis. Yet, it is important to consider the limitations and the choice of biomass source which is central when assessing the overall sustainability of bioplastics.

In addition to direct decrease in fossil-dependency, the alternative feedstock possibility provided by bioplastics also allows for more secure plastic supply in case the oil market faces remarkable changes. The oil market can be expected to change in the future decades while it is expected that the transportation sector is heavily decarbonized. Thus, the market of other oil-based commodities is expected to face changes. Additionally, as the number of economically viable oil fields decreases, changes in the market can be further amplified. This highlights that studying bioplastics should not be done from the climate change mitigation perspective alone but also to offer further options for the plastics industry in the changing world.

The work towards this thesis was motivated mainly by the goal of building a module describing bioplastics in the SuCCESs model to assess the mitigation potential of the decarbonization of the plastics industry. Although a number of approximations was required for the modelling, the goal is achieved. The results indicate that modelling bioplastics in an IAM is a worthy topic of study since bioplastics form an interesting problem balancing land-use and carbon storage with the use of fossil resources. Based on the recent views by Stegmann et al. (2022b), this thesis is one of the first studies to include bioplastics production in IAMs. Moreover, this thesis is also one of the first studies made using the SuCCESs model. Utilizing the model has, in addition to the results and the thesis, been beneficial in the validation and learning on the use of the model.

All in all, bioplastics are undoubtedly a commodity worth further techno-economic studies. Future studies should consider biodegradable plastics, since the possible benefits of these are not limited to emission reductions, but they would also help in reducing the accumulation of plastic waste.

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A Propylene production

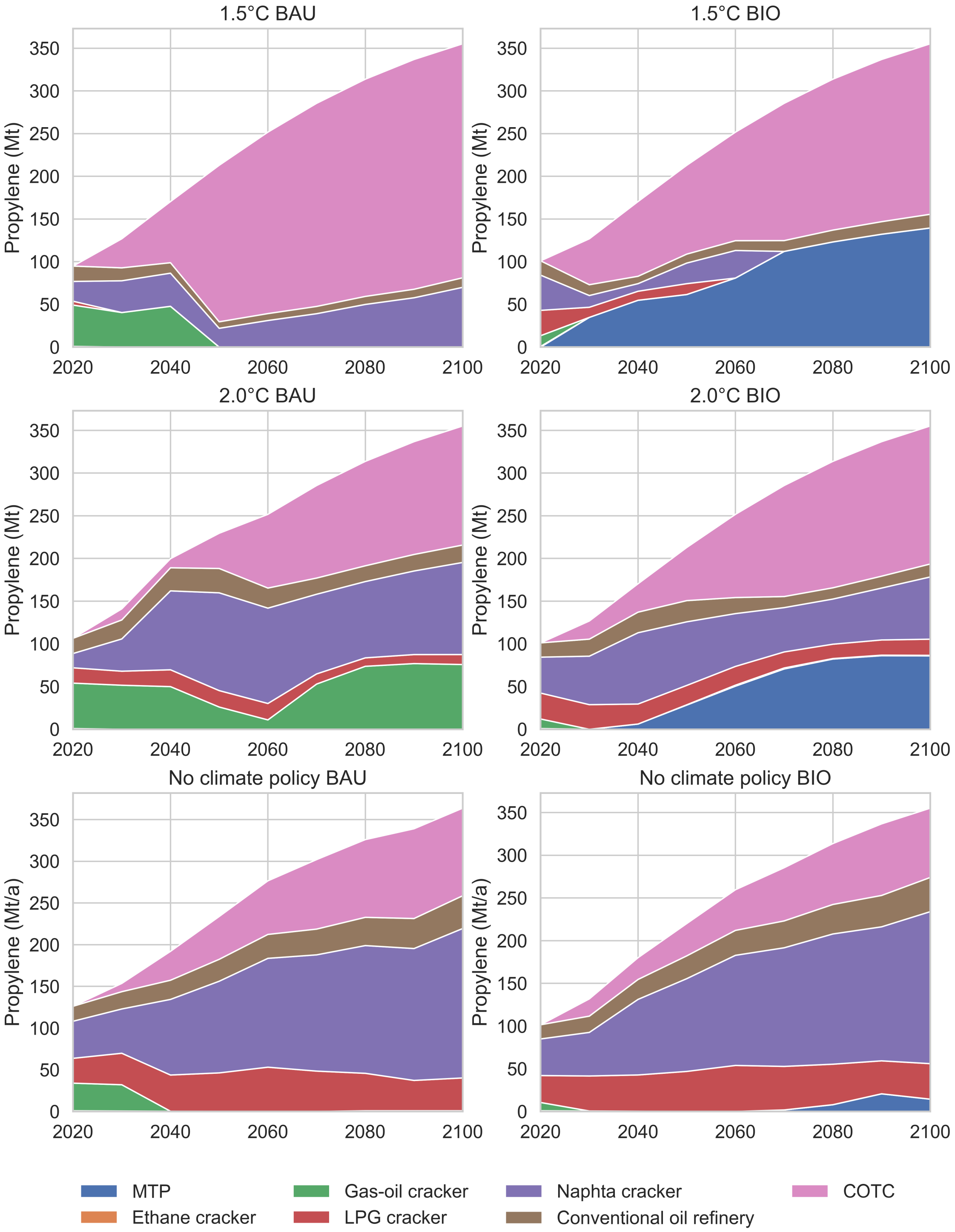

Figure A1: Production of propylene similarly described as in other commodities.