



BIOMASS-TO-CHEMICALS IN ENERGY TRANSITION SCENARIOS:
THE CASE OF BRAZIL

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Orientador(es): Alexandre Salem Szklo

Pedro Rua Rodriguez Rochedo

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Para Henrique, Isadora e Olivia.

“Instruction does much, but encouragement everything.”
- J. W. von Goethe

“Above all, don’t fear difficult moments. The best comes from them.”
- Rita Levi-Montalcini

“Imagination is more important than knowledge. Knowledge is limited.”
- Albert Einstein

“If at first the idea is not absurd, then there is no hope for it.”
- Albert Einstein

“It's extraordinary how inventive one can be with ethanol right now.”
- Daniel Yergin

“Everything is hard before it is easy.”
- J. W. von Goethe

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BIOMASS-TO-CHEMICALS EM CENÁRIOS DE TRANSIÇÃO ENERGÉTICA:
O CASO DO BRASIL

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Programa: Planejamento Energético

Esta tese visa contribuir para uma melhor representação da biomassa em Modelos de Avaliação Integrada, de forma a avaliar os usos não energéticos da biomassa na bioeconomia, associados aos seus usos energéticos. Para tanto, foram realizados três estudos com foco em petroquímicos básicos, nas necessidades materiais associadas à transição energética e na possível competição entre biomassa e derivados de petróleo. O primeiro estudo compara quatro rotas de produção de eteno de acordo com seu custo estimado de produção no Brasil. O segundo estudo aprofunda a análise sobre a relevância da disposição final e os benefícios da conversão de bioplásticos em material de longa vida. O terceiro estudo consolida os estudos anteriores e tem como objetivo avançar o entendimento do papel da biomassa em cenários de transição energética no Brasil, através da inclusão de um módulo petroquímico no modelo de avaliação integrada do Sistema Brasileiro de Uso da Terra e Energia desenvolvido na COPPE e denominado BLUES. Os resultados dos estudos mostram tanto que a produção de biocombustíveis em um cenário de restrições climáticas também gera co-produtos para produzir biomateriais, substituindo nafta petroquímica, quanto que a transição nos sistemas energéticos pode gerar excedentes de hidrocarbonetos/carboidratos que para servir de matéria-prima para a produção de materiais.

Abstract of Thesis presented to COPPE/UFRJ as a partial fulfillment of the requirements for the degree of Doctor of Science (D.Sc.)

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This thesis aims to contribute to a better representation of biomass in Integrated Assessment Models (IAMs), in order to assess the non-energy uses of biomass in the bioeconomy, associated with its energy uses. To this end, three studies were carried out with a focus on basic petrochemical products, the material needs associated with the energy transition, and the possible competition between biomass and oil products. The first study compares four ethylene production routes according to its estimated cost of production in Brazil. The second study further analyzes the relevance of the final disposal and the benefits of converting bioplastics into long-lived material. The third study consolidates previous studies and aims to advance the understanding of the role of biomass in energy transition scenarios in Brazil, through the inclusion of a petrochemical module in the Integrated Assessment Model of the Brazilian System for the Use of Land and Energy developed at COPPE and called BLUES. The results of the studies show that the production of biofuels under a scenario of carbon emission constrains co-generates products to produce biomaterials, replacing petrochemical naphtha, and that the transition in energy systems can also generate surplus hydrocarbons / carbohydrates that serve as raw material for the production of materials, as well.

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1. Introduction

1.1. Transition to a bio-based economy

Energy transitions have profoundly influenced human evolution (Smil, 2019) and vice-versa. The most emblematic examples of energy transition are the gradual shifts from biomass to fossil fuel as primary energy supply, from animate (human and animal) to inanimate energy converters (water wheels, wind mills), and from coal steam power to oil, gas and electricity (Fouquet, 2010; Grubler, 2012). Historical energy transitions were shaped by combustion of fossil fuels, which led to the rising atmospheric concentration of CO₂, from 285 parts per million (ppm) in 1850 to 397 ppm in 2000 and to 413 ppm in 2020 (NASA, 2020). In today's climate constrained world, a transition to a low carbon economy is crucial to preserve biodiversity, global energy security and social justice.

A low carbon economy can be achieved through a transition from a fossil-based to a renewable based economy, where the bio-based economy (BBE) should play a significant role. This transition is driven by the depletion of fossil fuels and by climate change, which itself is mainly caused by fossil fuels combustion (Broeren et al., 2017; Grubler, 2012; Smil, 2010). Scholars remark that the transition to a bio-based economy will have a considerable effect on society (Pearson and Foxon, 2012; Smil, 2010; Sovacool, 2016) since it will require new ways of fulfilling basic human needs and providing services such as food, housing, transport, energy and material. This holistic transformation of economy and society that is fundamentally based on balancing environmental concerns with human activities is seen as a Third Industrial Revolution (Pearson and Foxon, 2012). Thus, beyond the substitution of fossil-fuels, the transition to a BBE demands the creation of benefits for workers by creating new jobs and also for consumers by avoiding risks for them (Spierling et al., 2018). Sustaining economic growth within planetary boundaries can be achieved by changing existing patterns of production and consumption for a BBE (Sanz-Hernández et al., 2019).

1.2. Role of biomass in the bio-based economy

Biomass is a renewable resource and sequesters CO₂ from the atmosphere through photosynthesis. This feature brings the possibility of a zero net CO₂ emission when biomass is burned for energy purposes. Nonetheless, biomass production requires land,

impacting land use and land management, which in turn could impact food security (Daioglou et al., 2019; Rose et al., 2014), biodiversity and greenhouse gas emission, as well. The role of biomass in the BBE depends on land use dynamics, the volume and type of replaced fossil fuels and potential feedbacks in the energy system (Daioglou et al., 2019).

The ultimate goal of the transition to a BBE is that biomass fulfills multi-objectives: it provides food, bioenergy, and bio-based products while soil fertility is maintained. In addition, if biomass production associated with land use policies is properly managed, it can provide ecosystemic services (Parron et al., 2014; Strand et al., 2018). To achieve this it is necessary to maximize the valorization and the environmental benefits of biomass supply chains through high-efficient biomass conversion technologies (IEA, 2014). Therefore, scientists foreground the concept of biorefining, which is “the sustainable processing of biomass into a spectrum of marketable products and energy” (IEA, 2008). This concept is analogous to petroleum refining, which produces fuels and products from petroleum. However, for the case of biorefining, biomass resources (wood, grasses, corn, etc.) are converted into biofuels, power and chemicals (Cherubini, 2010). Biorefineries can produce drop-in products, such as bio-ethylene, bio-propylene, etc, which have direct fossil-based counterparts; bio-based platforms hardly produced from fossil feedstocks, such as succinic acid, lactic acid, etc¹; and even new bio-based products, such as polylactic acid (PLA), polyhydroxyalkanoates (PHAs) (Karan et al., 2019). Nevertheless, drop-in products have easier short-to-mid-term market acceptance since they can be processed at a large scale in already established infrastructure, and are already associated to a complex and verticalized industrial chain, from the first to the third generation of plastic products. Hence, drop-in products can contribute to mitigate GHG emissions in the short term at larger scales, while novel products require longer time for commercial introduction and marketing effort (de Jong, 2014; Dusselier et al., 2014; IEA Bioenergy, 2020), since they require the establishment of the industrial chain for converting the bioplatforms into final products².

¹ These are bio-based products, such as dicarboxylic acids and hydrocarbons with carboxylic and hydroxyl terminations, and/or protein-based polymers, which are produced in small quantities and hardly from petroleum derivatives, as of today.

² Santos (2013) proposes a methodology to assess the potential of biorefineries to produce chemical bioplatforms such as succinic acid. In her study, succinic acid is produced from sugarcane bagasse, which, however, is only available in rural areas that lack industrial infrastructure and specialized labor. Two strategies are considered, then: sugarcane bagasse could be transported to an industrial cluster to produce

Aspects of the biorefinery concept are already used commercially in the co-production of ethanol and animal feed from sugar and starch crops, and also the co-production of biodiesel, animal feed and glycerol from oil crops (Gerssen-Gondelach et al., 2014; IEA Bioenergy, 2020). However, the majority of biorefineries today are still based on a single conversion technology and not entirely following the principles of a biorefinery concept (Cherubini, 2010; Stegmann et al., 2020).

To have a better understanding of the role of biomass in the global energy system, scientists develop mitigation scenarios using integrated assessment models (IAMs) (Hare et al., 2018). These models examine energy technologies, energy use choice, land use changes and societal trends integrated in an energy, land use and climate system to estimate how greenhouse gas (GHG) emissions may evolve in the future under different assumptions. IAMs are used to answer two broad types of questions: “what would happen if...?” and “how could we get to...?”. Despite answers to these questions being uncertain, they constitute a valuable guidance for policy evaluation, since they explore the choices that will cause or prevent GHG emissions (Hare et al., 2018; Parson and Fisher-Vanden, 1997).

IAMs project biomass as a crucial energy carrier to reduce GHG emissions in the world’s energy system (Daioglou et al., 2019; Gambhir et al., 2019b; Rogelj et al., 2018; Rose et al., 2014). Bioenergy is often highlighted by these models due to its versatility in producing electricity, gases, heat, hydrogen or liquids (Rose et al., 2014), and its possibility to create negative GHG emissions (NETs) if combined with carbon capture and storage (BECCS³) (Gambhir et al., 2019; Hilaire et al., 2019; Junginger et al., 2019; Rose et al., 2014). In fact, several studies (Detz and van der Zwaan, 2019; Fuss et al., 2014; Gasser et al., 2015; Hilaire et al., 2019; Obersteiner et al., 2018; D. van Vuuren et al., 2017) stress that a large-scale deployment of NETs is crucial to keep global warming below 1.5°C to meet the Paris Agreement. Besides, biomass can achieve NETs when it is used as a feedstock (non-energy use) for long lifetime material production (Junginger et al., 2019; Oliveira et al., 2020b), what we call here BIOCCUS (biomass with carbon

succinic acid and the final product, or succinic acid production is located close to ethanol distilleries, and then transported to an industrial cluster to produce the final product.

³ Bioenergy with carbon capture and storage.

capture utilization and storage), when the use of biomass in material production functions as a carbon storage. Nonetheless, the scientific literature lacks studies that evaluate the non-energy-use of biomass associated with its energy use, e.g., biomass conversion into (petro)chemical products under an energy transition framework. The following section shows how this thesis addresses this gap by developing a framework that allows to systematically assess the non-energy use of biomass in BBE.

1.3. Achieving negative emissions through bio-based chemicals

The chemical and petrochemical sector is a prime example of the non-energy use of energy carriers⁴. In fact, this sector is a key “blind spot” in the global energy debate since much of its fossil hydrocarbons enter the sector as feedstock (non-energy use), not undergoing combustion. Interestingly, the sector is the largest industrial fossil fuel user, accounting for 28% of the global industrial final energy consumption (IEA, 2018, 2017) and yet only the third-largest industrial CO₂ emitter, representing 18% of all industrial CO₂ emission (IEA, 2018). For this reason, the sector needs a holistic strategy to reduce GHG emissions in both energy and material flows. Bio-based materials, circular economy and product innovations are expected to play a critical role in decarbonizing the chemical sector (Bauer et al., 2018a; Karan et al., 2019; MacArthur, 2017; Oliveira et al., 2020b; Spierling et al., 2018). Moreover, the conversion of biomass into a chemical product can be a NET option (Kemper, 2015; Moreira et al., 2016; Oliveira et al., 2020b), as mentioned before.

Bio-based chemicals could also lower many countries’ dependence on fossil fuels, and stimulate local economies (IRENA, 2013a). Low-cost and readily available feedstock has been a cornerstone of value creation in the chemical sector, as seen in the low-cost champions for key petrochemicals (Griffin et al., 2018; International Energy Agency, 2018; McKinsey, 2018): the USA, with its cheap shale gas, and the Middle East, with stranded gas reserves. Companies around the world are therefore locating themselves in those regions to take advantage of cheap feedstock (Griffin et al., 2018; Hammond and O’Grady, 2017). However, the urgency with which the world economy needs to be decarbonized could lead to the emergence of other regions with renewable feedstock such

⁴ Other non-energy uses include coke oven and oil refinery products such as waxes, lubricants, aromatics and bitumen in the energy transformation sector (Daioglou et al., 2014).

as biomass (Ren, 2010; Ren et al., 2006). These regions' source of competitiveness would be to produce high value added chemicals, such as plastics, at the lowest cost in terms of producer costs including GHG emission abatement costs. Brazil has large potentials in this respect: it is one of the world's major agricultural producers (MAPA, 2018a); it is the second largest ethanol producer (RFA, 2017); and, along with the USA, it has the lowest ethanol production costs (Gupta and Verma, 2015; RFA, 2017).

In fact, Brazil already operates the largest world bio-ethylene plant with a production capacity of 200 kt per year (Rosales-Calderon and Arantes, 2019). The production of bioplastics using sugarcane is possible in Brazil due to the country's climatic advantages and the extent of land available to grow sugarcane. For this annual production of bio-based polyethylene, 65,000 ha of sugarcane plantations are required, which equals 0.2% of Brazil's arable land (de Vargas Mores et al., 2018). Hence, this thesis aims to test a first hypothesis that Brazil could be a potential pioneer in large scale bio-based plastics production due to its well-established sugar and alcohol sector. Furthermore, if a local or global CO₂ market is considered, Brazil could boost the use of biomass to produce plastic, potentially achieving NETs, and improving its petrochemical competitiveness. Therefore, the *Research Question 1* of this thesis is: *Can Brazil become a large-scale low cost bio-ethylene producer via its ethanol sector, under a strong global climate governance (for example, expressed by a relevant CO₂ price)?*

Besides developing strategies to reduce GHG emissions in energy and material flows, the petrochemical sector has to deal with a controversial societal debate: plastic pollution. Around one third of plastics consumed ends up as terrestrial or marine pollution (de Souza Machado et al., 2018; WWF, 2019), accounting for 100 million metric tonnes of plastic waste in 2016 (de Souza Machado et al., 2018). Plastic and microplastic pollution pose negative effects on marine environment and on its food chain, including human beings (Laskar and Kumar, 2019). Microplastics contaminate tap and bottled water, which leads to possible negative effects on human health (GEF, 2018a; Jefferson, 2019). There are over 150 million tonnes of plastic waste in the ocean today (Laskar and Kumar, 2019; MacArthur, 2017; McKinsey Center and Ocean Conservancy, 2015) and, in 2050, there will be more plastics, by weight, than fishes in the ocean, unless action is taken (GEF, 2018a; MacArthur, 2017). Single-use plastics such as grocery bags, food packaging,

bottles, straws, containers, cups and cutlery are the biggest contributor to this pollution (MacArthur, 2017; UN Environment, 2018).

Plastic pollution is an issue linked to the last step of the life cycle of plastics: final disposal. The use of plastics in long-term applications, such as construction, can reduce plastic pollution and GHG emissions during their lifetime. Also, if bio-based plastics are considered, the biogenic carbon absorbed during biomass cultivation and then captured in plastics could result in NETs (Oliveira et al., 2020b).

Zheng and Suh (2019) evaluate four strategies to reduce the carbon footprint of plastics on a global scale: 100% sugarcane and corn-based plastics, 100% renewable energy, 100% recycling, and halving plastic growth in demand. According to them, for the lowest GHG mitigation potential to happen (93% GHG reduction from the baseline in 2050), the four strategies should be implemented in concert. However, the study lacks the evaluation of a fifth option, which will also be assessed in this thesis: orient bio-based plastics production towards long-lifetime products as a strategy to achieve negative emissions. Plastics could further compete in specific applications with energy-intensive construction materials, such as cement and steel, coming back to a historical strategy of the industry to expand markets by substituting traditional materials. Moreover, as the usage of plastics in construction means long-lived applications concentrated in few sites, the waste output associated with this application will be delayed and could be easily handled, compared to the disperse and low scale waste output from packaging.

Hence, this thesis also aims to test the hypothesis that using plastics in long-term applications would bring environmental advantage due to the reduction of plastic waste accumulation. Therefore, the *Research Question 2* of this thesis is: *How does the final disposal of biomass-derived plastics affect the feasibility of negative CO₂ emission associated with BIOCCUS?*

Despite Brazil's vast production of plantation crops, its potential for producing bio-based plastics relies on the developments of the economy, technology and environmental policy (Lap et al., 2019). Also, biomass supply depends on the type of land available and potential land-use change (LUC) GHG emissions. The deployment of biomass for energy use, food or chemical production has to be consistent with avoiding deforestation and

contributing to climate change mitigation (Daioglou et al., 2019). This also means that it has to be consistent with avoiding energy, food and, as implemented in this thesis, material competition – what this study proposes as a *trilemma* (Oliveira et al., 2017) . Therefore, to have a clear understanding on the role of biomass in energy transition scenarios, it is worth considering the volume and type of fossil fuels replaced, land availability, the costs of biomass conversion to energy and/or materials, and the possible direct and indirect LUC emissions⁵ (Daioglou, 2016; Searchinger et al., 2008; Wicke et al., 2015). In this case, IAMs are a useful tool to assess the trade-offs between different biomass uses since they can describe both the land and energy systems and their dynamic changes over time (Daioglou, 2016).

Rose et al. (2014) look across 15 IAMs to evaluate the role of bioenergy in tackling climate change. Most of the models show bioenergy as a significant part of the energy transformation, constituting up to 35% of global primary energy in 2050 and 50% in 2100. Biomass uses include biofuels, biogas, hydrogen production and biopower. Rogelj et al., (2018) analyse 6 IAMs that project the use of bioenergy in large amounts in scenarios to keep warming below 1.5°C. They find that bioenergy from residues presents fewer trade-offs than dedicated bioenergy crops. The models project different global bioenergy potentials ranging from < 50 to > 500 EJ per year. Hanssen et al., (2019) analyse the potential of biomass residues to supply energy across 8 IAMs. The results also vary substantially suggesting that residues could meet 7-50% of bioenergy demand in 2050 and 2-30% towards 2100. Daioglou et al. (2014) include in an IAM the demand of the non-energy sector, finding that it will increase from 30 EJ in 2010 to 100 EJ by 2100. In this model, non-energy use is aggregated into four products: high value chemicals (HVCs), representing the total demand of ethylene, propylene, butadiene and aromatics; ammonia; methanol; and refinery products such as bitumen, aromatics and lubricants. The authors find that until 2050 only fossil fuels meet the demand for HVC production. Annual emissions from non-energy increase from 164 Mt CO₂ per year to 677 Mt CO₂ in

⁵ Direct LUC (dLUC) emissions is a process by which bioenergy/biomaterial production causes direct land use change by converting a previous land use to a bioenergy/biomaterial crop production. Indirect LUC (iLUC) emissions occurs when bioenergy/biomaterial production indirectly causes land use change by converting forests to cropland somewhere in the globe to meet the demand for commodities displaced by the production of feedstock for bioenergy/biomaterial (Prins et al., 2012).

2100. However, biomass can supply over 40% of the total required primary energy, reducing emissions to 544 Mt CO₂ per year.

Most IAMs have dealt with biomass conversion from the perspective of the energy-food dilemma (Bauer et al., 2018b; Heck et al., 2018; Luderer et al., 2014; Rose et al., 2014; Torvanger, 2019), neglecting or simplifying its competition for chemical conversion (materials production). An exception is Daioglou et al. (2019, 2014), which include in their modeling exercise the demand of the non-energy sector, although in an aggregate manner for basic petrochemicals.

As mentioned before, this study highlights that, actually, in more ambitious GHG abatement scenarios, there could be a trilemma of biomass (energy-food-materials), instead of the usual dilemma approach of IAMs.

On one hand, a likely increase of urban mobility electrification might lead to surpluses of automotive fuels, including liquid biofuels⁶. In this case, the use of biomass surpluses for chemical production could serve as an alternative market, which would also lead to carbon capture from chemical reactions. Furthermore, the demand of chemicals is expected to grow in energy transition scenarios. For instance, to reduce fuel consumption, plastic-based materials are integrated in vehicle as a strategy to reduce their overall weight. Also, light-weight plastics can help addressing the challenges of making longer turbine blades to increase generation efficiency, while innovative chemical materials can help increase the durability of wind turbines, reducing cost of maintenance (IEA, 2018).

On the other hand, alternative uses of biomass can be limited by land availability (Fargione et al., 2010; Plevin, 2017; United Nations University, 2010), water resources constrains (Bonsch et al., 2016; Fargione et al., 2010; Hejazi et al., 2013), biodiversity (Creutzig et al., 2012; Fargione et al., 2010; Visconti et al., 2016), land property issues (Barreiro et al., 2017; Rinaldi et al., 2015) and direct and indirect GHG emissions (Popp et al., 2014; Searchinger et al., 2008; Wicke et al., 2015). For instance, the scenarios run by Daioglou et al. (2019) indicated that biomass supply will represent 8% to 35% of the

⁶ In Brazil and the USA, light vehicles can be fueled 100% with ethanol or gasoline, while gasoline is blended with ethanol (27% in Brazil and 10% in the USA, in volume basis) (EIA, 2019; PETROBRAS, 2019).

total primary energy demand by 2050, depending on the stringency of the GHG mitigation ambition - e.g., in scenarios coping with the 1.5°C target, bioenergy makes up 26% to 35% of primary energy demand, or 115 to 180 EJ per year. This biomass supply can be challenging given its interactions with the issues mentioned before.

Hence, this thesis also aims to fulfill this gap in biomass representation in IAMs, providing a valuable contribution to the evaluation of the non-energy uses of biomass in the BBE and to the investigation on how biomaterials can help to mitigate climate change. An integrated analysis of energy, land and material systems enables to test, for instance, if carbon storage in biomaterials would impact the remaining carbon emission budgets of other economic sectors; if the production of biofuels in a climate constrained scenario could also generate co-products to produce biomaterials; or if a transition in the energy systems would generate surpluses of hydrocarbons that could serve as feedstock for material production. Therefore, the *Research Question 3* of this thesis is: *What is the role of biomass in climate mitigation scenarios when considering biomass competition for energy, food and chemicals in an integrated manner?*

In this case, the Brazilian IAM model called Brazilian Land Use and Energy System (BLUES) will be improved to better detail a material module associated with petrochemicals. By running this improved version of BLUES, this thesis aims to investigate the interactions between biomass demand for energy, food and materials, given land, GHG emissions (from fuel combustion and direct and indirect land use change) and water availability constraints.

Each research question is addressed in a separate paper,⁷ which in a sequential way cover question 1 (more specific) up to question 3 (which seeks to assess holistic impacts of a NET strategy based on biomaterials). Figure 1 shows the system boundary of each research question and how they relate to each other. The papers attempt to cover the gap

⁷ *Research Question 1* is addressed in the paper “Bio-ethylene from sugarcane as a competitiveness strategy for the Brazilian Chemical industry” (Oliveira et al., 2020b) published in the Journal Biofuels, Bioproducts and Biorefining. *Research Question 2* is addressed in the paper “Achieving negative emissions in plastics life-cycle through the conversion of biomass feedstock” published in the Journal Biofuels, Bioproducts and Biorefining. And *Research Question 3* is addressed in the paper “The role of biomaterials for the energy transition from the lens of a national integrated assessment model” which was submitted to the Climatic Change Journal.

in the literature on the potential of chemicals to achieve NETs, providing a valuable contribution to debates on non-energy use of biomass in mitigation scenarios.

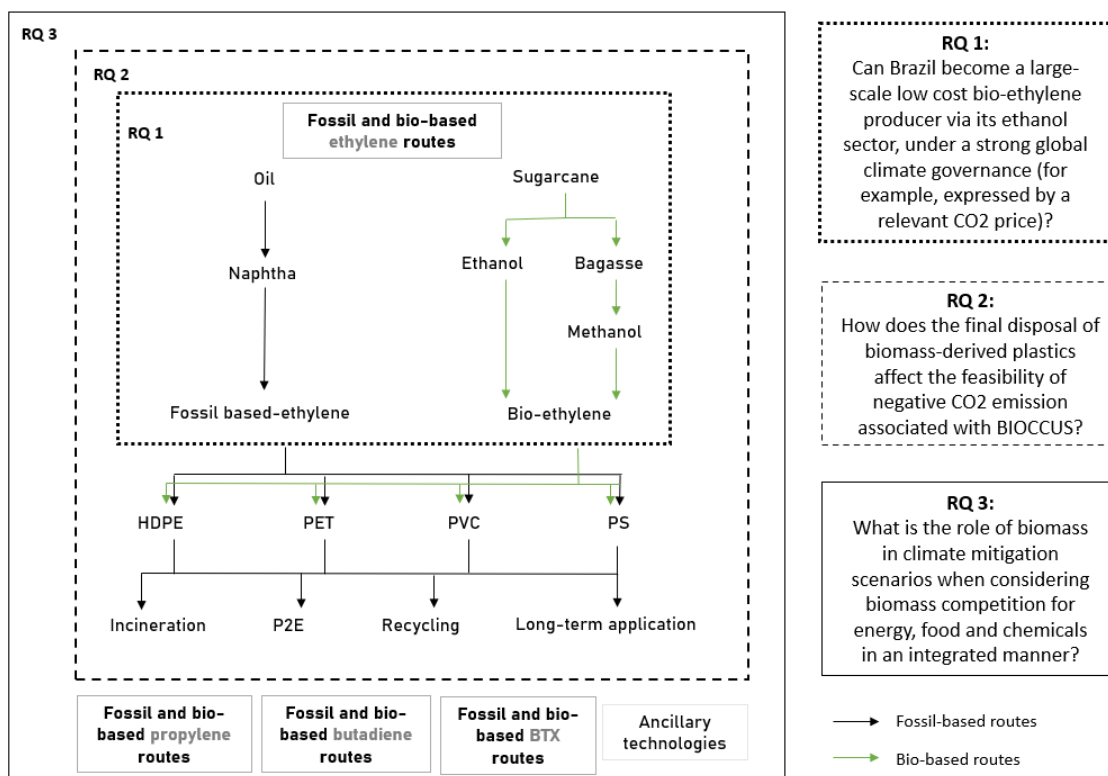


Figure 1: System boundary of the research questions

1.4. Thesis outline

In order to develop the methods required to answer the research questions posed above, this thesis is divided into 5 chapters, including this Introduction. It is worth noting that given the urgency to decarbonize the petrochemical industry and to find chemicals that are currently produced at a large-scale, this study assesses only the production of drop-in chemicals. In Chapter 2, the study “Bio-ethylene from sugarcane as a competitiveness strategy for the Brazilian chemical industry” is presented. This work aims to answer *Research Question 1* through testing the hypothesis that bio-ethylene could be a strategy for NETs, with Brazil being a potential pioneer and beneficiary of this strategy. The Brazilian chemical industry would become more competitive through the production of bio-ethylene and this would be achieved by applying the revenues from carbon credits associated with using ethanol and sugarcane bagasse as feedstock for bio-ethylene production. Three ethylene production routes were compared according to their estimated

costs of production in Brazil under a simplified life-cycle analysis (LCA) from cradle to gate.

Chapter 3 presents the study “Achieving negative emissions in plastics life-cycle through the conversion of biomass feedstock”. This work deepens the analysis on the benefits of converting bioplastics into long lifetime material, which was proposed in Chapter 2, aiming to answer the *Research Question 2* of this thesis. Here, GHG life-cycle emissions of ethylene were expanded through further steps: the conversion of ethylene into final products (plastics) and their final disposals. The plastics studied are high-density polyethylene (HDPE), polyvinyl chloride (PVC), polyethylene terephthalate (PET) and expanded polystyrene (EPS). For final disposal option it was considered incineration, incineration with energy recovery (plastic to energy, P2E) and recycling. Moreover, it was assessed the use of plastic for long-term application (construction & infrastructure). In this study, it was tested the hypothesis that using plastics in long-term applications would bring environmental advantage due to the reduction of plastic waste accumulation, delaying its final disposal and related emissions for decades; due to the achievement of NETs by bio-based plastics; and due to the demand reduction for emission-intensive construction materials.

The study entitled “The role of biomaterials for the energy transition from the lens of a national integrated assessment model” is then presented in Chapter 4. This chapter aims to answer the *Research Question 3* of this thesis by including the biomass *trilemma* (energy-food-chemicals) in the Brazilian Land Use and Energy System (BLUES) model. For that, it was incorporated in the BLUES model the conversion routes of fossil and bio-based petrochemicals to meet the demand of ethylene, propylene, butadiene and the mixture of benzene, toluene and xylenes (BTXs). Moreover, it was included technologies that produce the required inputs to meet petrochemical demands, here defined as ancillary technologies. This effort intends to expand the competing applications of biomass in IAMs. The objective here is to test if and how hydrocarbons currently used for the transportation sector may have their conversion chain modified for the production of materials and to estimate the impacts of this transition on GHG emissions and land use change.

Finally, Chapter 5 concludes this thesis, integrating the individual results from the preceding chapters in order to answer the research questions, give policy recommendations and propose future research.

It is worth noting that the Chapters 2-4 are self-contained pieces of work. They can be read individually. However, together, they constitute an investigation of the role of biomass in energy transitions scenarios that goes from a LCA of the fossil and bio-based ethylene, the assessment of the final disposal of the products derived from fossil and bio-based ethylene to an integrated assessment of the entire energy and land-use Brazilian system.

2. Bio-ethylene from sugarcane as a competitiveness strategy for the Brazilian Chemical industry

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2.1. Abstract

The urgency with which the world economy needs to be decarbonised could lead to the emergence of regions with the capacity to produce renewable feedstock such as biomass, whose competitiveness could be to produce high value-added chemicals at the lowest cost. The biomass embodied in a chemical product could reduce carbon emissions leading to net CO₂ removal. The aim of this study was to test the hypothesis that bio-ethylene could make the Brazilian chemical industry more competitive. This would be achieved by applying the revenues from carbon credits associated with using ethanol and sugarcane bagasse as feedstocks for bio-ethylene production. Three production routes were compared according to their estimated cost of production in Brazil under a simplified life cycle analysis: sugar cane derived ethanol to ethylene (with and without CO₂ capture and storage - BECCS); bio-methanol to olefin; and conventional steam cracking of naphtha. When associated with the production of long-lived materials, the ethanol to ethylene with BECCS route achieved the lower CO₂ break-even price (\$ 75/ t CO₂), followed by ethanol to ethylene without BECCS (\$ 82/ t CO₂) and bio-methanol to ethylene (\$ 106/ t CO₂). Our findings highlight the advantage for the Brazilian chemical industry of implementing a national, or even better, a global carbon pricing instrument.

2.2. Introduction

The Paris Agreement signed at COP21 in December 2015 sets a global objective to limit the rise in the average global air temperature at the Earth's surface to "well below 2°C" above pre-industrial levels (UNFCCC, 2015). According to the IPCC Special Report (IPCC, 2018), CO₂ emissions from 2018 onwards need to remain a carbon budget below

of 420 GtCO₂ to keep the rise in temperature below 1.5°C with a probability of 66%. Current emissions (including land-use change emissions) are already close to 40 GtCO₂eq per year (EASAC, 2018). Therefore, the target of limiting the temperature increase at 1.5°C becomes difficult (Millar et al., 2017) highlighting the urgency with which various technological options to achieve net carbon-dioxide removal (CDR) (Fuss et al., 2018; Walsh et al., 2017).

The chemical and petrochemical sector is the largest industrial energy user, accounting for 28% of the world's industrial final energy consumption (IEA, 2017), 10% of the world's total final energy consumption (IEA, 2017) and 7% the of greenhouse gas (GHG) emissions associated with industry (IEA, 2013). At the same time, the climate debate in this sector is one of the key "blind spots" in the global energy debate (IEA, 2018) and differs from what happens in other industrial sectors. It uses fossil fuels both for energy as well as a feedstock for the production of materials (Ecofys, 2018), resulting in a possible industrial process to capture carbon. As the chemical products are used in a wide variety of applications, the reduced emissions in this sector contributes to reducing the emissions in many other sectors through their products, adding value to their value chain (CEFIC, 2013; Ecofys, 2018). For instance, plastic insulation materials such as polystyrene or polyurethane result in energy savings from home heating and cooling and related CO₂ savings (CEFIC, 2013).

Chemical production based on low-cost, readily available feedstock has been a cornerstone of value creation in the industry, as seen in the United States with its cheap shale gas and in the Middle East with stranded gas reserves. They represent the low-cost champions for key petrochemicals (Griffin et al., 2018; IEA, 2018; McKinsey, 2018). Therefore, companies around the world are locating themselves in those regions to take advantage of cheap feedstock (Griffin et al., 2018; Hammond and O'Grady, 2017). However, the urgency with which the world economy needs to be decarbonised could lead to the emergence of others regions with renewable feedstock such as biomass (Ren, 2010; Ren et al., 2006) This could become a source of competitiveness that would produce high value added chemicals at low cost including the cost of GHG emission abatement.

Bio-based chemicals could significantly reduce the environmental impact of the chemical industry, lower many countries' dependence on fossil fuels and stimulate local economies (IRENA, 2013b). Moreover, the conversion of biomass into a chemical product can be a CDR option (Kemper, 2015; Moreira et al., 2016; Tagomori et al., 2019). This is particularly important, as CDR has become widely selected by Integrated Assessment Models (IAMs) to meet the requirements of keeping global temperature rise under the 2°C limit (Krey et al., 2014; Minx et al., 2018; Smith et al., 2016; UNFCCC, 2015; D. P. van Vuuren et al., 2017).

Brazil is one of the world's major agricultural producers (MAPA, 2018a) and supports a vast production of plantation crops like sugarcane, the predominant feedstock for its ethanol industry (Welfle, 2017). Along with the United States, Brazil leads the world in production of ethanol with those two countries accounting for 85% of global ethanol production (RFA, 2017). Historically, Brazil has had the lowest production cost (\$0.16-0.22/l) (Gupta and Verma, 2015) compared to United States (US) (\$0.25-0.40/l) (Gupta and Verma, 2015), Europe (\$0.36-0.57/l) (Gupta and Verma, 2015) or China (\$0.32/l) (Gupta and Verma, 2015). However, with the recent rapid increase in ethanol production in the US⁸, combined with the decreased investment in ethanol production in Brazil (since 2009) (Ferraz et al., 2010), both countries currently report similar ethanol production costs (between \$ 0.51- 0.58/Lge⁹ in US and \$0.54-0.62/Lge in Brazil) (IEA, 2019).

Even though, despite its current similar production costs compared to sugarcane ethanol (IEA, 2019), corn ethanol does not generate enough lignocellulosic material for chemical production. This also means that the Brazilian sugarcane industry can use both ethanol and surplus bagasse to produce chemicals. Actually, Brazil rates as a top producer of soybeans and coffee (Carvalho, 2017). The country generates significant amounts of biomass residues from harvesting and processing agricultural products such as sugarcane, soybeans and rice (Portugal-Pereira et al., 2015).

Interestingly, the use of biomass is well regarded for energy production such as bioenergy in transport, for heating or cooking in households or for conversion into electricity

⁸ Ethanol production in US increased 9.100% from 1980 to 2018, surpassing Brazilian production in 2006 (RFA, 2017).

⁹ Litre of gasoline equivalent.

(Daioglou et al., 2015; Gerssen-Gondelach et al., 2014; Welfle, 2017; Wicke et al., 2015). Some IAMs have identified the importance of biomass in the energy system to meet emission reduction targets (CALVIN et al., 2014; Daioglou, 2016; Luckow et al., 2010; Rose et al., 2014). Traditionally, the scientific literature has dealt with biomass conversion to energy from the perspective of the energy-food dilemma (Abdelradi and Serra, 2015; Cobuloglu and Büyüктаhtakin, 2015; Zhang et al., 2018). However, the scientific literature still lacks studies that evaluate CDR technologies through the conversion of biomass into chemical products.

Given the abundant source of biomass in Brazil along with the advantage that the chemical sector has in capturing CO₂ in its final products, this study aims to evaluate the potential gain in competitiveness of the Brazilian chemical industry through processing biomass. At present, the main source of competitive advantage in the petrochemical sector is the cost of, and, to a lesser extent, economies of scale (Deloitte, 2018). The hypothesis proposed in this study is that, if the carbon price is high enough, the Brazilian petrochemical industry can become competitive in cost through a quality premium price due to environmental differentiation (fewer GHG emissions when compared to fossil fuel based production).

To test this hypothesis, ethylene was selected as the case study. Ethylene is by far the most important building block in the petrochemical industry with a wide applicability (Spallina et al., 2017a). The global production capacity of ethylene exceeds 140 million tonnes per year (OGJ, 2015). Ethylene represents 51% of total olefin production in Brazil (ABIQUIM, 2015). Most of the ethylene is polymerized into polyethylene plastics such as HDPE¹⁰, LLDPE¹¹ and LDPE¹², but it is also used for the production of cosmetics, solvents, paints. Three ethylene production routes were compared according to their estimated levelized cost¹³ of production in Brazil and their environmental impact was examined using a simplified life cycle analysis, to investigate whether the use of biomass as feedstock could become a source of revenue in scenarios with different CO₂ prices.

¹⁰ High-density polyethylene.

¹¹ Linear low-density polyethylene.

¹² Low density polyethylene.

¹³ The levelized cost of each bio-ethylene process allows comparison among them, since it is an economic assessment of the annualized total cost to build and operate a bio-ethylene plant divided by the total annual bio-ethylene production (Gerssen-Gondelach et al., 2014; Tagomori et al., 2018).

The processes are: sugar cane derived ethanol to ethylene (with and without BECCS¹⁴); bio-methanol to olefin; and conventional steam cracking of naphtha, which was defined as the benchmark route for comparison.

The next section of this paper shows the current state of the Brazilian chemical industry, aiming to show its current lack of competitiveness. Section 3 describes the methodology applied to assess the levelized costs of ethylene from naphtha, ethanol and bio-methanol, as well as the methods used for the sensitivity analysis. Section 4 presents the break-even carbon prices of the selected routes, the results of the sensitivity analysis and the discussion of the final results. Finally, section 5 concludes the paper.

2.3. Brazil's chemical industry

The Brazilian industry share in the country's GDP has been decreasing since the early 1990s (Bacha and Bonelli, 2006; Cano, 2012; GAULARD, 2015). This process is also happening in some developed economies (Palma, 2014), but the deindustrialization process in Brazil took place at an early stage in the country's development (Cano, 2012), when Brazil's per capita income was much lower than in the developed countries (Palma, 2014). Moreover, this process has occurred in a country with a population with a low level of schooling and an economy where, instead of the tertiary sector expanding, it has returned to one where the primary sector dominates.

Aside from deindustrialization, Brazil has suffered from a deep economic recession and political crisis, losing competitiveness in the international market. According to the World Economic Forum (2017a), in 2017, the country reached the worst position of the past ten years in global competitiveness ranking and its industrial production fell back to 2004 levels. This compromises economic growth as well as affecting generation of jobs and income.

The chemical industry is one of the more onward and upward integrated industrial sector in Brazil (Rathmann, 2012). Nevertheless, the country has increased its dependence on imported chemicals. This trend may be reinforced over the next few decades, especially due to the lack of recent investment (Figure 2), including the announcement of the

¹⁴ Bio-energy with Carbon Capture and Storage.

Brazilian state-controlled company, Petrobras, of cancelling the petrochemical sector expansion (ETENE, 2016).

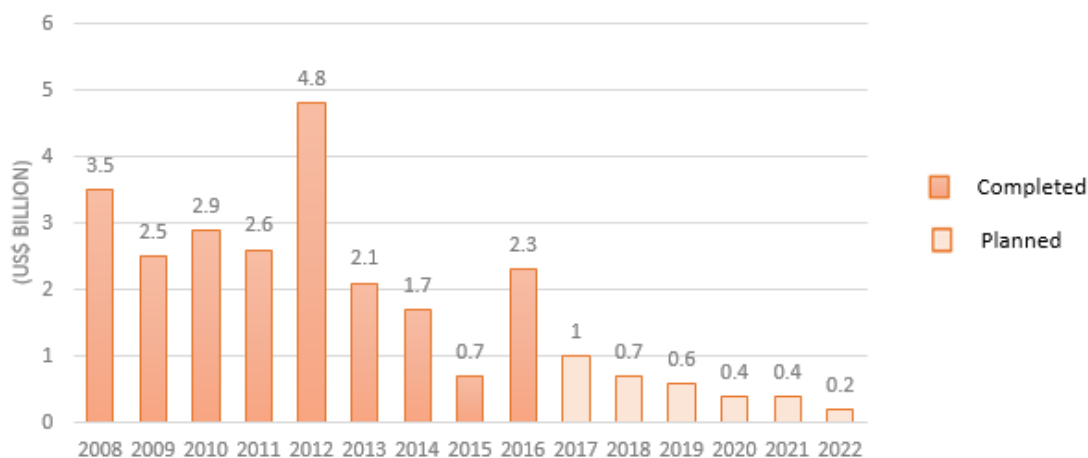


Figure 2: Investments in Brazilian Chemical industry

Source: Based on Deloitte (2018)

In 2017, the Brazilian chemical industry accounted for 10% of country's industrial GDP (Deloitte, 2018) but dropped in turnover from sixth to eighth position worldwide. To retake its position, Brazil's chemical sector is betting on the removal of several barriers that affect its competitiveness: high costs of feedstock, excessive bureaucracy, high price of electricity and high logistic costs (Deloitte, 2018). This study focuses on one of these barriers: the high costs of feedstock. Brazil's petrochemical industrial facilities face one of the highest naphtha prices in the world (Deloitte, 2018). Besides, domestic natural gas is expensive and is associated with the offshore production of crude oil (Deloitte, 2018).

In summary, taking into account the strong influence that divestment in the chemical industry has had on the Brazilian economy, the sector has to reinvent itself to be able to compete as a global player. In this regard, the Brazilian chemical sector could consider its comparative advantages, such as the low cost of sugarcane that has already encouraged the production of bioethanol for the production of ethylene. Since 2010, BRASKEM has operated a commercial plant with a production capacity of 200 kt per year of polyethylene from bio-ethylene (Gallo et al., 2014). Under current market conditions, ethylene from ethanol would not compete with ethylene from naphtha or natural gas, simply because ethanol prices tends to follow the price of gasoline (Cavalcanti et al., 2012a, 2012b; Hallack et al., 2020). While petrochemical naphtha is less expensive than gasoline, the

same applies to ethane from natural gas (particularly, for stranded reserves) (Platts, 2018a). Therefore, this study assesses whether bio-ethylene has an environmental advantage (expressed as lower CO₂ emissions than ethylene derived from fossil fuel), and whether those emissions if valued (or priced) could generate a financial advantage for this product. This could also be seen as an economic benefit from mitigating CO₂ emissions in the Brazilian chemical sector.

2.4.Methods

The selected routes to produce ethylene assessed by this study were conventional steam cracking of naphtha, ethanol to ethylene (with and without BECCS), and bio-methanol to olefin (MTO¹⁵), representing the current most promising routes for ethylene production from biomass. The estimated Levelized Costs (LC) and GHG emissions intensity of these bio-production routes were compared to their fossil fuel counterpart. The GHG emissions intensity of each route was assessed from cradle-to-gate calculated on adopted a mass-based allocation method¹⁶. To find the break-even carbon price of these bio-products, the LCs were subject to a range of different carbon prices (from US\$ 0 to US\$ 220 /tCO₂).

The LCs calculated for each route follows Equation 1.

Equation 1:

$$LC_i = \frac{CAPEX_i + FOM_i + VOM_i + FEEDSTOCK_i - REVENUE_i}{PRODUCTION_i} \pm CARBON_i$$

Where,

LC_i = Levelized costs of route i (\$/t ethylene);

i = Ethylene route;

$CAPEX_i$ = Annualized capital expenditure for route i (\$/year);

FOM_i = Fixed operations and maintenances costs for route i (\$/year);

VOM_i = Variable operations and maintenances costs for route I (\$/year);

$FEEDSTOCK_i$ = Costs with feedstocks for route i (\$/year);

¹⁵ Methanol to olefins.

¹⁶ Allocation can be done according to the relative mass, volume, energy or economic value of the products and coproducts. This study has adopted a mass-based allocation; therefore, the environmental impact is distributed between the outputs based on mass.

$REVENUE_i$ = By-products revenues for route i (\$/year);
 $PRODUCTION_i$ = Total production of route i (t ethylene/year);
 $CARBON_i$ = CO₂ emissions costs or revenue for route i (\$/t ethylene), calculated accordingly to Equation 2.

Equation 2:

$$CARBON_i = Annual\ emissions_i \times Carbon\ price$$

Where,

$Annual\ emissions_i$ = Annual CO₂eq emissions from route i (tCO₂eq/ t ethylene);

$Carbon\ price$ = Carbon price (\$/ t CO₂eq).

Table 1 shows assumptions for the LC costs for the overall routes.

Table 1: Economic assumptions

Annual discount rate ⁽¹⁾	9.8%
Economic lifetime ⁽¹⁾	30 years
Base-year	2017
Exchange rate ⁽²⁾	1.13 €/ \$

⁽¹⁾ It was assumed that 10% of the investment was financed at a 15.0 % annual interest rate (Oliveira, 2017) and 90% from the Brazilian public development bank, BNDES, at a 8.5% annual interest rate (BNDES, 2019).

⁽²⁾ Average exchange rate from Statista (2019) for 2017.

Primary data for CAPEX and OPEX for the processes assessed by this study were adjusted to US\$₂₀₁₇, according to the Chemical Engineering Plant Cost Index – CEPCI (Chemical Engineering, 2019)

2.4.1. Assessment of ethylene production routes

This study compared three ethylene production routes: sugarcane derived ethanol to ethylene, bio-methanol to olefin (using sugarcane bagasse as feedstock) and conventional steam cracking of naphtha. For the first option, there is already a plant of 200 kt/year installed in Brazil (ETENE, 2016). It is based on a simple, established process, whose main advantage is the large Brazilian sugar cane industry, but whose drawback is the cost of ethanol supply. The second route was also based on a by-product of the sugar cane industry, i.e. bagasse. It is less expensive than ethanol but its conversion requires a more complex process. Finally, the fossil fuel route based on naphtha was selected, since it is

the major process adopted in Brazil (ETENE, 2016) and even in China, which is globally the major importer of petrochemicals and a potential market for exports from Brazil.

Before detailing the routes, it is worth noting that the emission factor of each process depends on the final disposal of the final product (ethylene into its derivative). For instance, if the bio-ethylene is converted into polyethylene plastic bag, which is a single-use product, it can be incinerated, recycled or landfilled at the end of life. Each one of these final disposals emit GHG emissions. However, the ethylene product could be converted into long life-time products, as a strategy of carbon sink. In this case, if all the carbon embodied in 1 tonne of bio-ethylene is considered as biogenic carbon storage 3.14^{17} tCO₂ would need to be subtracted from the bio-ethylene's total life-cycle GHG emissions.

While this paper does not detail the assessment of the final disposal, this step is crucial to understand the real benefits of bio-based routes. Therefore, this study assessed a best-case for bio-ethylene products' final disposal (Table 2), which means that the biogenic carbon captured in the sugarcane production is embodied into a long-lifetime product; and a worst-case for bio-ethylene products' final disposal, when the biogenic carbon is fully released in the atmosphere at their end-of-life.

For the best-case of bio-ethylene products' final disposal, this paper considers bio-plastics as construction material, such as façade panels, windows or water pipes (The Constructor, 2019a). In Brazil, the construction industry was the largest consumer of plastics in 2017, followed by the food industry, accounting for 23.8% (ABIPLAST, 2017a) and 20.2% (ABIPLAST, 2017b), respectively.

Table 2: CO₂ emissions range from final disposal of bio-ethylene¹

	Worst case	Best case
	(t CO₂/ t ethylene)	(t CO₂/ t ethylene)
Bio-ethylene	0	-3.14

¹ Not considering emissions from transportation

¹⁷ The molar mass of ethylene (C₂H₄) and carbon dioxide (CO₂) is 28 g/mol and 44 g/mol, respectively. Stoichiometrically, if burned, one molecule of ethylene emits 2 molecules of CO₂, i.e., 3.14 g CO₂/ g ethylene (2 x 44 / 28).

2.4.1.1. Steam cracker of naphtha

Steam cracking of naphtha are the dominant technologies for the production of light olefins, representing 40% and 38% respectively of global production, in 2017 (Platts, 2018b, 2018a). In Brazil, naphtha represents 92% of petrochemical feedstock and Petrobras is practically the only naphtha and natural gas producer in the country, meeting part of national demand with its own production and with imports (ETENE, 2016). This process is energy intensive (60% of energy required in the ethylene production plant is consumed in the cracker) and it is responsible for high CO₂ emissions¹⁸ (Ren et al., 2008; Xiang et al., 2015).

This process produces mostly ethylene (32% by mass, on average), but also propylene, butadiene, aromatics – the so-called high value chemicals (HVCs) – pyrolysis gasoline, and fuel grade by-products such as hydrogen and methane used to fuel the process or to be exported (Ren, 2010; Ren et al., 2006). Table 3 shows the yields on a mass basis for each HVC considered in this route. The cost data for a naphtha steam cracker is presented in Table 4.

Table 3: High value chemical yields of naphtha steam cracker

High value chemicals	Yield (wt%)
Ethylene	0.32
Propylene	0.17
C4 ⁽¹⁾	0.13
BTX ⁽²⁾	0.104

⁽¹⁾ C4 cracking fractions are the mixture of butane and butadiene.

⁽²⁾ Mixture of benzene, toluene and xylene.

Source: Ren et al. (2006)

¹⁸ Different allocation methods influence the final CO₂ emissions of a process that outputs various co-products. Still, the scientific literature agrees with the high CO₂ emission intensity of ethylene production, ranging from a minimum value (according to which emissions are allocated for each co-products according to mass or energy) to a maximum value (according to which emissions are allocated to solely the main product).

Table 4: Cost data for a naphtha steam cracker

Capacity (Mt/y) ⁽¹⁾	0.50
Capacity factor (%)	0.90
Ethylene prod. (Mt/y)	0.45
Propylene prod. (Mt/y)	0.24
C4 prod. (Mt/y)	0.18
BTX prod. (Mt/y)	0.14
CAPEX (M\$_{2017/y}) ⁽²⁾	147.68
FOM (M\$_{2017/y}) ⁽³⁾	56.03
VOM (M\$_{2017/y}) ⁽⁴⁾	761.71
Propylene price (\$_{2017/t}) ⁽⁵⁾	766.67
Butadiene price (\$_{2017/t}) ⁽⁵⁾	1002.92
BTX price (\$_{2017/t}) ⁽⁵⁾	751.67
Naphtha prices (\$_{2017/t}) ⁽⁶⁾	541.00

- (1) The plant capacity is the average capacity of naphtha steam crackers in Brazil (OGJ, 2015).
- (2) From TNO estimates based on market prices (2016) (TNO, 2018).
- (3) Fixed O&M costs from Ren (2010).
- (4) Variable O&M costs includes the annual costs with naphtha as feedstock.
- (5) From INTRATEC (2019).
- (6) From COMEXSTAT (2019).

The route from naphtha to ethylene was assessed on a cradle-to-gate basis (Figure 3). The starting point of the life-cycle analysis is the emissions from the upstream operation of oil and gas production accounting for 21.60 Mt CO₂ eq in 2017 (Petrobras, 2017), when 130.55 Mt of oil were produced (ANP, 2018a). The distance from the well to refinery was assumed to be 50 km¹⁹ and the oil transportation was based on pipelines with an electricity consumption of 1.51 kWh/bbl (Nimana et al., 2017). The electricity is assumed to be purchased from the grid with an emission factor of 0.0927 kg CO₂/kWh (MCTIC, 2019). Emissions from oil refining totaled 22.8 MtCO₂ eq in 2017 (Petrobras, 2017) for the 87 Mt of oil processed (ANP, 2018a). The total amount of oil products obtained from oil in Brazilian refineries in 2017 reached 84.6 Mt, with naphtha representing 2.5% of total output. This small fraction of naphtha is explained by the fact that fuel prices in the 2011-2014 period were controlled by Brazilian government. That kept fuel prices below

¹⁹ The assumed pipeline distance from well to refinery is conservative. For instance, the distance of the pipeline that connects Ilha d'água Oil Terminal to the refinery REDUC (Refinaria Duque de Caxias), both in Rio de Janeiro, is 14 km, while the pipeline distance from Barueri Oil terminal to the refinery REPLAN (Refinaria de Paulínea), both in São Paulo, is 50 km (Petrobras, 2019).

international parity in order to prevent inflation and led to an increase in the country's gasoline demand (ALMEIDA et al., 2015; Oliveira and Almeida, 2015). To attend this growing gasoline demand, unfinished naphtha, from Brazilian refineries, was blended into the gasoline pool, decreasing supply for the petrochemical sector. This study sought to fix that distortion, by using the average mass yield of naphtha from 2007 to 2017, which corresponds to 4.8% (ANP, 2018a).

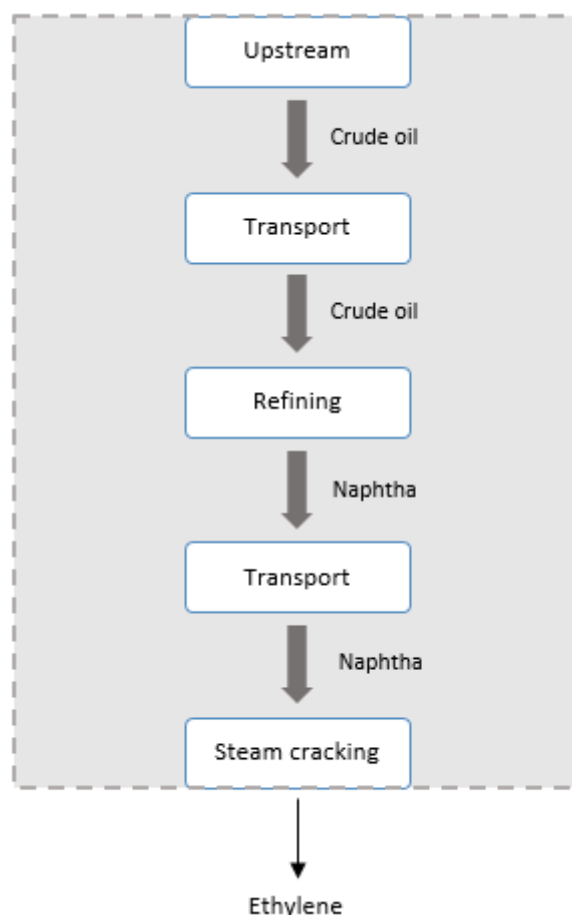


Figure 3: Life cycle system boundaries for naphtha steam cracking route

The transport of naphtha from the refinery to the petrochemical industry was also assumed to be a distance of 50 km and made through pipelines (Nimana et al., 2017). For the steam cracking process a mass yield of ethylene/HVC of 0.48 and an emission factor of 0.66 tCO₂/t ethylene (Spallina et al., 2017b) were assumed.

Table 5 indicates the emission factor calculated for this route. The final number is in accordance with the emission factor proposed by Simapro software version 8.5.2.0 (1.13 t CO₂eq/t ethylene).

Table 5: GHG emissions for naphtha steam cracking

Step	tCO₂ eq/ t ethylene
Upstream	0.01
Transportation 1	1.72x10 ⁻⁷
Refinery	0.36
Transportation 2	3.55x10 ⁻⁶
Steam cracking	0.66
Total	1.02

2.4.1.2. Ethanol to ethylene

Historically, ethylene was made from dehydration of ethanol up to the expansion of the petrochemical industry in the mid-1940, when ethylene started to be produced from thermal cracking of hydrocarbons (EIA, 2019; Tsiropoulos et al., 2015). The costs assumed for the ethanol-based route were derived from a simulation using the Aspen Plus® software Version 10 detailed in SECCHI et al. (2018), based on a real Brazilian ethanol-to-ethylene plant. The plant was simulated with a capacity of 200 kt per year, which corresponds to the capacity of the bio-ethylene plant in Brazil. However, this study adopted a capacity of 500 kt per year of ethylene to be consistent with the naphtha steam cracking plant that was also assessed. The costs (Table 6) were calculated using a scaling coefficient of 0.6258 (MELLO et al., 2019).

Table 6: Costs for the ethanol to ethylene route

Capacity (kt/y)⁽¹⁾	500.00
Capacity factor	0.90
CAPEX (M\$_{2017/y})⁽¹⁾	44.09
OPEX (M\$_{2017/y})⁽¹⁾	75.29
Ethanol costs (M\$_{2017/y})⁽²⁾	517.89
Ethanol price (\$_{2017/t})⁽²⁾	661.42

⁽¹⁾ Based on SECCHI et al. (2018).

⁽²⁾ From INTRATEC (2019).

Again, the system was assessed from cradle-to-gate (Figure 4)Figure 3.

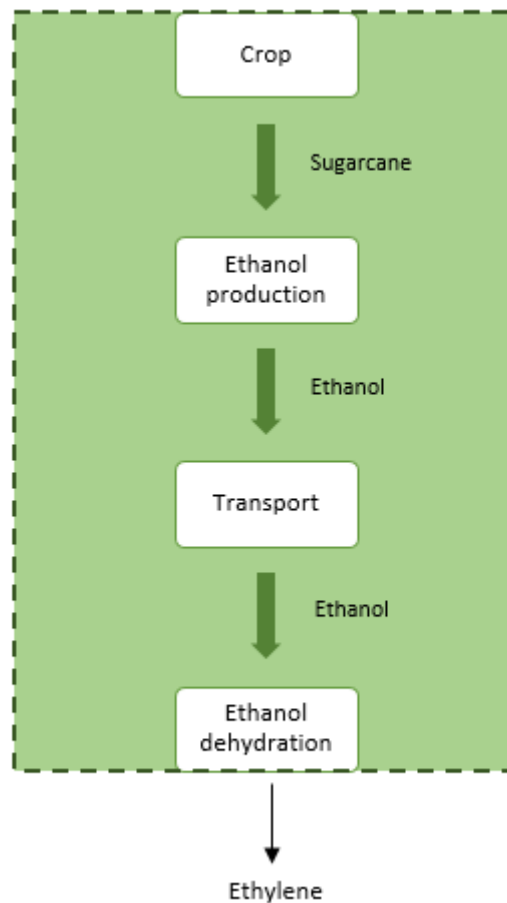


Figure 4: Life cycle system boundaries for the ethanol to ethylene route

The production of bioethanol from sugarcane has been reported many times in the literature (Alvarenga and Dewulf, 2013; Seabra et al., 2011; Seabra and Macedo, 2008; Tsiropoulos et al., 2014; Walter et al., 2015). The main products from processing sugarcane are ethanol, bagasse for cogeneration (of electricity and steam) and electricity for the grid (from surplus bagasse). The first step in this whole-of-life system is the cultivation of sugarcane (Table 7).

Table 7: GHG emissions for sugarcane cultivation ⁽¹⁾

Sugarcane cultivation steps	EF (gCO₂eq/MJ ETOH)
Sugarcane farming	6.8
Field emissions	6.7
Agricultural Input	3.8
Sugarcane transportation	1.4

(1) Sugarcane trash burning in São Paulo (major sugarcane producer State in Brazil) will be completely phased out by 2021 to meet State Law N° 11.241/2002. Therefore, the emissions from this step were not included in this LCA (Carvalho et al., 2017; European Commission, 2018)

Source: Seabra et al. (2011)

The emission factor for ethanol production is 2.6 g CO₂eq/MJ ethanol and the bagasse for cogeneration yield is 8.7 kg/ t cane, according to Seabra et al. (2011). The possibility of carbon capture from ethanol fermentation was also considered. It is a commercially proven technology with low specific costs (\$11 /t CO₂) (Tagomori et al., 2018). Ethanol production is an important opportunity for Bio-energy with Carbon Capture and Storage (BECCS) deployment. Actually, most current BECCS projects use CO₂ captured from ethanol production as input for enhanced oil recovery (Carbo, 2011; Kemper, 2015; Reiter and Lindorfer, 2015; Tagomori et al., 2018).

A distance of 50 km (Machado, 2014; Tagomori et al., 2019) to transport by truck from the ethanol distillery to the dehydration plant was assumed. The specific consumption of diesel is 0.020 l/t.km (Nimana et al., 2017) and the emission factor for diesel combustion is 75.243 kg CO₂ eq/TJ (IPCC, 2006a).

The specific energy consumption of the ethanol dehydration step was set as 0.04 GJ (natural gas)/t ethylene (Haro et al., 2013a). The emission factor of natural gas is 0.056 t CO₂/GJ (IPCC, 2006a). Finally, as mentioned before, the “best case” of bio-ethylene final disposal capture 3.14 t CO₂/ t ethylene, while the “worst case” does not capture biogenic CO₂

Table 8 summarizes the emission factor calculated for this route. It is worth noting that the GHG emissions presented in Table 8 was converted from tCO₂eq/ t ethanol to tCO₂eq/ t ethylene by a mass-based allocation.

Table 8: GHG emissions for ethanol to ethylene route

Steps	EF (t CO ₂ eq/ t ethylene)
Crop	0.04
Ethanol production	0.12
Ethanol production with BECCS	-0.45
Transportation	0.00 ⁽¹⁾
Dehydration	0.00 ⁽²⁾
Total	0.17
Total with BECCS	-0.41
Final disposal (“best case”)	-3.14
Final disposal (“worst case”)	0.00

⁽¹⁾ Transport by truck emits 0.0046 t CO₂/t ethylene.

⁽²⁾ Dehydration process emits 0.0022 t CO₂/t ethylene.

2.4.1.3. Methanol to olefins

Finally, this study also assessed the methanol to olefins (MTO) route. In this case, methanol is produced via syngas from gasification of sugarcane bagasse (IRENA, 2013a; Renó et al., 2011). The bio-methanol is then used as a feedstock to produce ethylene and propylene in a ratio between 0.5 and 1.5 to 1 (Chen et al., 2005) – the so-called MTO process. In this study, ethylene was assumed to be the main product, and propylene as the byproduct. Table 9 summarizes the costs for this route.

Table 9: Costs for MTO route

Capacity (kt/year)	500.00
Capacity factor	0.90
Ethylene/propylene ⁽¹⁾	0.90
CAPEX (M\$₂₀₁₇/year) ⁽²⁾	73.00
OPEX (M\$₂₀₁₇/year) ⁽²⁾	3.57
Price propylene (\$/t) ⁽³⁾	766.67
Methanol/HVC ^{2 (4)}	2.70
Price bio-methanol (\$/t)⁽⁵⁾	380.00

⁽¹⁾ Based on Amghizar et al. (2017).

⁽²⁾ From TNO estimates based on market prices (2016) (TNO, 2018).

⁽³⁾ From INTRATEC (2019).

⁽⁴⁾ From TNO estimates based on market prices (2016) (TNO, 2018). HVC herein is the mixture of ethylene and propylene.

⁽⁵⁾ From Huisman et al (2011).

Again, the system was assessed from cradle-to-gate (Figure 5).

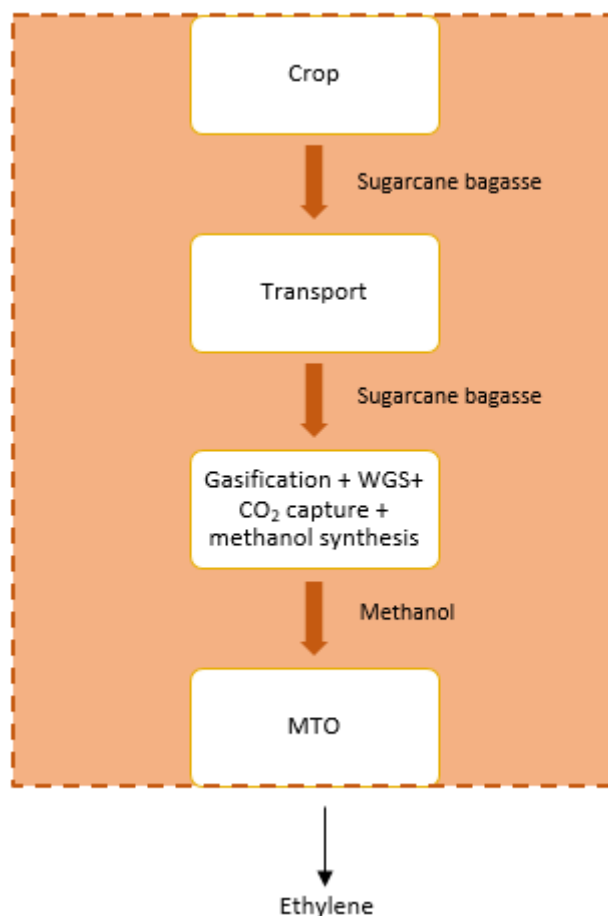


Figure 5: Life cycle system boundaries for MTO route (feedstock: sugarcane bagasse)

Note: WGS = water gas shift

The sugarcane cultivation step is the same as used in the ethanol to ethylene route. However, in this case, the surplus of bagasse that would be sold to thermoelectric plants to generate electricity for the grid is, instead, used for methanol production via syngas. The mass yield bagasse/total products²⁰ is 0.024 (Seabra et al., 2011). Trucks transport the bagasse for an assumed 50 km distance, from the distillery to the gasification and methanol synthesis plants. Diesel specific consumption is 0.020 l/t.km (Nimana et al., 2017), with an emission factor of 75.243 kg CO₂ eq/TJ (IPCC, 2006a).

The emission factor for the gasification and methanol synthesis steps is 1.83 t CO₂/ t methanol (Renó et al., 2011), including electricity and steam consumption, as well as

²⁰ The total products of the distillery is assumed to be ethanol, bagasse for cogeneration and bagasse surplus for methanol production.

process emissions. The electricity consumption is 0.093 kWh/ t methanol (Renó et al., 2011) and steam consumption is 0.00173 t/ t methanol (Renó et al., 2011). After the gasification, a water-gas shift (WGS) reaction is used to adjust the H₂:CO ratio in the syngas by converting CO and steam into H₂ and CO₂ (Dechema, 2017; Renó et al., 2011; Tagomori et al., 2019). CO₂ is removed with a capture rate of 95% (Tagomori et al., 2019). The MTO process emission factor is 0.10 tCO₂/t ethylene according to Liptow et al. (2015) (Liptow et al., 2015). The “best case” of final disposal for this route capture 3.14 t CO₂/ t ethylene, while the “worst case” does not capture biogenic CO₂

Table 10 indicates the emission factors for this route.

Table 10: GHG emissions for MTO route.

Step	EF (t CO₂ eq/ t ethylene)
Crop	0.08
Transportation	0.01
Gasification, WGS, CO₂ removal, methanol synthesis	0.23
MTO	0.10
Total	0.42
Final disposal (“best case”)	-3.14
Final disposal (“worst case”)	0.00

2.4.1.4. Sensitivity Analysis

The price of feedstock influences the variable operating costs of the processes assessed. Therefore, a sensitivity analysis was performed on the naphtha, ethanol, and bagasse prices. For this purpose, an uncertainty range of -50% to 100% was applied to the feedstock prices. Market feedstock prices were based on INTRATEC (2019) and COMEXSTAT (2019). It should be noted that a variation in the naphtha price also affects the prices of steam-cracking by-products.

In addition, a sensitivity analysis on bio-based plants’ capital expenditure (CAPEX) was also conducted. Economic analysis tends to underestimate the capital costs and overestimate the plant performance if compared with values observed for first-of-a-kind

(pioneer plant) (de Jong et al., 2015). Therefore, an uncertainty range of -50% to 100% was applied to the CAPEX of both bio-based ethylene processes.

The break-even carbon prices were calculated subject to variations in relative prices of the feedstocks (naphtha/ethanol and naphtha/bagasse) and in CAPEX of both bio-based plants. Break-even carbon prices allows the levelized costs of bio-based and fossil ethylene be equal. This study applied the Solver optimization tool in Microsoft Excel to determine how the desired break-even prices could be achieved by changing the feedstock prices for each of the selected routes and by ranging the bio-based plants' CAPEX. It should be noted that the sensitivity analysis was assessed assuming only the “best case” for ethylene final disposal, i.e., its conversion into long life-time products.

2.5. Results and discussion

2.5.1. Break-even CO₂ prices for the worst and best cases of ethylene final disposal

Figure 6 presents the results of the modelled routes for the “worst case” final disposal. When the biogenic carbon capture is not considered in the bio-ethylene's life-cycle GHG emissions, the break-even carbon prices are extremely high: \$ 241/ t CO₂, \$ 384/ t CO₂ and \$ 645/ t CO₂ for the ethanol to ethylene route with BECCS, ethanol to ethylene without BECCS and bio-methanol to ethylene, respectively. Moreover, the bio-based ethylene routes' behavior in this situation shows that the higher the carbon price the more costly these routes become, except for ethanol to ethylene route with BECCS that already presents a negative life-cycle emission as shown in Table 8.

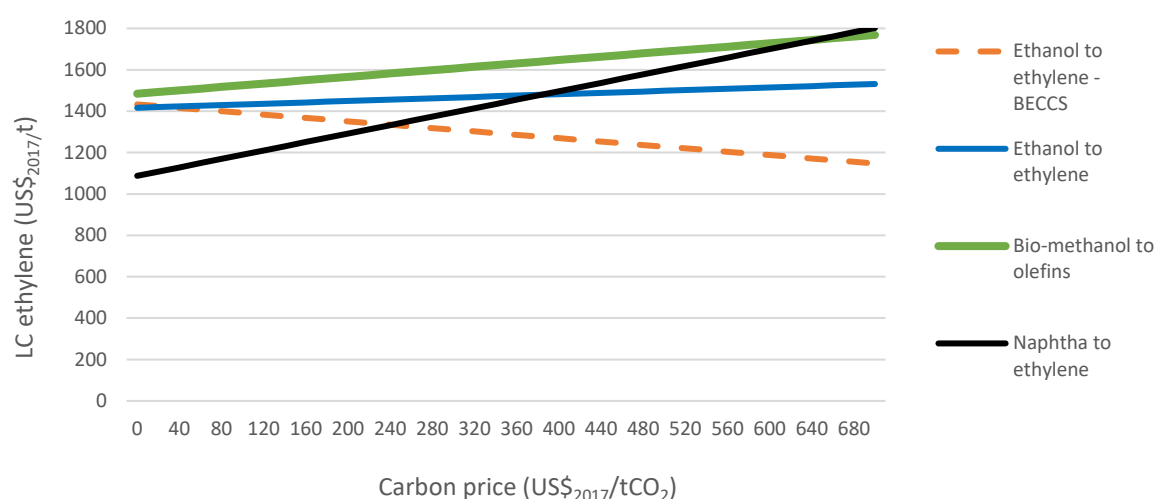


Figure 6: Levelized costs for ethylene production (“worst case”)

Figure 7 shows the results for the “best case” final disposal. The lines with negative slope correspond to the routes to produce ethylene using biomass as feedstock. This behavior is explained by their capacity to generate negative emissions: the higher the carbon price the cheaper these routes become. For instance, for a carbon price of US\$ 120/ tCO₂ , the costs associated with the ethanol to ethylene route with BECCS, the ethanol to ethylene route without BECCS, and the bio-methanol to ethylene route decrease to US\$ 1.006, \$1.060 and US\$ 1.156/ t ethylene, respectively. This means that, even though the bio-based routes are more costly, the cost becomes lower than their fossil counterpart, when the external cost of emitting CO₂ to the atmosphere through a carbon prices is taken into account. In other words, the revenue derived from CO₂ emissions abatement (quantity times price) more than compensates for the higher producer costs from biomass. At the end, the CO₂ break-even prices (that equalize bio-routes costs with naphtha route costs) are US\$ 75/ t CO₂ for the ethanol to ethylene route with BECCS, US\$ 82/ t CO₂ for the ethanol to ethylene route without BECCS, and US\$ 106/ t CO₂ for the bio-methanol to ethylene route.

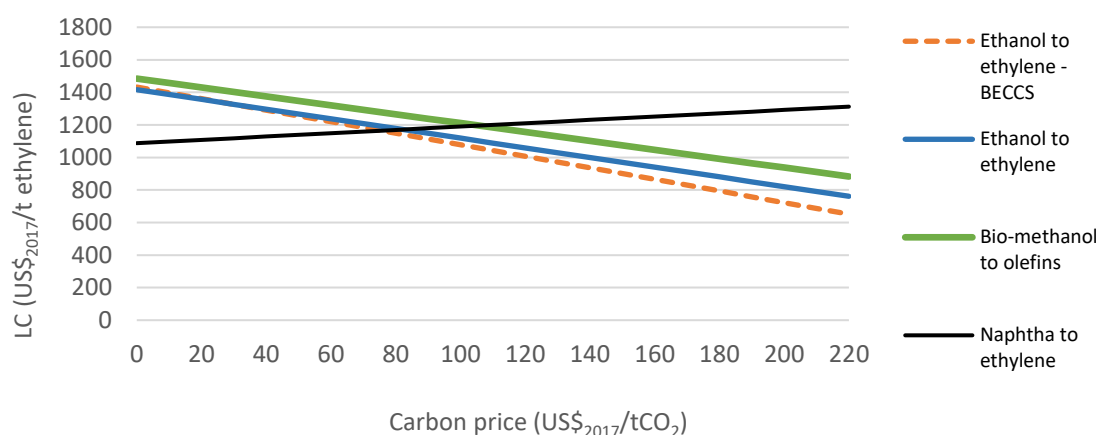


Figure 7: Levelized costs for ethylene production (“best case”)

As the feedstock cost accounts for 70% of the total production costs of bio-ethylene in the ethanol to ethylene route, this could give Brazil’s chemical industry a competitive advantage. Moreover, the production of ethanol from sugarcane in Brazil produces bagasse as a residue that can be sold for electricity generation or, in the case of this study, to produce bio-ethylene. Therefore, appropriate use of bagasse could improve the economics of the sugarcane ethanol production in Brazil. For instance, a dedicated facility using the sugarcane ethanol-to-ethylene process and converting the surplus bagasse into olefins through MTO would output 0.04 tonnes of ethylene per tonnes of sugarcane, with an average levelized cost of \$ 1,435.64/ t ethylene (based on weighting the share of each product from each route) and an average CO₂ break-even cost of \$ 86/ t CO₂ (idem).

During COP 21, Brazil announced the target to reduce GHG emissions by 37% compared to 2005 levels by 2025, and the intention to reduce emissions by 43% by 2030 (Brasil, 2017). In the recent past, the country has already considered the use of market mechanisms to reduce GHG emissions, as presented in its Nationally Determined Contribution (Gurgel and Paltsev, 2017; MCTIC, 2016). However, there is no clear indication of how these instruments will be used (Brasil, 2017). It signals that long-term investments need to be made in order to decarbonize the economy (Santos, 2018; Santos et al., 2018; Tvinnereim and Mehling, 2018). This paper does not aim to discuss the design of a carbon pricing instrument for Brazil, but instead it shows that a local or a global CO₂ market could boost the use of abundant primary energy sources in Brazil to produce ethylene. Moreover, it shows that, under a carbon pricing mechanism, the bio-

based chemical industry, based on sugarcane, could competitively produce ethylene when compared to the alternative process from naphtha.

The hypothesis tested in this study is that the Brazilian petrochemical industry can benefit from a leadership in cost through a quality premium of bio-ethylene; and this could favor an industry under a severe crisis.

In other words, there would be a co-benefit for Brazil to mitigate CO₂ emissions in the chemical sector, expressed in terms of competitiveness gains, if the CO₂ abated is priced and the ethylene produced is used in long-lived materials. The range of carbon prices available in the literature (Matthews et al., 2015; Rochedo et al., 2018; Soares-Filho et al., 2016) to reach a below 2° C world (\$ 162 – 505 per tCO₂) is higher than the range of bio-ethylene break-even prices founded in this study for the “best case” (\$ 75 - 106 per tCO₂). Nevertheless, the break-even prices found here are still above the price found in carbon markets already established in the world. For instance, the carbon price from the European Union Emissions Trade System (EU ETS) was on average only \$ 28 per tCO₂ in 2019 (Investing, 2019).

2.5.2. Sensitivity analyses

Table 11 shows the break-even CO₂ prices associated with the variation in the relative prices of feedstocks (naphtha/ethanol and naphtha/bagasse) for the best case of final ethylene disposal. As the relative feedstock prices increase, the break-even price for the bio-methanol to ethylene route become lower than that for the ethanol to ethylene route. This result was expected since the ethanol to ethylene process is more sensitive to a variation in feedstock price. Instead, a reduction in the relative prices can make the bio-ethylene feasible without the need for pricing the CO₂ (when the break-even CO₂ price is negative). This can happen sometimes, especially just before the driving season in the USA (starting from May-June) when the price of gasoline (and, thus, the price of naphtha) increases (GAO, 2005), and when the sugarcane supply season also starts in Brazil (USDA, 2009).

Table 11: Break-even CO₂ prices across a range in relative feedstock prices.

Feedstock relative price variation	Break-even CO₂ price in US\$/t ethylene (from ethanol)	Break-even CO₂ price in US\$/t ethylene (from bio-methanol)
-50%	-61.80	-9.70
-25%	10.20	47.98
0%	82.20	105.68
25%	154.20	163.37
50%	226.20	221.05
75%	298.21	278.74
100%	370.21	336.43

Table 12 shows the break-even CO₂ prices associated with the variation on bio-based plants' CAPEX. Actually, it is expected that pioneer (first-of-a kind) plants will face higher costs than nth. of-a-kind plants (de Jong et al., 2015), meaning that it is wise to consider a conservative break-even CO₂ price range of 100-150 US\$/tCO₂ for implementing a strategy aiming at producing bio-ethylene from sugar cane in Brazil. This range might decrease due to learning effects and yield increases as the strategy consolidates.

Table 12: Break-even CO₂ prices across a range in bio-based plants' CAPEX.

CAPEX variation	Break-even CO₂ price in US\$/t ethylene (from ethanol)	Break-even CO₂ price in US\$/t ethylene (from bio-methanol)
-50%	69.94	84.08
-25%	63.81	73.28
0%	82.20	105.68
25%	88.33	116.48
50%	94.46	127.28
75%	100.59	138.08
100%	106.73	148.88

2.6. Conclusions

Our findings indicate that bio-ethylene from sugar cane could become competitive with the naphtha derived ethylene for a price range of around 75-150 US\$/tCO₂, depending on the conversion of ethylene into long life-time products and the costs of pioneer plants. This competitiveness would be represented by both the revenues generated from carbon credits, as well as by the attractiveness to investors searching for regions with available, cheap and renewable feedstock.

Actually, bio-based chemicals could be an important step in the transition to a sustainable economy. From a technical point of view, the proposed transition could be closer than expected, however, the geopolitical situation and economic aspects, such as feedstock prices, are unstable market factors that make any assessment uncertain (Moreira et al., 2016). Therefore, the production costs estimated in this study depend not only on the future carbon prices, but also on the prices of crude oil, sugar, fuels and feedstocks. Moreover, first-of-a-kind plants always present high project and process contingencies and need learning to improve competitiveness.

The uncertainty of our results also stems from the LCA approach. Even though this study is based on a cradle-to-gate analysis, the disposal of ethylene products is crucial to understanding the real benefits of producing bio-ethylene for the Brazilian chemical industry. Therefore, the final disposal of ethylene was assessed in a simplified manner in this case, looking at the “best case” and the “worst case” final disposal for the bio-based routes, i.e., the final product is transformed into a long-lifetime product; or it is incinerated, emitting the total amount of biogenic carbon captured during sugarcane production. Also, the GHG emissions of bio-based chemicals vary across a wide ranges of values, due to the multiplicity of methodological choices regarding allocation procedures, system boundaries and functional units and assumptions made in the LCA studies that were reviewed (Alonso-Fariñas et al., 2018; Alvarenga and Dewulf, 2013; Amghizar et al., 2017; Haro et al., 2013b; Liptow et al., 2015; Liptow and Tillman, 2012; Renó et al., 2011; Tsiropoulos et al., 2015),

For this reason, a comparison between our results and others found in the literature is difficult and calls for a more uniform procedure. Still on the LCA uncertainties, the

present study did not consider the emissions from land use change for ethanol production. The reason behind this approach is that the expansion of sugarcane area will hardly cause indirect deforestation in the Brazilian Amazon rain forest (Seabra et al., 2011; Walter et al., 2015). Studies based on satellite images shows that the deforestation due to sugarcane expansion from 2005 to 2008 was around 0.18 Mha (Prins et al., 2012). This slight indirect impact can be explained by livestock intensification, expansion of sugarcane over pastures areas and improvement in the yields of different crops (Walter et al., 2015). Besides, the forecast ethanol demand in the coming 15 years will require no more than 6 Mha (FIESP, 2018) of the 64 Mha suitable for sugarcane production (MAPA, 2018b).

The sensitivity analysis performed in this study shows that the ethanol to ethylene route is more sensitive to a variation in feedstock price (ethanol price) than the other routes selected. It is worth noting that the price of bagasse used in this study is low since it is a residue from ethanol production. In future, the bagasse price may increase with an increase in demand for it. The sensitivity analysis also shows that if that occurs, the break-even price for the bio-methanol to ethylene route is lower than for the ethanol to ethylene route.

Further studies should also evaluate other feedstocks for the production of ethylene such as alternative sources of biomass besides bagasse. They could as well assess the methanol production from the hydrogenation of CO₂, being H₂ produced through water electrolysis.

3. Achieving negative emissions in plastics life-cycle through the conversion of biomass feedstock

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3.1. Abstract

Plastics are one of the fastest-growing group of bulk materials in the world. Yet, one third of plastic waste ends up as terrestrial or marine pollution. As a strategy to lower the carbon footprint of plastics, this study aims to test the hypothesis that using plastics in long-term applications would bring environmental advantage due to the reduction of plastic pollution; the achievement of negative CO₂ emissions (NETs) by bio-based plastics; and the demand reduction for emission-intensive construction materials, such as iron, aluminum, wood and cement. Cradle to grave life-cycle GHG emissions of high-density polyethylene (HDPE), polyvinyl chloride (PVC), polyethylene terephthalate (PET), and expanded polystyrene (EPS) were performed for four ethylene production routes. For the final disposal, this study assessed incineration; incineration with energy recovery; recycling; and the orientation of plastics for replacing emission-intensive material construction (long-term applications). Findings show that using plastics as long lifetime materials could lead to NETs, particularly in the cases of bio-based HDPE, bio-based PET, and bio-based EPS. Hence, an opportunity arises in producing plastics for long-term applications to reduce both the carbon footprint and the plastic waste generation that may enter the marine environment.

3.2. Introduction

Plastics are one of the largest groups of chemical products and the fastest-growing group of bulk materials in the world (Geyer et al., 2017a; IEA, 2018), apart from cement and steel (USGS, 2017; World Steel Association, 2017). Their unrivalled features include

durability, light-weight, high strength-to-weight ratio, hardness, ease of design and manufacture, and low cost (Gu and Ozbakkaloglu, 2016; PlasticsEurope, 2018). Yet, plastics' durability feature represents a controversial debate in the society (Monteiro, 2018; Pinto, 2012). On one hand, its low degradability, non-toxicity and water, chemical and decay resistance can be advantageous as an alternative to traditional materials such as glass, metal, or wood. In addition, the low degradability of plastics increases their lifetime if they are applied in long-term applications. On the other hand, since plastics waste is still mismanaged, around 60% of the plastics produced from 1950 to 2015 ends up as terrestrial or marine pollution, accounting for 4,900 million metric tons of plastic waste (Geyer et al., 2017a). The report "The marine plastic footprint" (IUCN, 2020) estimates that 12 million metric tonnes of plastics leak to the marine environment every year.

Plastic and microplastic pollution pose negative effects on marine environment and on its food chain, including human beings (Laskar and Kumar, 2019). Microplastics contaminate tap and bottled water, which leads to possible effects on human health (GEF, 2018a; Jefferson, 2019). There are over 150 million tonnes of plastic waste in the ocean today (Laskar and Kumar, 2019; MacArthur, 2017; McKinsey Center and Ocean Conservancy, 2015) and, in 2050, there will be more plastics, by weight, than fish in the ocean, unless action is taken (GEF, 2018a; MacArthur, 2017). Single-use plastics such as grocery bags, food packaging, bottles, straws, containers, cups and cutlery are the greatest contributor to this leakage (MacArthur, 2017; UN Environment, 2018).

Complete elimination of post-consumer plastics bets on destructive thermal treatment such as combustion or pyrolysis (Geyer et al., 2017b). Despite addressing the accumulation of plastic waste that may end in the marine environment, these solutions contribute to further increase GHG emissions, even if the energy embodied in the plastic is partially recovered. Besides environmental pollution, the upstream of plastic industry (petrochemical industry) is one of the key "blind spots" in the global energy debate since much of its fossil hydrocarbons enters the sector as feedstock and do not undergo combustion. The sector, thus, achieves the contradictory feat of being the largest industrial fossil fuel user, accounting for 28% of the global industrial final energy consumption (IEA, 2018, 2017) and yet only the third-largest industrial CO₂ emitter, representing 18% of all industrial CO₂ emission (IEA, 2018).

For this reason, the sector needs a holistic strategy to both reduce GHG emissions in energy and material flows and stop plastic pollution especially in marine environments. Bio-based materials, circular economy and product innovations are expected to play a critical role in decarbonizing the chemical sector while harnessing the many benefits of plastics (Bauer et al., 2018a; MacArthur, 2017; Oliveira et al., 2020b).

Zheng and Suh (2019) evaluate four strategies to reduce the carbon footprint of plastics in global scale: 100% sugarcane and corn-based plastics, 100% renewable energy, 100% recycling and halving plastic growth in demand. According to them, for the lowest GHG mitigation potential to happen (93% GHG reduction from the baseline in 2050), the four strategies should be implemented in concert. However, the study lacks the evaluation of a fifth option: orient plastics production through the conversion of biomass feedstock towards long-lifetime products as a strategy to achieve negative emissions.

Spierling et al. (2018) estimated that bio-based plastic could save 241 to 316 MtCO_{2eq} per year by substituting 65.8% of all conventional plastics. Bio-based plastics can act as a negative emission technology (NET²¹) depending on the plastic's final disposal (Oliveira et al., 2020b). Actually, NETs have been widely selected by Integrated Assessment Models (IAM) to meet the requirements of temperature limits of 1.5°C (Krey et al., 2014; Smith et al., 2016; UNFCCC, 2015). Nonetheless, the scientific literature on IAMs still lacks evaluating NETs through the conversion of biomass into chemical products (Oliveira et al., 2020b). Exceptions are Daioglou et al. (2019, 2015, 2014), which include in their modeling exercise the demand of the non-energy sector, although in an aggregate manner for basic petrochemicals; and Lap et al. (2019) who explored in an IAM the biomass competition between energy and chemicals, however, the analysis was restricted to few petrochemicals and leaves the competition between energy and food out of the scope. Therefore, we aim to fill this gap, understanding that, if used in long-term applications, bioplastics could be capable of removing atmospheric GHG, what we call here BIOCCUS (biomass with carbon capture utilization and storage).

²¹ NETs is defined by the 2018 IPCC special report (IPCC, 2018). Other technologies considered NETs are afforestation, soil carbon sequestration, direct air capture with storage (DAC-S) and bioenergy with carbon capture and storage (BECCS) (Tanzer and Ramírez, 2019)

After packaging, the construction industry is already the second largest consumption of plastics, accounting for 16% of global consumption (Geyer et al., 2017b; IEA, 2018), being polyvinyl chloride (PVC) the most adopted plastic, especially for pipes, windows and door frames (IEA, 2018). The use of plastic in long term application, such as construction, may delay their end of life emissions by around 35 years (Geyer et al., 2017b), depending on the application. Bio-based infrastructure therefore could act as a long-term²² NET (Churkina et al., 2020; Oliveira et al., 2020b), if strong regulatory measures are taken to certificate this long-term use. Also, as a mitigation strategy, plastics could compete in specific applications with energy-intensive construction materials, such as cement and steel, rediscovering a historical strategy of the industry to expand markets by substituting traditional materials as an approach to adapting to climate emergency imperatives. Besides, several countries have already banned single-use plastics (UNEP, 2018a); if this trend persists it will naturally pressure the plastics industry to search for new markets. In addition, by substituting traditional construction materials, it reduces deforestation caused by their mining (Churkina et al., 2020).

The use of plastics for long-term application, such as construction, can reduce GHG emissions during their lifetime, since this application stores the plastic (and the carbon in its molecular structure) for decades delaying their final disposal. Though the same may occur in single-use applications, long-term applications avoid both emissions from recycling or incineration, and potential marine pollution due to plastic mismanagement. Also, if bio-based plastics are considered, the biogenic carbon absorbed during biomass cultivation and then captured in plastics could result in negative emissions (Oliveira et al., 2020b). Therefore, given the urgency to deal with plastic waste and to decarbonize the petrochemical industry, this paper investigates what plastics' final disposal option achieves the lowest carbon footprint or even negative emissions. The hypothesis tested is that orienting plastic production to the construction sector, instead of applications that require extensive recycling or incineration, such as packaging, would result in an environmental advantage due to three reasons: the biogenic carbon embodied in the plastic would be stored in a long-lifetime material (Oliveira et al., 2020b); if plastic waste is used for construction purposes, it would reduce plastic waste accumulation (Sule et al., 2017), delaying for decades its final disposal and related emissions; and it would reduce

²² Long-term material application in the construction or infrastructure sectors have a useful lifetime of around 35 years (Geyer et al., 2017a).

the demand for emission-intensive construction materials such as cement, aluminium, steel and wood from deforestation.

The increase of the usage of plastics in construction does not mandatorily lead to plastic reduction in packaging. However, the drop of plastic use in packaging is already happening and several countries have been banning single-use plastics (UN Environment, 2018). On the other hand, the use of plastic in construction has been increasing since the emergence of plastic in 1950 (Geyer et al., 2017b). Therefore, we considered in our study that the use of plastics in construction could be an alternative to compensate the packaging market loss, which should be accelerated by more stringent environmental policies. In other words, we considered a twin objective by both promoting the usage of plastics in construction and accelerating the market loss in package. Actually, this is already happening in the two major Brazilian cities (EBC, 2019; Latin News, 2020).

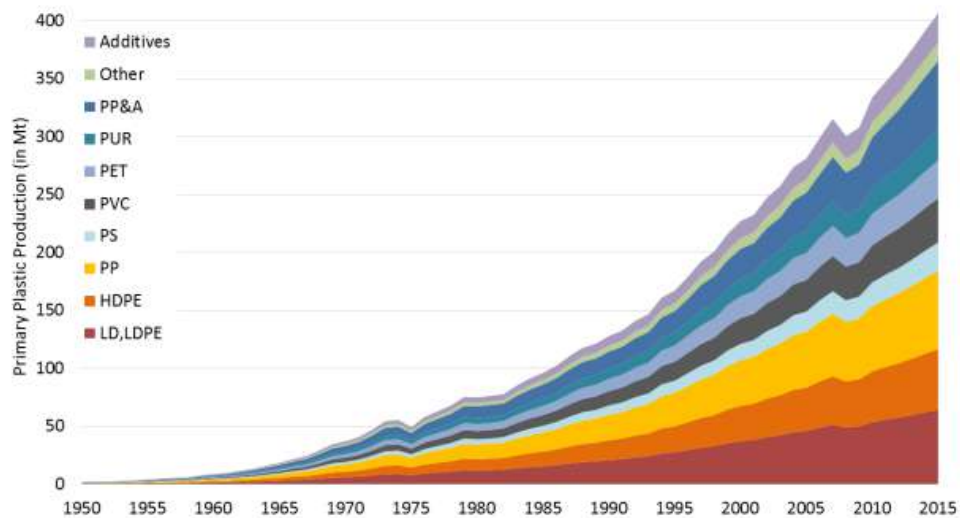
The next section of this article shows the landscape of waste plastic. Then, the paper describes the methodology applied to assess the carbon footprint of the plastics selected according to their final disposal. Finally, we present the results and discussion of this assessment.

3.3.Landscape of plastic waste

The global plastics production was around 2 Mt (Geyer et al., 2017b) in 1950 and has increased 200 times since then (MacArthur, 2017; WWF, 2019). In 2016, the global production of plastics reached 396 Mt, emitting 2 Gt of CO₂, representing around 6% of total global CO₂ emissions per year (WWF, 2019). The global plastic capacity has increased 4% per year since 2000 (WWF, 2019). Should this trend continue, plastic production is expected to increase in 40% until 2030 (WWF, 2019) when compared to 2000.

According to UN Environment's global mapping (UNEP, 2018b), China leads plastic production and consumption, followed by North America and Western Europe, with 28%, 19% and 19%, respectively for production and 20%, 21% and 18%, respectively for consumption. Latin America and Caribbean is the 7th largest plastic producer in the world, accounting for 4% of global plastic production and 8% of global plastic consumption.

Polypropylene (PP), low-density polyethylene/linear low-density polyethylene (LDPE/LLDPE), polyvinyl chloride (PVC), high-density polyethylene (HDPE), polyethylene terephthalate (PET) and polystyrene (PS) are the most used plastic polymers in the world (Geyer et al., 2017a; UNEP, 2018b) which cover 21%, 20%, 11.8%, 16.3%, 10.2%, 7.6%, respectively. Figure 8 shows historical global primary plastics production per polymer type.



LD, LDPE = Low-density and linear low-density polyethylene; HDPE = High-density polyethylene; PP = polypropylene; PS = polystyrene; PVS = polyvinylchloride; PET = polyethylene terephthalate; PUR = polyurethanes; PP&A= polyester, polyamide, and acrylic.

Figure 8: Global primary plastics production according to polymer type from 1950 to 2015.

Source: Geyer et al. (2017b)

Packaging is the main application for plastic followed by construction, accounting for 36% and 16%, respectively, of total plastic usage in 2017 (Geyer et al., 2017b; IEA, 2018). Figure 9 shows the consumption of plastics by end-use sector.

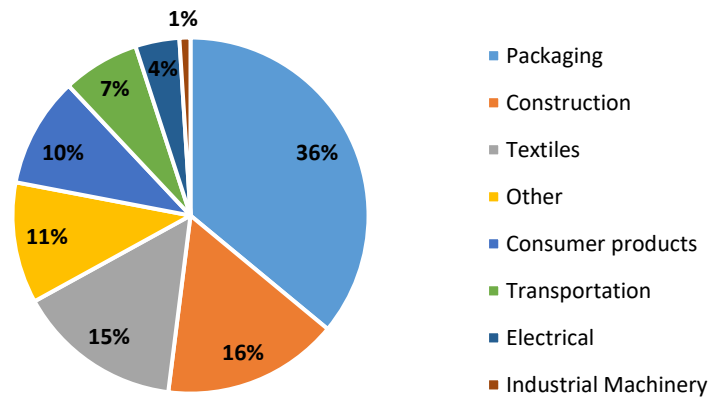


Figure 9: Estimated consumption of plastic by end-use sector.

Source: Based on Geyer et al. (2017b) and IEA (2018)

Geyer et al. (2017b) estimated that, in 2015, 407 Mt of virgin plastics entered the use phase and 302 Mt left it as waste. The products' lifetimes rely on polymer type and industrial use, as shown in Figure 10. For instance, plastics for construction leave the use phase decades later than packaging plastics, which present a lifetime of one year maximum (Geyer et al., 2017b).

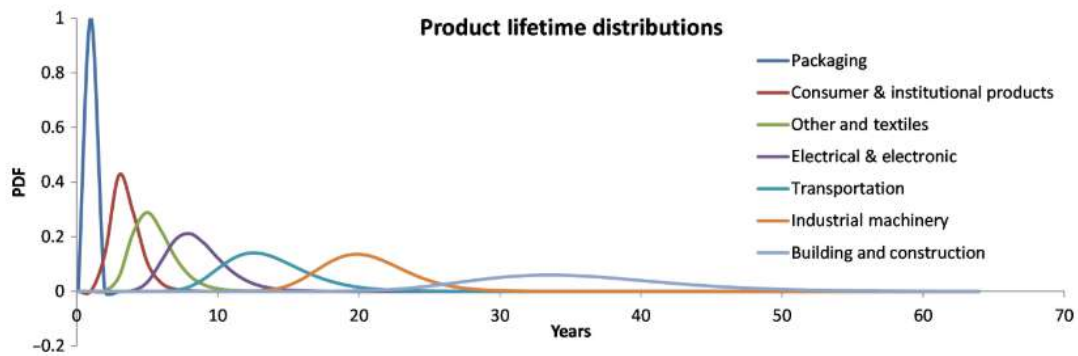


Figure 10: Product lifetime distributions for eight industrial use sectors plotted as lognormal probability distribution functions (PDF).

Source: Geyer et al (2017b)

In the end of their lifetime, the plastics waste follows three main trajectories (Geyer et al., 2017b): recycling, what delays their final disposal; incineration, what destroys them thermally with or without energy recovery; and landfilling, when they are discarded in a sanitary landfill. Due to plastic waste mismanagement, open dumps and natural

environment are both current final disposal options for plastics (Bhattacharya et al., 2018). Also, recycling is considered for n recycles loops. After that, the plastic is sent to any of the final disposal options left. As mentioned before, this study does not analyze the disposal of plastics in landfills.

3.3.1. Recycling

Recycling is the backbone of circular economy (Worrell, 2019) and an “essential tool out of a whole toolbox to better manage natural resources” (Worrell and Reuter, 2014). Nonetheless, recycling a plastic can lead to a down cycle process, in which the plastic returns to the cycle with a lower quality (Dilkes-Hoffman et al., 2019; Flock, 2018). Therefore, the quality of recycling plastic needs to be improved and the plastic’s properties should be maintained to increase the “circularity” of plastics (Eriksen et al., 2019; Hopewell et al., 2009).

The average recycling rate in European Union is 30% (OECD, 2018; World Economic Forum, 2017b), while in developing countries is around 20-40% (OECD, 2018), with exception of India whose recycling rate is around 60% (Sustainable Recycling Industries, 2018). In the US only 9.1% of plastics were recycled in 2015 (USEPA, 2018) and the recycling rates in low-to-middle-income countries are largely unknown (OECD, 2018). Despite the higher recycling rate of high-income countries, most of the so-called recyclables plastic waste is being shipped abroad and dumped in local communities in low and middle-income countries, especially in Southeast Asia (Greenpeace, 2018). This phenomenon is being seen as “the recycling myth” (Greenpeace, 2018).

In 2018, China banned the imports of recyclable plastics in order to improve life quality (National Geographic, 2019). Until then, the country imported up to 56% of the world's plastic garbage to recycle (DW, 2019). This decision has engendered a new stage in the world recycling industry (Greenpeace, 2018; OECD, 2018; WWF, 2019), in which exporters nations have to find alternatives to get rid of their plastic waste, such as recycling. Also, in 2020, China decided to ban non-degradable bags in major cities by the end of 2020 and in the whole country in 2022 (Ministry of Ecology and Environment. National Development and Reform Commission, 2020).

According to Geyer et al. (2017b), plastic waste totaled 6,300 Mt between 1950 and 2015. Of this, 9% have been recycled (Jefferson, 2019; MacArthur, 2017) and only 10% of this have been recycled more than once (MacArthur, 2017). Recycling delays final disposal, rather than avoids (Geyer et al., 2017b) it, since most of the plastics are recycled into lower-value applications that are not recycled again after use (MacArthur, 2017).

Plastic waste is a complex material mixture comprising a large group of individual polymers with different chemical and technical characteristics that hinder the recycling process (Eriksen et al., 2018; Faraca and Astrup, 2019; Ragaert et al., 2017). Moreover, post-consumer plastics contain organic and inorganic substances as contaminants that lead to a recycled plastic with poor material properties that (Eriksen et al., 2018), in turn, limits the applicability of the recycled plastic. Organic contaminants may degrade or migrate during recycling, while inorganic such as metals impurities and residues from catalysts may persist in the product after the recycling process (Eriksen et al., 2018).

There are two main types of plastic recycling: mechanical (primary and secondary) and chemical (tertiary) (Monteiro, 2018; Ragaert et al., 2017; Rudolph et al., 2017). The choice among both recycling methods depends on the degree of contamination of the plastics with organic or inorganic substances and also on the molecular structure of the plastic (Rudolph et al., 2017). Firstly, mechanical recycling is the most established method due to its low cost and high reliability (Monteiro, 2018; Pinto, 2012; Ragaert et al., 2017; Rudolph et al., 2017), keeping the polymer's structure basically intact (Rudolph et al., 2017). If the source of plastic waste is pre-consumer, therefore clean and without contamination, the primary mechanical recycling is used. Post-consumer plastic waste is highly contaminated and requires additional steps like collecting, sorting and cleaning (Ragaert et al., 2017; Rudolph et al., 2017). Figure 11 shows the steps included in the secondary mechanical recycling. After the plastic waste is collected, it is sorted based on size, colour, density and chemical composition and then it is baled for transport purposes. In order to remove the contaminants, the product is washed and then it passes through grinding and pelletizing to finally be transformed into raw materials for new plastics (Ragaert et al., 2017).



Figure 11: Steps of secondary mechanical recycling

Source: Based Ragaert et al. (2017)

The recyclability of plastics is determined by the design of the product and the degree to which they can incorporate recycled materials (Ragaert et al., 2017). “Design for Recycling” is heavily promoted by European Union within the concept of Circular Economy as a strategy to ensure that the products developed will be recycled at their end-of-life (Parliament, 2018). For the recyclability purpose, the plastic should “maintain its mechanical and chemical properties” (Worrell and Reuter, 2014) and “be able to be sorted by recycling companies” (Worrell and Reuter, 2014) in an acceptable cost-to-performance ratio (Worrell and Reuter, 2014).

Some plastics are more recycled than others. In order to assist their sorting prior to recycling, the resins present on the bottom of plastic packaging an identification code ranging from 01 to 07 in the following order (IEA, 2018): polyethylene terephthalate (PET), high-density polyethylene (HDPE), polyvinyl chloride (PVC), low-density polyethylene (LDPE), polypropylene (PP), polystyrene (PS), and others (O), which includes polycarbonate, acrylonitrile butadiene styrene, styrene acrylonitrile, polymethyl methacrylate, polyacrylonitrile, polyvinyl acetate, and many others.

As opposed to mechanical recycling, chemical recycling enables to recover the petrochemical components in plastics. It means that the polymers are chemically converted in monomers through a chemical reaction in the presence of a catalyst (Grigore, 2017). This process enables new polymerizations with the resulted monomers to reproduce the original polymer or a related polymeric product (Ragaert et al., 2017). Despite the advantage in achieving the quality of virgin polymer (Worrell and Reuter, 2014), chemical recycling has higher costs than mechanical recycling and requires a large scale to become economically feasible (Ragaert et al., 2017; Worrell and Reuter, 2014). Currently, this process is economically reasonable for polymers such as polyethylene

terephthalate (PET), polymethyl methacrylate (PMMA) and polyether ether ketone (PEEK) (Ragaert et al., 2017; Rudolph et al., 2017; Worrell and Reuter, 2014). However, as this is an energy-intensive and yet an emerging method, we will only consider mechanical recycling in our assessment.

3.3.2. Incineration

If plastic waste presents high degree of contamination, incineration is an option for plastic final disposal (Perugini et al., 2005). The main advantages of incineration process are the reduction need for landfill disposal, and the possibility of recovering energy to produce heat and electricity (Chen et al., 2019; Hou et al., 2018). The drawback of this method is the release of CO₂ to the atmosphere when plastics are burned (UK WIN, 2019). Also, in poor countries, plastic waste is incinerated in open fields for cooking or heat (Verma et al., 2016), exposing people to toxic and carcinogenic emissions such as chlorinated and brominated dioxins and furans for plastics containing chlorinated and brominated additives (GEF, 2018b; UN Environment, 2018). Even in developed countries with emission control plants, there is risk of exceeding the limit value for toxic emissions. Measurements in an incinerating plant in Norway have revealed that the emissions of dioxins, furans and other toxic pollutants were far beyond the limits set by the European laws (Zero Waste Europe, 2019). According to Hamilton et al. (2019), in 2019, the production and incineration of plastics will emit 850 Mt of GHG, equal to the emissions from 189 coal power plants. If the trend in plastic production and incineration continues, it is estimated that, in 2050, plastic alone could consume 10-13% of the total remaining carbon budget, undermining the efforts to keep warming below 1.5°C (Hamilton et al., 2019).

3.3.3. Long lifetime plastics

Plastic applications in construction usually lead to energy savings due to better insulation (SPI, 2016). Plastics usually presents ductility, thermal properties advantages, resistance to chemical attack, electric insulation properties, and light weight (Institute of Building Structures and Structural Design, 2013; PlasticsEurope, 2017; The Constructor, 2019b). Plastics in construction also reduce total costs, are easy to install and require minimal maintenance (PlasticsEurope, 2011). Besides, substituting traditional materials with lightweight plastic can result in indirect GHG emissions reduction in transportation

(Lackner, 2015). Hence, long-term applications of plastics in the construction sector could be an interesting solution to reduce waste generation of materials such as cement and steel²³. For instance, the Dutch PlasticRoad concept consists of a prefabricated and modular road structure based on recycled plastics (PlasticRoad, 2019). The expected lifetime of the PlasticRoad is two to three times longer than of traditional road paving and the expected construction time would be reduced by 70% (PlasticRoad, 2019). Due to longer lifespan and reduction of transport involved in its construction, PlasticRoad also presents a smaller carbon footprint than traditional road structures (PlasticRoad, 2019). Table 13 presents examples of plastic use in construction and building.

Table 13: Examples of plastic use in the construction industry

Use	Plastic
Façade Panels	Sandwich panels covering with PVC, plasticized plates and polyurethane foams;
Exterior covering	Polyester coated concrete by moulding from an existing plate; Epoxy resins and polyesters on various supporting media
Weather Boarding	Polyester; PVC; Polymethyl methacrylate
Windows	PVC casing on metal moulding; PVC/ wood; Polyester glass fibre and phenolic foam core
Wall Lining	Coating – polyvinyl acetate; Sprayed lining polyurethane; Wall tiles – polystyrene ; polyethylene
Roof Covering	Flat or corrugated sheets – polyester, PVC, polymethylmethacrylate; Gutters – Rigid PVC polyester
Sanitary Equipment	Sinks – polymethylmethacrylate, polyester, polyamides; Pipeworks – PVC; Showers – polymethylmethacrylate, polyester, polyethylene
Insulation	Polystyrene; PVC; Polyurethane
Damp-proofing	Polyethylene

Source: Based on The Constructor (2019a) and Rudolph et al. (2017)

Several studies (Al-Hadithi and Hilal, 2016; Jassim, 2017; Saikia and De Brito, 2012; Sule et al., 2017) have shown the applicability of waste plastic in the construction industry as cementitious based materials. In this case, recycled plastics are reused to substitute virgin materials in infrastructures. This scheme is advantageous since it reduces the concrete density, increases concrete's toughness behavior, improves the concrete's abrasion resistance, and increases concrete's thermal insulation properties (Saikia and De

²³ Substituting aluminium could perhaps reduce GHG emissions, but certainly not waste generation as aluminium has recycling rates around 98.00% in Brazil (ABAL, 2020).

Brito, 2012). Also in 2011, several companies have developed eco-plastic bricks that exceeded the performance of concrete walls when used in emergency rooms (SPI, 2016).

3.4.Methods

To test this hypothesis, this study assesses the carbon footprint of plastics. The case study was assessed for Brazil, since the country is, together with the USA, a world leader in ethanol production (RFA, 2017), presenting one of the lowest ethanol production costs (\$ 0.16–0.22/l) (Gupta and Verma, 2015). Also, Brazil is one of the world's major agricultural producer (MAPA, 2018a), and could become a competitive producer of bio-based plastics under stringent scenarios for GHG mitigation (Oliveira et al., 2020b).

This study focused on polymers derived from ethylene, since it is by far the most important building block in the petrochemical industry (Spallina et al., 2017b) and the most used plastic polymers in the world with applicability in the construction sector. The plastics studied are high-density polyethylene (HDPE)²⁴, polyvinyl chloride (PVC), polyethylene terephthalate (PET) and expanded polystyrene (EPS), covering 16.3%, 11.8%, 10.2% and 7.6% of the world's production, respectively (Geyer et al., 2017a).

GHG emissions from ethylene production and from intermediate products, polymerization, and transformation into final product, transportation and final disposal were accounted for each plastic. For the first plastic production step, four ethylene production routes were used according to a previous study of ours (Oliveira et al., 2020b): conventional steam cracking of naphtha; sugar-cane-derived ethanol to ethylene without bio-energy with carbon capture and storage (BECCS); sugar-cane-derived ethanol to ethylene with BECCS; and bio-methanol to olefin. For final disposal option it was considered incineration; incineration with energy recovery (plastic to energy, P2E); and recycling. Moreover, it was assessed the use of plastic for long-term application (construction & infrastructure) as a final disposal; and the substitution of emission-intensive material construction (cement, aluminum, steel, wood from eucalyptus planted forest and wood associated with deforestation in the Amazon) by a plastic material.

²⁴ Low-density polyethylene (LDPE) and linear low-density polyethylene (LLDPE) were not selected for the case study since their use as long-life time plastic (construction sector) is low (5.5%) (Geyer et al., 2017b) when compared to HDPE (20.2%) (Geyer et al., 2017b).

Landfilling is the main global final disposal for plastic packaging, followed by leakage to the environment, recycling and incineration, accounting for 40%, 32%, 14% and 14% in 2015, respectively (UN Environment, 2018). Nonetheless, landfilling was not considered in this study since it is the least preferred option for waste management²⁵(UN Environment, 2015) and it is not encouraged by policy (Chen et al., 2019). Also, despite recent efforts (Woods et al., 2016), LCA method still faces several challenges to assess the impacts of plastic mismanagement resulting in potential plastic pollution in the ocean environment.

The carbon footprints of HDPE, PVC, PET and EPS were assessed from cradle to grave using a mass-based allocation method based on principles of ISO 14067:2018(ISO, 2018). GHG emissions data were collected for the following life-cycle stages: production of ethylene, production of intermediate products, polymerization, transportation, transformation, and final disposal. Production of ethylene were used according to Oliveira et al. (2020b): conventional steam cracking of naphtha; sugar-cane-derived ethanol to ethylene without bio-energy with carbon capture and storage (BECCS); sugar-cane-derived ethanol to ethylene with BECCS; and bio-methanol to olefin. Transportation in all cases is assumed to be made by truck for a distance of 100 km. The specific consumption of diesel is 0.020 L/t.km (Nimana et al., 2017) and the emission factor for diesel combustion is 75.243 kg CO₂ eq/TJ (IPCC, 2006a). The steps of production of each plastic are described below, starting with the ones common to all: ethylene production and final disposal options. Then, each plastic production will be described separately.

Ethylene production

GHG emissions from each ethylene production route were based on Oliveira et al. (2020b) as shown in Table 14. Ethylene's emission factors were assumed for Brazil (Oliveira et al., 2020b; Seabra et al., 2011; Walter et al., 2015).

²⁵ Uncontrolled release of methane, soil and ground water contamination by leachate, unpleasant odors and spread of pathogenic microorganisms are some of the waste landfilling's drawbacks (European commission, 2011).

Table 14: GHG emissions for ethylene routes

Ethylene route	Emission Factor (t CO ₂ eq/ t ethylene)
Naphtha steam-cracking	1.02
Ethanol to ethylene w/ BECCS	0.16
Ethanol to ethylene w/o BECCS	-0.41
Bio-methanol to olefins	0.41

Source: Oliveira et al. (2020b)

Conversions from ethylene and other inputs to intermediate products and to polymers were calculated by mass accordingly to Figure 12.

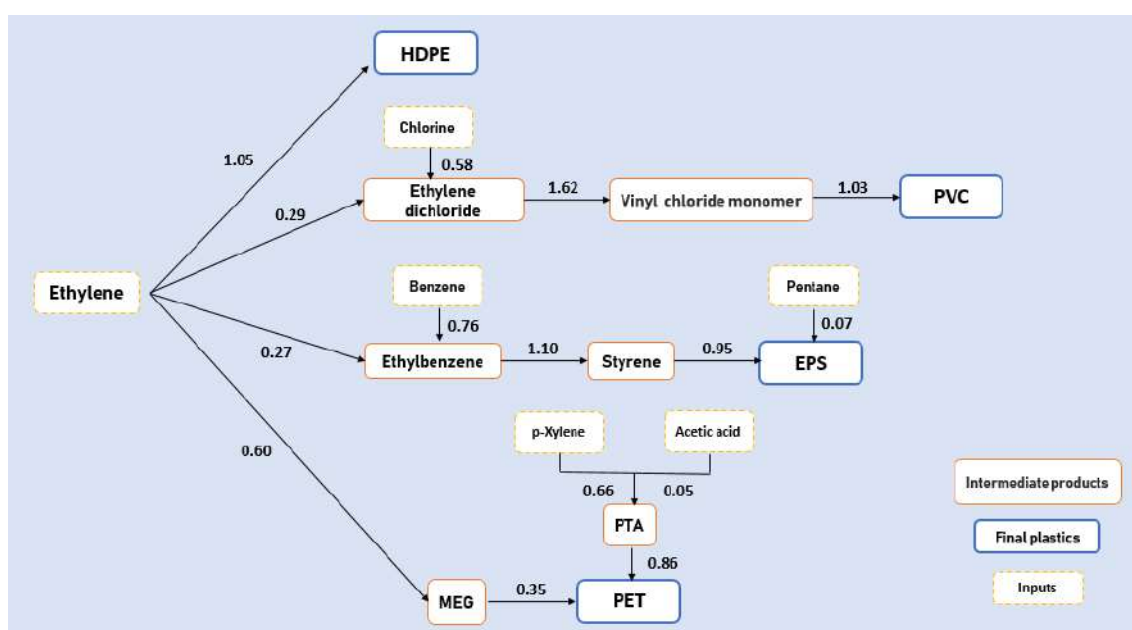


Figure 12: Mass conversions in tonne of feedstock per tonne of product considered for HDPE, PVC, PET and EPS production

Source: Based on Platts (2017) and Boulamanti and Moya (2017)

3.4.1. Final Disposal and Material Substitution

The basic options considered for final disposal in this study include: (i) incineration; (ii) mechanical recycling; and (iii) application in the construction and infrastructure sector (C&IF).

The incineration process can happen with or without energy recovery (plastic to energy, P2E). All carbon stored in HDPE, PVC, PET and PS is assumed to be released as CO₂ in the incineration process. The repeating unit of HDPE is ethylene (C₂H₄) whose molar

mass is 28 g/mol/g. Stoichiometrically, if burned, one molecule of ethylene emits two molecules of CO₂, i.e., 3.14 g CO₂/ g ethylene ($2 \times 44 / 28$). By analogy, it was calculated CO₂ emissions for each type of plastic when incinerated, according to Table 15.

Plastic to energy (P2E) is considered when the incineration process recovers energy from the plastic burning in a cogeneration plant (CHP) and uses it to produce electricity. The heat produced by each plastic is accounted for by their respective lower heating value (LHV). The incinerator electricity generation efficiency was assumed as 23% (WRAP, 2008). The Brazilian grid emission factor is used to estimate the avoided CO₂ emissions (0.58 tCO₂/MWh) (MCTIC, 2017a). Table 15 **Error! Reference source not found.** shows the lower heating value (LHV), the amount of electricity generated and emissions avoided from the grid for the P2E option. It is worth noting that incinerating plastics with energy recovery would mitigate emissions in the system “P2E – grid”, even though this final disposal option increases marginally grid emissions.

Table 15: Incineration emission factors, LHV and electricity generated for HDPE, PVC, PET and EPS

Plastic	Repeating unit (molar mass in g/mol/g)	N° of CO ₂ molecules released	LHV (MJ/kg)	Electricity generated (MJ/kg plastic)	Emission factor incineration (t CO ₂ /t plastic)	Non-emitted CO ₂ from the grid due to P2E (t CO ₂ /t plastic)
HDPE	C ₂ H ₄ (28)	2	42.47	9.77	3.14	1.59
PVC	C ₂ H ₃ Cl (62)	2	21.51	4.95	1.42	0.81
PET	C ₁₀ H ₈ O ₄ (192)	10	22.95	5.28	2.29	0.86
EPS	C ₈ H ₈ (104)	8	38.67	8.89	3.38	1.45

For the mechanical recycling option, the waste plastic needs to be shredded, extruded, and agglomerated. Electricity consumption of each step of mechanical recycling is shown in Table 16. It was assumed 10% of material loss (Rossi et al., 2015) in each recycling cycle, meaning that 1 kg of recycled plastic avoids producing 0.9 kg of virgin plastic and its related emissions.

Plastics undergo some degradation in each recycling cycle and the impurities may become concentrated after subsequent cycle (Rigamonti et al., 2018; WRAP, 2008), limiting the number of cycles that they can afford (Rigamonti et al., 2018). Therefore, recycling does not guarantee that the plastic will return to the cycle with the same quality (Dilkes-

Hoffman et al., 2019; Flock, 2018). For a closed-loop consideration, this study assumed only one recycling cycle for each plastic, following the method adopted by Shonfield (2008).

Table 16: Electricity consumption for plastic's mechanical recycling

Recycling step	Electricity consumption (kWh/t plastic)
Shredding	24
Extruders	270
Agglomerators	175
Total	469

After one closed-loop recycling cycle, the plastic must be diverted towards another final disposal option. Hence, this study considered the association of recycling with incineration and with waste plastic post-application in long lifetime materials, called herein Construction & Infrastructure (C&IF). Plastic use in C&IF assumes that the carbon will be locked in for the period the infrastructure exists. Moreover, the plastic could substitute traditional construction materials (cement, aluminum, steel, and wood), reducing CO₂ emissions in the C&IF sector. Regarding the use of wood in the construction sector, this study assumed the use of eucalyptus that already accounts for 72% (Indústria Brasileira de Árvores, 2017) of all planted forests in Brazil, and also wood associated with deforestation in the Amazon. The emission factors of eucalyptus wood and of wood associated with deforestation were calculated based on the wood volume of the forest (290 m³/ha (Angelkorte, 2019; Santos et al., 2017) and 180 m³/ha (Araujo, 2006), respectively), the basic density of the wood (0.49 g/cm³ (Oliveira et al., 2005) and 0.65 g/cm³ (Silveira et al., 2013), respectively), and the emission factor from silviculture of eucalyptus and from deforestation-induced land-use change (-61 tCO₂eq/há (Sato et al., 2019; Zimmer et al., 2013) and 94.2 tCO₂eq/ha (Köberle, 2018a), respectively). It worth noting that the use of wood from planted forest in the construction sector can also act as carbon sink as discussed in Churkina et al. (2020). However, in Brazil, exploitation of illegal wood is still representative, being the Amazon forest the main affected by this activity (Governo de São Paulo, 2019; Rochedo et al., 2018). For instance, in 2017, 60% of the wood exploration in the State of Pará was illegal (Imazon, 2019).

Every material replaced by the bioplastic would count as a CO₂ credit for avoiding the emission factor of its production (see Table 17).

Table 17: Emission factor of cement, aluminium, steel and wood

Construction material	Emission factor (t CO ₂ eq/ t material)
Cement	0.58
Aluminium	4.44
Steel	1.84
Wood	-0.43
Wood (deforestation)	0.80

Source: MCTIC (2017b) and Costa (2012)

It was assumed that plastics could substitute cement, aluminum, steel and wood in a mass or volume 1:1 proportion, according to Table 18. If an 1:1 (v/v) proportion was assumed, the new emission factors were calculated based on the materials bulk density rates (see Table 19). It is worth noting that the material substitution rate and the selection of plastics for long-term material assumed here is a simplification method used to calculate the impacts of this measure on GHG emissions. The values adopted are fairly conservative, given that we considered only a small share of construction materials widely used and that plastics would not be an alternative for structural, load-bearing materials. A more detailed evaluation of the use of plastics in infrastructure should be conducted to refine the results of this mitigation measure.

Table 18: Material substitution examples and assumptions

	HDPE	PVC	PET	EPS
Cement	1:1 (m/m) Plastic cement(Jassim, 2017)	1:1 (v/v) Water and Sewage Pipes (FICCI, 2017)	1:1 (m/m) Concrete†(Prasad and Jaysawal, 2017)(Sulyman et al., 2016)	1:1 (v/v) EPS concrete, Floor and wall panels (Doran and Cather, 2014; Ede, 2015; SPI, 2016)
Aluminum	1:1 (v/v) Showers, Cabinets	1:1 (v/v) Pipes, Windows(SPI, 2016)	1:1 (v/v) Cabinets	N/A
Steel	1:1 (v/v) Non-structural applications*	1:1 (v/v) Non-structural applications*	1:1 (v/v) Non-structural applications*	N/A
Wood	1:1 (v/v) Flooring, Windows, Cabinets	1:1 (v/v) Flooring, Windows, Cabinets(Xue, 2011)	1:1 (v/v) Flooring, Windows, Cabinets	1:1 (v/v) Door linings and frames
Wood (deforestation)	1:1 (v/v)	1:1 (v/v) Flooring, Windows,	1:1 (v/v) Flooring, Windows, Cabinets	1:1 (v/v) Door linings and frames

Flooring, Windows, Cabinets	Cabinets(Xue, 2011)
-----------------------------------	------------------------

†Partially substitute cement in concrete. *Non-structural applications such as rack systems, mobile homes, gutters, chimney liners, among others.

Table 19: Construction and infrastructure materials densities

Material	Bulk density (kg/m³)
<u>Plastics</u>	
HDPE	941-970 (Doran and Cather, 2014)
PVC	1380-1500 (Doran and Cather, 2014)
PET	1380 (Doran and Cather, 2014)
EPS	10-50 (Doran and Cather, 2014)
<u>Construction materials</u>	
Cement	1440 (The Constructor, 2019c)
Aluminum	2700 (Doran and Cather, 2014)
Steel	7850 (Doran and Cather, 2014)
Wood	490 (Oliveira et al., 2005)
Wood (deforestation)	650 (Silveira et al., 2013)

In sum, this article evaluated the following plastics' final disposal options:

- Incineration (INC);
- Plastic to Energy (P2E);
- Recycling + Incineration (R+INC);
- Recycling + Construction & Infrastructure (R + C&IF);
- Construction & IF (C&IF);
- Construction & IF + Cement substitution (C&IF + CS);
- Construction & IF + Aluminium substitution (C&IF + AS);
- Construction & IF + Steel substitution (C&IF + SS);
- Construction & IF + Wood substitution (C&IF + WS);
- Construction & IF + Wood (deforestation) substitution (C&IF + WDS).

3.4.2. Carbon footprint of plastics

Figure 13-Figure 16 present the life-cycle system boundaries assessed for HDPE, PVC, PET and EPS production, respectively. For HDPE production (Figure 13), emissions from ethylene polymerization were estimated by deducting from HDPE cradle to gate GHG emissions (1.20 tCO₂/ t HDPE) (Ecoinvent Centre, 2015) by ethylene monomer cradle to gate GHG emissions, calculated based on Oliveira et al. (2020b). Electricity consumption for the transformation process was based on the injection-molding process (1.47 kWh/kg HDPE) (Ecoinvent Centre, 2015). Estimated carbon footprint of HDPE is shown in

Table 20.

For PVC production (Figure 14), GHG emissions from chlorine production were calculated based on the electricity demand of a chlor-alkali electrolyser (3000 kWh/ t product), attributing 48% of mass allocation to chlorine. Electricity consumption for EDC and VCM production was based on Boulamanti and Moya (2017) (0.08 MWh/ t EDC and 0.53 MWh/ t VCM, respectively). Energy for EDC and VCM production was assumed to be produced by a fuel oil boiler with an efficiency of 85%, consuming 5.30 MJ/ t EDC (Boulamanti and Moya, 2017) and 5.03 MJ/ t VCM (Boulamanti and Moya, 2017) thermal energy. Emission factor of fuel oil is based on IPCC (2006b). Polymerization in suspension was assumed with a steam consumption of 2.5 GJ/ t PVC (ComanițĂ et al., 2016), being generated by a fuel oil boiler with an efficiency of 85%, while electricity consumption was based on ComanițĂ et al. (2016) (0.9 GJ/ t PVC). Pipe extrusion was considered for the transformation step, consuming 1.08 MWh/ t PVC of electricity. Estimated carbon footprint of PVC is shown in Table 21.

Electricity consumption for ethylene oxide and MEG (Figure 15) was based on Boulamanti and Moya (2017) (0.33 MWh/ t ethylene oxide and 0.08 MWh/ t MEG, respectively). Fuel oil consumption for ethylene oxide and MEG production was assumed as 3.1 MJ/ kg ethylene oxide (Boulamanti and Moya, 2017) and 9.1 MJ/ kg PET (Boulamanti and Moya, 2017). For PTA production, it was assumed 0.25 MWh/ t PTA of electricity consumption and steam consumption of 3.87 MJ/ kg PTA, which is produced by fuel oil boiler with an efficiency of 85%. Emission factor of fuel oil is based on IPCC (2006b). Cradle to gate GHG emissions for p-xylene was based on PlasticsEurope (2013) (1.43 t CO₂eq/t p-xylene) and for acetic acid was estimated based on CPME (2016) (0.08 t CO₂eq/t PTA). Steam consumption for PET polymerization was assumed as 2.71 GJ/ t PET (CPME, 2017), being generated by a fuel oil boiler with an efficiency of 85%, while electricity consumption was assumed as 0.19 MWh/ t PET (CPME, 2017). Gate to gate GHG emissions of subsequent polymerization step (solid-state polymerization) was also included in the PET polymerization step (0.10 t CO₂eq/ t PET) (Shen et al., 2011). Blow molding was considered for the transformation step, consuming 1.47 MWh/ t PET of electricity. Estimated carbon footprint of PET is shown in Table 22.

Cradle to gate GHG emissions for benzene (Figure 16) was based on PlasticsEurope (2013) (1.86 t CO₂eq/t benzene) and for pentane was based on PlasticsEurope (2005) (1.4 t CO₂eq/t benzene). Electricity consumption for ethylbenzene and styrene was based on Boulamanti and Moya (2017) (0.03 MWh/ t ethylbenzene and 0.12 MWh/ t styrene, respectively). Steam consumption for ethylbenzene and styrene production was assumed as 2.98 GJ/ t ethylbenzene (Boulamanti and Moya, 2017) and 6.57 GJ/ t styrene (Boulamanti and Moya, 2017), respectively, being generated by a fuel oil boiler with an efficiency of 85%. For EPS production, it was assumed an electricity consumption of 0.16 MWh/ t EPS (PlasticsEurope, 2015) and steam consumption of 1.29 GJ/ t EPS (PlasticsEurope, 2015). In addition, it was considered that the steam would be generated by a fuel oil boiler with an efficiency of 85%. Estimated carbon footprint of EPS is shown in Table 23.

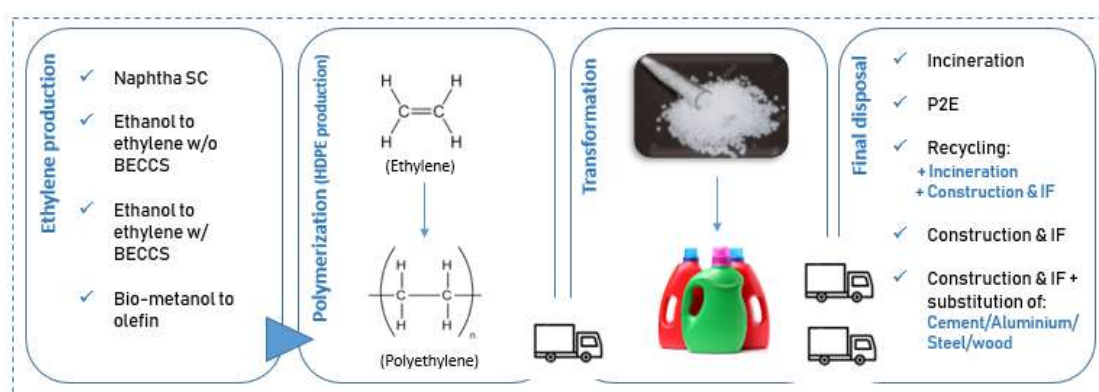


Figure 13: Life-cycle system boundaries for HDPE production

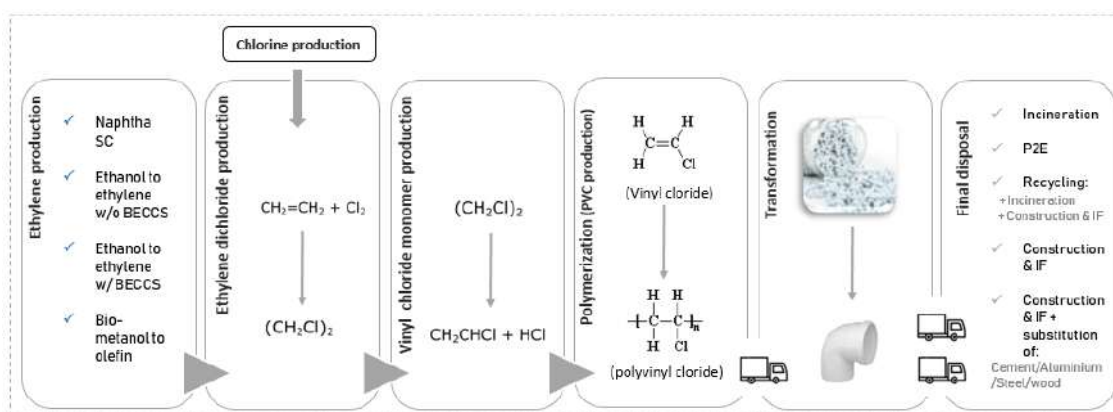


Figure 14: Life-cycle system boundaries for PVC production

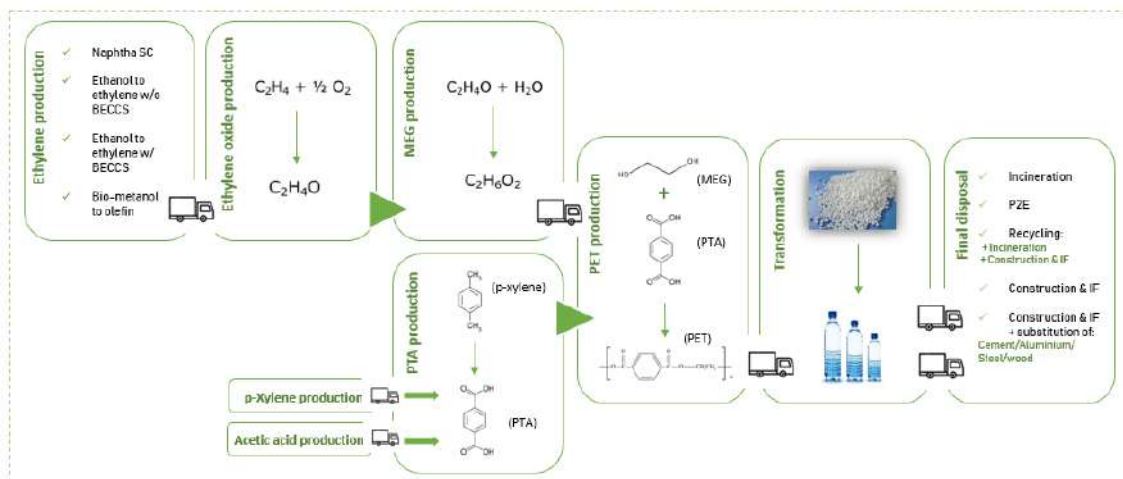


Figure 15: Life-cycle system boundaries for PET production

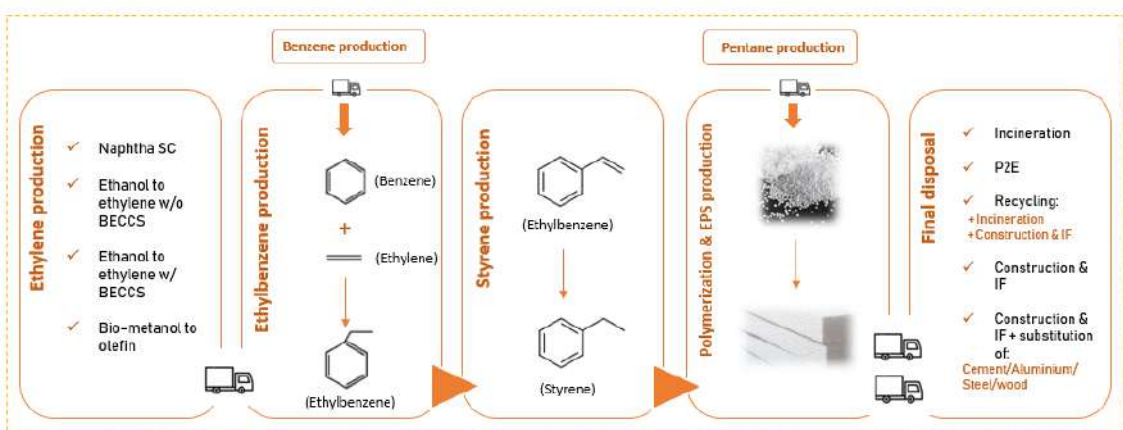


Figure 16: Life-cycle system boundaries for EPS production

Table 20: Carbon footprint of HDPE

Steps	Emission factor (tCO₂eq/ t HDPE)
Ethylene production	
Naphtha steam-cracking	1.07
Ethanol to ethylene w/o BECCS	0.18
Ethanol to ethylene w/ BECCS	-0.42
Bio-methanol to olefins	0.43
Polymerization	0.13
Transportation to transformation	0.01
Transformation	0.86
Transportation to distributors	0.01
Transportation to final disposal	0.01
Final disposal	
Recycling	0.28
Incineration	3.14
P2E	1.55
Construction & IF	0.00

Source: Oliveira et al. (2020b), Platts, (2017), Boulamanti and Moya (2017), MCTIC (2017a), Shonfield (2008), Nimana et al. (2017)

Table 21: Carbon footprint of PVC

Steps	Emission factor (tCO₂eq/ t PVC)
Ethylene production	
Naphtha steam-cracking	0.48
Ethanol to ethylene w/o BECCS	0.08
Ethanol to ethylene w/ BECCS	-0.19
Bio-methanol to olefins	0.19
Chlorine production	0.51
EDC production	0.89
VCM production	0.56
Polymerization	0.37
Transportation to transformation	0.01
Transformation	0.64
Transportation to distributors	0.01
Transportation to final disposal	0.01
Final disposal	
Recycling	0.28
Incineration	1.42
P2E	0.61
Construction & IF	0.00

Source: Oliveira et al. (2020b), Platts (2017), Boulamanti and Moya (2017), MCTIC (2017a), Shonfield (2008), Nimana et al. (2017)

Table 22: Carbon footprint of PET

Steps	Emission factor (tCO₂eq/ t PET)
Ethylene production	
Naphtha steam-cracking	0.21
Ethanol to ethylene w/o BECCS	0.03
Ethanol to ethylene w/ BECCS	-0.09
Bio-methanol to olefins	0.09
Ethylene transportation	0.01
Ethylene oxide production	0.05
Ethylene oxide transportation	0.01
MEG production	0.02
MEG transportation	0.01
p-xylene production	0.81
p-xylene transportation	0.01
Acetic acid production	0.07
Acetic acid transportation	0.01
PTA production	0.13
Polymerization	0.21
Transporte to transformation	0.01
Transformation	0.86
Transportation to distributors	0.01
Transportation to final disposal	0.01
Final disposal	
Recycling	0.28
Incineration	2.29
P2E	1.43
Construction & IF	0.00

Source: Oliveira et al. (2020b), Platts (2017), Boulamanti and Moya (2017), MCTIC (2017a), Shonfield (2008), Nimana et al. (2017)

Table 23: Carbon footprint of EPS

Steps	Emission factor (tCO₂ eq/ t EPS)
Ethylene production	
Naphtha steam-cracking	0.28
Ethanol to ethylene w/o BECCS	0.04
Ethanol to ethylene w/ BECCS	-0.12
Bio-methanol to olefins	0.11
Ethylene transportation	0.01
Benzene production	1.48
Benzene transportation	0.01
Ethylbenzene production	0.30
Styrene production	0.64
Pentane production	0.10
Pentane transportation	0.01
EPS production	0.09
Transportation to distributors	0.01
Transportation to final disposal	0.01
Final disposal	
Recycling	0.28
Incineration	3.38
P2E	1.94
Construction & IF	0.00

Source: Oliveira et al. (2020b), Platts (2017), Boulamanti and Moya (2017), MCTIC (2017a), Shonfield (2008), Nimana et al. (2017)

3.5. Results and discussions

Figure 17Figure 24 present the carbon footprint of each plastic for the options that achieve the highest (ethylene from steam cracking of naphtha) and the lowest (ethanol to ethylene with BECCS) life-cycle GHG emissions. The results that include ethanol to ethylene without BECCS and bio-methanol to olefins routes can be found in Annex A. Table 24 presents the options that achieve the highest and lowest carbon footprints (with and without credits) and the corresponding final disposal options for all the plastics assessed. In our study, the difference between “Total emission with credits” and “Total emission without credits” stands for the CO₂ credits accounted (or not) for material substitution;

for avoiding ethylene production and transportation when the waste plastic is recycled; and for avoiding electricity generation in P2E. These credits are not considered in “Total emissions without credits”, which aims to reveal in which cases bioplastics achieve negative emissions i.e. when life-cycle emissions do not surpass photosynthetic CO₂ capture, thus effectively removing CO₂ from the atmosphere. Also, CO₂ capture was disaggregated in the results so steps’ emissions, credits and capture could be compared.

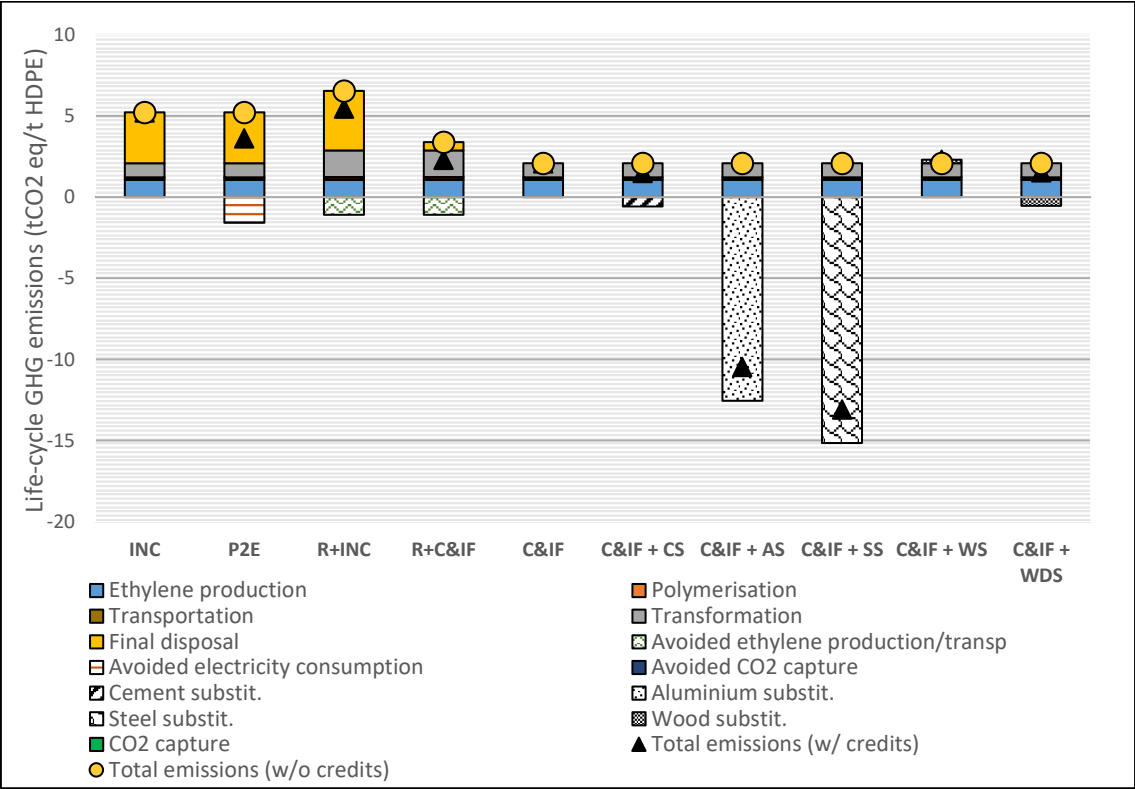


Figure 17: Carbon footprint for HDPE (ethylene from steam cracking of naphtha)

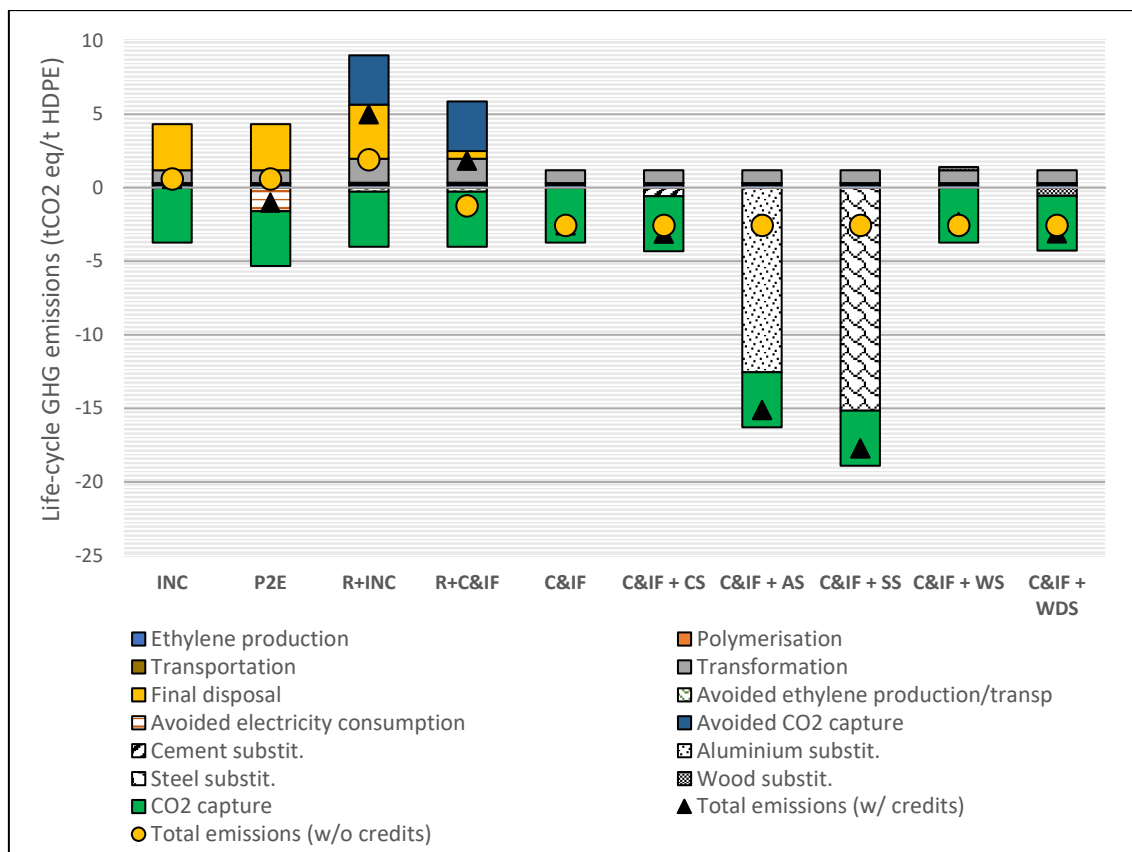


Figure 18: Carbon footprint for HDPE (ethanol to ethylene with BECCS)

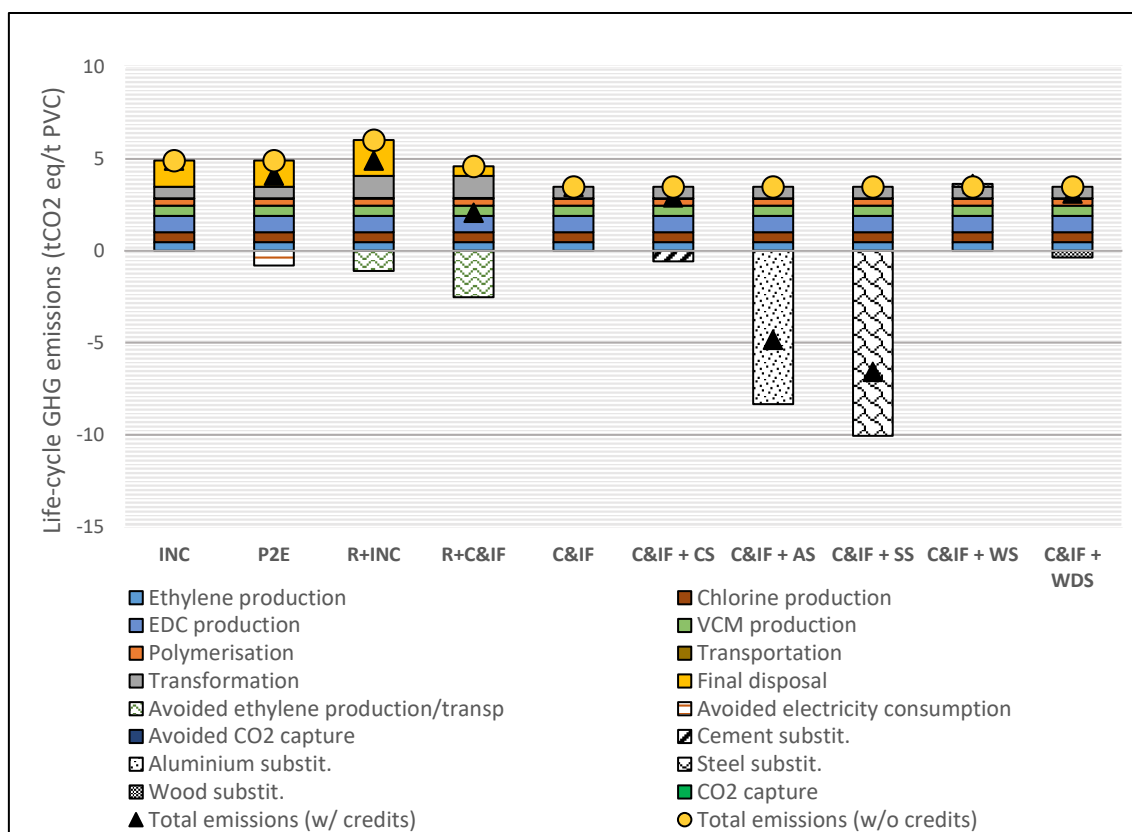


Figure 19: Carbon footprint for PVC (ethylene from steam cracking of naphtha)

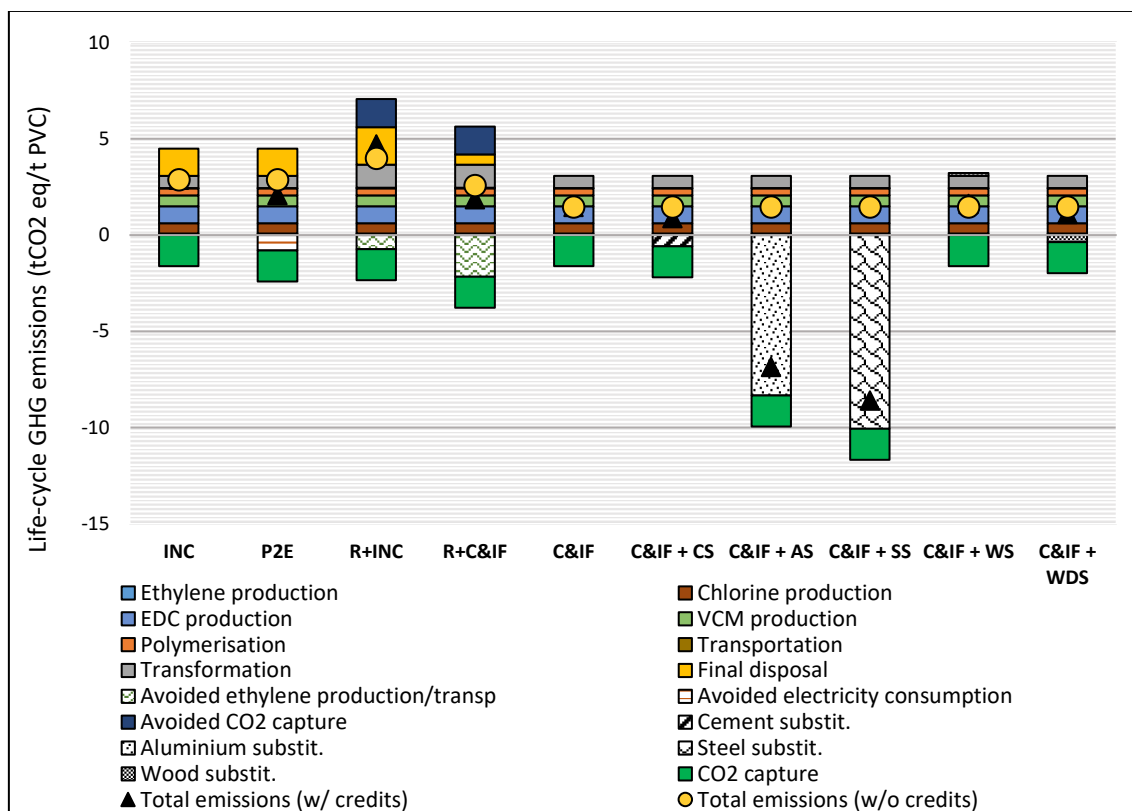


Figure 20: Carbon footprint for PVC (ethanol to ethylene with BECCS)

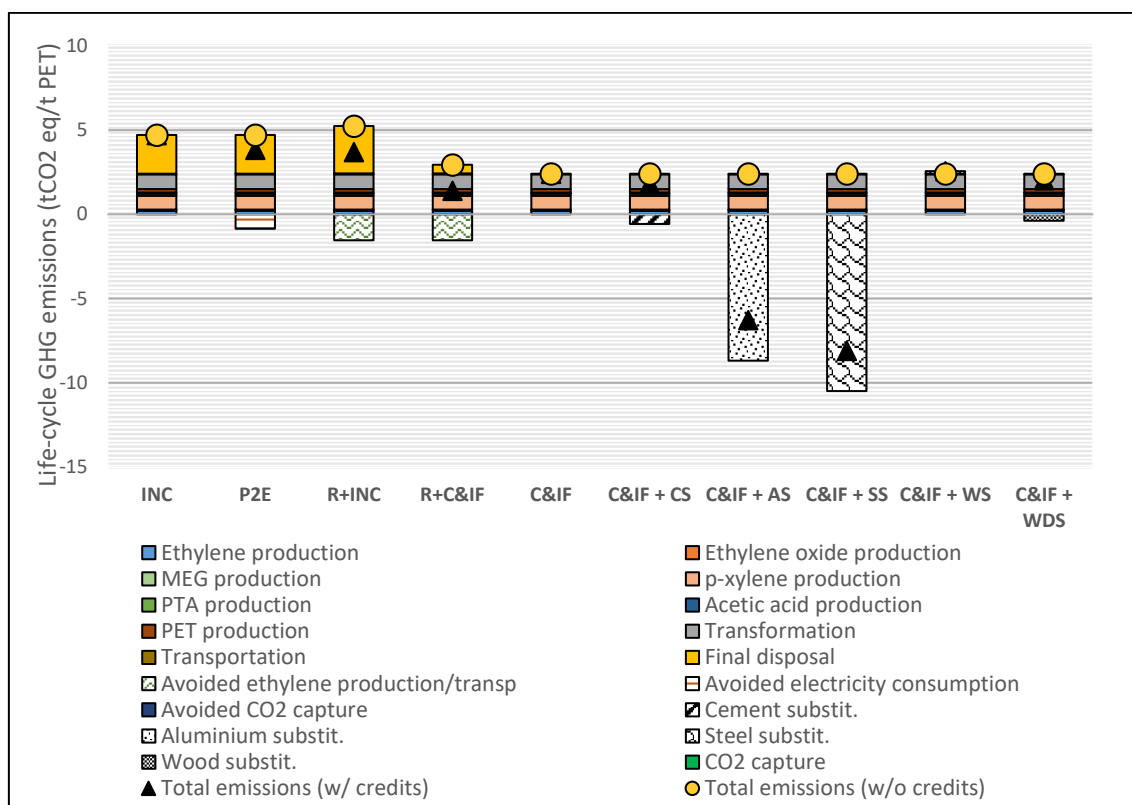


Figure 21: Carbon footprint for PET (ethylene from steam cracking of naphtha)

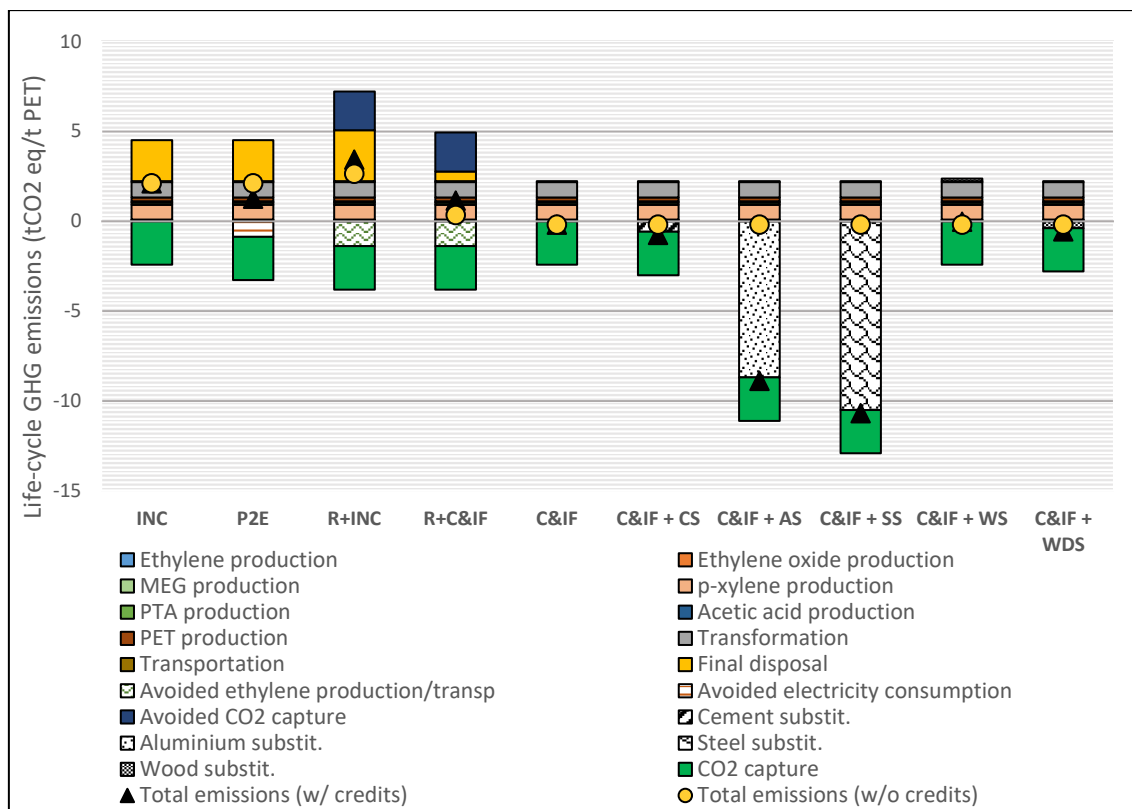


Figure 22: Carbon footprint for PET (ethanol to ethylene with BECCS)

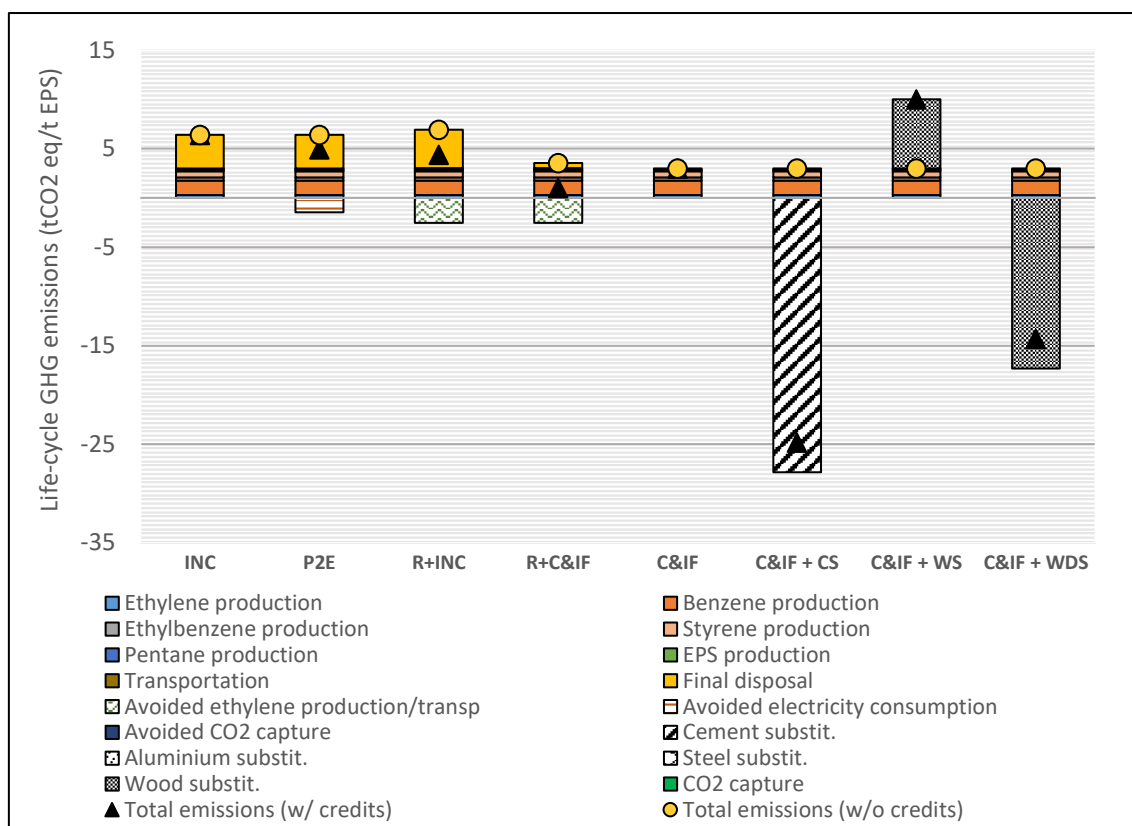


Figure 23: Carbon footprint for EPS (ethylene from steam cracking of naphtha)

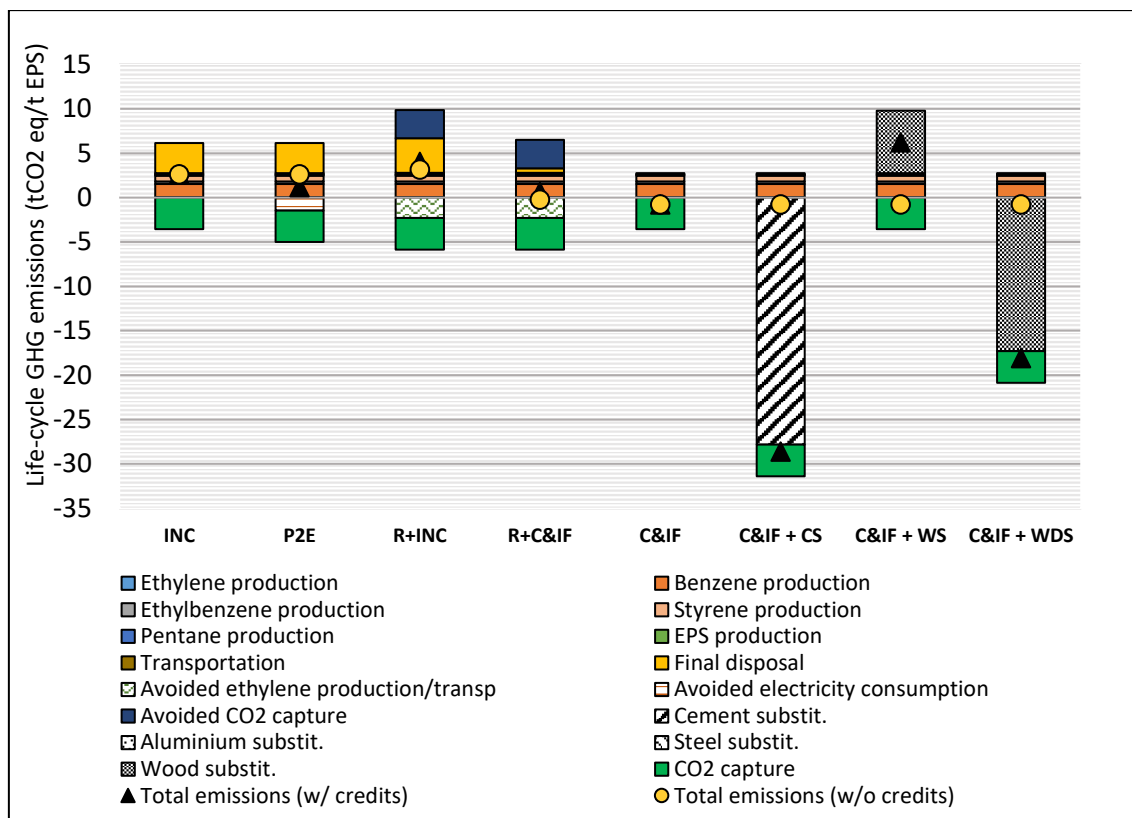


Figure 24: Carbon footprint for EPS (ethanol to ethylene with BECCS)

The results presented in Figure 17Figure 24 and in Annex A show that the routes that could be considered NETs are the ones in which the “Total emissions w/o credits” is below zero. NETs are only achieved in bio-based HDPE, PET and EPS production and the best case is always when ethylene is produced from sugarcane ethanol with BECCs and the final disposal option is the C&IF sector.

The exception therefore is bio-based PVC. For bio-based plastics production, 3.14 t CO₂/t HDPE, 1.42 tCO₂/t PVC, 2.29 tCO₂/t PET and 3.38 tCO₂/t EPS are captured in sugarcane cultivation. In bio-PVC production, because bio-based ethylene makes up for just a small portion of PVC’s molecular weight, life-cycle emissions surpass the CO₂ photosynthetic capture. Therefore, the production of bio-based PVC in Brazil may never result in negative emissions, unless EDC, VCM and Chlorine production emissions could be substantially reduced.

In some cases, where mitigation efforts surpass life-cycle emissions, net negative values are achieved. Though they do not represent negative emissions, it is implied that the overall emissions are reduced due to avoided feedstock production, electricity

consumption or traditional energy-intensive construction materials production. This is the case for all fossil-based plastics applied in the C&IF sector substituting: (i) aluminum or steel for HDPE, PVC and PET; and (ii) cement or deforestation wood for EPS.

When considering emissions with credits, the worst case (highest emission option) is the “Recycling + Incineration” option for all plastics and feedstocks assessed, except for fossil-based PET (worst case: “Incineration”) and fossil and bio-based EPS (worst case: “Construction & IF + Wood substitution”). For fossil-based plastics, “Recycling + Incineration” is usually the highest due to the 1-cycle recycling assumption, which makes recycling emissions surpass credits from avoided ethylene production. In other words, emissions from incineration are only postponed and avoided virgin material production emissions are not that relevant. When considering that plastics undergo more recycling cycles, recycling final disposal options tend to become less emission-intensive.

Also, “Recycling + incineration” option for bio-based plastics achieves higher carbon footprint when credits are considered because of the demand reduction of virgin bio-based ethylene (from ethanol or bio-methanol). Thus, it reduces the potential of carbon capture from sugarcane cultivation and BECCS. In addition, the more recycling cycles bioplastics undergo, the more carbon capture is avoided, which means that, for bio-based plastics, recycling is not the best final disposal when negative carbon emissions are the goal.

For fossil and bio-based EPS, “Construction & IF + Wood substitution” is the worst case when considering credits because of the lower bulk density of EPS compared to other plastics. Since wood from planted forests capture $-0.43 \text{ tCO}_2/\text{t wood}$, less carbon is captured if it is substituted in volume by EPS. On the other hand, when considering credits, the highest capture and mitigation option achieved is when EPS is produced from bio-ethylene with CCS and applied in “Construction & IF” substituting cement, also because of its light-weight property.

Finally, when BECCS in the ethanol production are considered for bio-based plastics, the carbon footprint of bio-ethylene is lower ($-0.41 \text{ t CO}_2 \text{ eq/ t ethylene}$) than the one without BECCS ($0.16 \text{ t CO}_2 \text{ eq/ t ethylene}$), as reported in Table 14. This negative emission potential in the bio-ethylene production step accumulates into the bio-based plastic production sequential steps. Then, options that include “construction & IF” preserve the

net negative emission potential of bio-based plastics, since they store biogenic carbon. Therefore, the best case for each ethylene derivative plastic is based on bio-ethylene produced with BECCS.

For illustration, considering a baseline scenario for HDPE demand (1.5% a.a. starting in 2010) and also considering that by 2050 this demand will be covered 100% by bio-based HDPE, 32.35 MtCO₂ of accumulated NETs will be achieved if the use of HDPE in construction increases 2.0 % p.a. in the same period. In this example, NETs represents less than 1% of the BECCS required to meet targets consistent with Brazil's contribution to a 2 °C world (Rochedo et al., 2018).

The results indicate that the advantages of bio-based plastic and even fossil-based plastic are enhanced by their use in long-lifetime materials. As of today, the main destination of plastics is not for construction purposes. However, under the desired carbon transition focus, the associated material transition could be based on the production of biodegradable plastics with short lifetime from biomass, and the production of the basic plastics oriented towards constructive uses. There would be room for this needed material transition in the desired low carbon transition, which will depend on growing materials demands to build the new renewable-based energy conversion facilities, the infrastructure for big data and energy transmission networks (fibers), and the smart buildings, cities and mobility. This means a transition in materials along with the low carbon transition.

Table 24: Carbon footprints of HDPE, PVC, PET and EPS

	Highest GHG emission option				Lowest GHG emission option			
	With credits	FD	Without credits	FD	With credits	FD	Without credits	FD
HDPE	tCO₂/t HDPE							
Steam-cracking of naphtha	5.45	R+INC	6.54	R+INC	-13.08	C&IF + SS	2.08	C&IF
Ethanol to ethylene w/o BECCS	5.05	R+INC	2.50	R+INC	-17.11	C&IF + SS	-1.95	C&IF
Ethanol to ethylene w/ BECCS	4.99	R+INC	1.91	R+INC	-17.71	C&IF + SS	-2.55	C&IF
Bio-methanol	5.07	R+INC	2.76	R+INC	-16.86	C&IF + SS	-1.70	C&IF
PVC	tCO₂/t PVC							
Steam-cracking of naphtha	4.91	R+INC	6.01	R+INC	-6.57	C&IF + SS	3.48	C&IF
Ethanol to ethylene w/o BECCS	4.73	R+INC	4.19	R+INC	-8.40	C&IF + SS	1.66	C&IF
Ethanol to ethylene w/ BECCS	4.71	R+INC	4.00	R+INC	-8.59	C&IF + SS	1.47	C&IF
Bio-methanol	4.74	R+INC	4.31	R+INC	-8.28	C&IF + SS	1.78	C&IF
PET	tCO₂/t PET							
Steam-cracking of naphtha	4.70	INC	5.24	R+INC	-8.09	C&IF + SS	2.41	C&IF
Ethanol to ethylene w/o BECCS	3.45	R+INC	2.77	R+INC	-10.56	C&IF + SS	-0.06	C&IF
Ethanol to ethylene w/ BECCS	3.44	R+INC	2.65	R+INC	-10.68	C&IF + SS	-0.18	C&IF
Bio-methanol	3.45	R+INC	2.82	R+INC	-10.51	C&IF + SS	-0.01	C&IF
EPS	tCO₂/t EPS							
Steam-cracking of naphtha	10.02	C&IF + WS	6.92	R+INC	-24.84	C&IF + CS	3.00	C&IF
Ethanol to ethylene w/o BECCS	6.39	C&IF + WS	3.30	R+INC	-28.46	C&IF + CS	-0.62	C&IF
Ethanol to ethylene w/ BECCS	6.23	C&IF + WS	3.14	R+INC	-28.62	C&IF + CS	-0.78	C&IF
Bio-methanol	6.46	C&IF + WS	3.37	R+INC	-28.39	C&IF + CS	-0.55	C&IF

FD: Final disposal option; INC: Incineration; P2E: Plastic to Energy; R+INC: Recycling + Incineration; R+C&IF: Recycling + Construction & IF; C&IF: Construction & IF; C&IF+CS: Construction & IF + Cement substitution (C&IF + CS); C&IF+AS: Construction & IF + Aluminium substitution; C&IF+SS: Construction & IF + Steel substitution; C&IF+WS: Construction & IF + Wood substitution (C&IF + WS); C&IF+WDS: Construction & IF + Wood (deforestation) substitution (C&IF + WDS).

3.6. Conclusions

Our findings show that using plastics as long life-time material could lead to net negative GHG emissions (NETs), depending on the feedstock, the polymer and the strategy for its final disposal. Fossil-based plastics could also mitigate GHG emissions when credits are accounted for material substitution in the construction sector. Therefore, the final disposal of the polymer is more relevant than its feedstock when emissions reduction in plastic life-cycle is desired. Particularly, in times of climate emergency, an opportunity arises in producing plastics for long-term applications to reduce the carbon footprint. Therefore, low carbon transition policies should be developed to promote the use of plastic in the construction sector, placing the chemical sector as potential enabler of NETs, and the use of biodegradable plastics for short-lifetime applications.

Results also show that bio-based HDPE, bio-based PET and bio-based EPS can be considered NETs when used in the construction sector. For PVC, negative values in emissions balance were achieved only when accounting the substitution of aluminium and steel for fossil-based PVC or any other material for bio-based PVC. This indicates that bio-based PVC may mitigate but not achieve negative emissions.

For fossil-based plastics, negative values in emissions balance are achieved only when it is used in construction, substituting the aluminum and steel content, indicating an interesting mitigation strategy for the fossil-based plastics industry. Actually, these final disposal options represent the lowest carbon footprint of three out of the four plastics (HDPE, PVC, PET) and for all ethylene production routes assessed (steam cracking of naphtha, ethanol to ethylene without BECCS, ethanol to ethylene with BECCS, bio-methanol to olefins). This result was expected since the emission factors of aluminium and steel production are higher than those associated with the other materials assessed. On the other hand, since it is unlikely that EPS substitute aluminium or steel extensively, we excluded it from our analysis. Hence, the lowest carbon footprint options for EPS is when it substitutes cement and deforestation wood.

Even though our study has a global scope and could be reproduced to other countries, the assumption of replacing wood by plastics in construction is very specific for Brazil as the illegal wood exploitation is much above world average.

Recycling one time (without plastic downcycling) and then addressing the plastic waste to incineration was the worst option in terms of carbon footprint, not considering credits, for all types of (bio-based and fossil) plastics assessed. Recycling, in this case, delays rather than avoids emissions from final disposal. It is worth noting that the use of plastics in C&IF sector delays around 35 years (or more) their final disposal, therefore addressing the critical issue of reducing emissions in the short-term. Additionally, it is easier to permanently dispose the plastics concentrated in one use (C&IF), in scale and location, than in a dispersed manner such occurs with single-use plastics.

Considering the recycling as final disposal, life-cycle GHG emissions of bio-based plastics are higher when credits are included than when they are not. Each recycling cycle avoids the production of virgin bio-based ethylene, which, in turn, avoids the capture of biogenic carbon from biomass cultivation. Therefore, in terms of GHG emissions, recycling makes sense only for fossil-fuel based plastics. Our study assumed that the recycling of fossil-based plastics replaces virgin fossil-based plastics and the recycling of bio-based plastics replaces virgin bio-based plastics, which is a limitation of our study since the recycling of the bio-based plastics replaces mostly fossil-based virgin materials. Still, applying it in the construction & IF sector is a better option, except for EPS when substituting planted forest wood. Furthermore, the analysis did not consider indirect environmental benefits provided by a greater participation of plastics in the construction & IF sector, such as better insulation, which could reward extra carbon credits for reduction of fuel consumption.

Although bio-based ethylene and bio-based HDPE is already produced by Braskem in Brazil (Braskem, 2020), the cost of bio-based plastics production will hardly ever be competitive with those of their fossil-based counterparts. Proper incentives – financial and policy design - to support bio-based plastics development will be critical considering their demonstrated potential to play the role of NETs for limiting global warming to 1.5 °C. Also, when designing such incentives, the level of reward of each technology should account for the level of benefit produced, i.e. policy-making should provide additional incentives to carbon removal (NET) compared to carbon reduction (mitigation technologies).

Hence, if the plastic industry adapts to the imperatives of the 21st century – climate emergency and plastic pollution – by changing its feedstock and purpose, it could become a NET, little-waste generating industry. This, in turn, would represent a technology that provide both private – housing, insulation, lower cost – and collective, social – climate alleviation and waste reduction - benefits. Though the material substitution assumptions made by this study may not be exactly precise, the results indicate that a shift to construction & IF is an attractive opportunity to the plastics industry.

However, a weakness of this study stem from the assumption that the use of plastic in the construction sector is a final disposal, neglecting the next final disposal this plastic would have in the end of the construction lifetime. Since plastic use in construction has an average lifetime of 35 years (Geyer et al., 2017b), this option would enable carbon storage until later than 2050. Given the urgency to achieve net zero CO₂ emissions around 2050 to limit global warming to 1.5°C (IPCC, 2018), the hypothesis tested in this study would contribute to this global effort. Yet, it is important to stress that bio-based plastics used for long-term construction purposes can only be considered NET if an appropriate regulatory framework is established to ensure that the carbon photosynthetically captured will be stored in windows, floorings, cabinets, for several decades, before being correctly disposed or reused.

Uncertainties also rely on the assumption that, for PVC, chlorine is produced on site; for PET, p-xylene and acetic acid are produced off-site; for EPS, benzene and pentane are produced off-site. Depending on the petrochemical plant, these intermediate products are produced on site or off-site, thus demanding transportation in the last case. Uncertainties also arise from the simplification made for defining the substitution rate between plastics and common emission-intensive materials. This should be better evaluated in further studies given the relevance of the replacement of steel and aluminum in our findings. Actually, detailed research on substitution of traditional material construction by plastic should be conducted to understand the real potential of plastic in the construction sector. It is worth noting that if only plastic's carbon footprint is investigated, sending plastic waste to landfill, open dumps or littering it in the natural environment could be also an option to achieve NETs. However, those final disposal options are not encouraged by policy since they create local pollution and harms natural ecosystems, even though it could bring climatic benefit due to NETs.

This study did not allow the investigation on the direct and indirect impacts of biomass use on the energy-food-materials competition not even enables to test, for instance, if NETs achieved by plastics would impact the remaining carbon emission budgets of other economic sectors. Moreover, the demand reduction of naphtha for material purposes could impact the emissions from the refining sector, since the emergence of biorefineries to provide bio-based energy and feedstock could lead to the reduction of petroleum refining utilization rates, impacting the production of oil derivatives for energy purposes. In order to fill this gap, we incorporated a biomass trilemma (instead of the usual dilemma food-energy) in the Brazilian Land Use and Energy System (BLUES) model, which represents biomass competition between energy, food and materials, given land, GHG emissions (from fuel combustion and direct and indirect land use change) and water availability constrains. The results of this study are presented in Oliveira et al. (forthcoming).

Further studies should also evaluate life-cycle GHG emissions for other plastics, such as those derived from propylene and aromatics, as well as for other routes of ethylene production. Also, the methodology applied here could be adjusted to other countries with different grid emission factors, chemical industry and biomass feedstock.

Finally, future research should include the evaluation of the plastic chemical recycling. Although this recycling method is not readily available, it could have a great impact on the results of this study since it contributes to material circularity, closing the plastic loop. In this case, if the monomer is repurposed to something other than a fuel, the plastic carbon would be stored for as many cycles as possible without downgrade, performing similarly to being stored in buildings and infrastructure. However, given that this process is not spontaneous (being, thus, energy consuming and GHG emitting), it is safe to say that the carbon footprint would be necessarily higher (or less negative, in the case of biogenic carbon) than storing plastic carbon in long-lifetime products.

4. The role of biomaterials for the energy transition from the lens of a national integrated assessment model

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Climatic Change (submitted)

4.1. Abstract

Integrated assessment models (IAMs) indicate biomass as an essential energy carrier to reduce GHG emissions in the global energy system. However, few IAMs represent the possibility of co-producing final energy carriers and feedstock. This study fills this gap by developing an integrated analysis of energy, land and materials, which evaluates if the production of biofuels in a climate-constrained scenario can co-output biomaterials, being also driven by surpluses of hydrocarbons/carbohydrates from the transition to electromobility. The analysis was implemented through the incorporation of a materials module in the Brazilian Land Use and Energy System model. Findings show that bio-based petrochemical accounts for 33% of the total petrochemical production in a carbon mitigation stringent scenario, in 2050. Most of this comes as co-products from facilities that produce advanced fuels as main product. Moreover, from 2040 mobility electrification leads to a surplus of ethanol, which is repurposed for material production, compensating for the fuel market loss. Finally, the emergence of biorefineries to provide bio-based energy and feedstock reduces petroleum refining utilization in 2050, affecting the production of oil derivatives for energy purposes, and, hence, the GHG emissions associated with their production and combustion.

4.2. Introduction

Integrated assessment models (IAMs) indicate biomass as an essential energy carrier to reduce GHG emissions in the global energy system (Daioglou et al., 2019; Gambhir et al., 2019b; Rogelj et al., 2018; Rose et al., 2014). IAMs are a useful tool to assess the trade-offs between different biomass uses since they can describe both the land and

energy systems and their dynamic changes over time (Daioglou, 2016). Thereby, the deployment of biomass for energy use, food or chemical production has to be consistent with avoiding deforestation and contributing to climate change mitigation (Daioglou et al., 2019). Bioenergy is often highlighted by IAMs due to its versatility in producing electricity, gases, heat, hydrogen or liquids (Rose et al., 2014), and its possibility to create negative emissions (NETs) if combined with carbon capture and storage (BECCS²⁶) (Gambhir et al., 2019b; Hilaire et al., 2019; Junginger et al., 2019; Rose et al., 2014). Actually, several studies (Detz and van der Zwaan, 2019; Fuss et al., 2014; Gasser et al., 2015; Hilaire et al., 2019; Obersteiner et al., 2018; D. P. van Vuuren et al., 2017) stress that a large-scale deployment of NETs is crucial to keep warming well below 2°C to meet the Paris Agreement. Besides through BECCS, biomass can achieve NETs when it is used as a feedstock (non-energy use) for long lifetime material production (Junginger et al., 2019; Oliveira et al., 2020b, 2020c).

Most of the studies have dealt with biomass conversion from the perspective of the energy-food dilemma (Bauer et al., 2018b; Heck et al., 2018; Luderer et al., 2014; Rose et al., 2014; Torvanger, 2019), neglecting or simplifying its use for chemical conversion, although the petroleum revolution of the last century comprehended energy and food, but also materials (Perlin, 1989; Smil, 2004). Exceptions are Daioglou et al., (2019, 2014), who dealt with the demand of the non-energy sector, in an aggregated manner for basic petrochemicals; and Lap et al., (2019) who explored in an IAM the biomass competition between energy and chemicals, but restricting the analysis to few petrochemicals and leaving the competition between energy and food out of the scope. Nonetheless, the multiple uses of biomass have to be consistent with avoiding competition between energy, food and, as implemented in this study, materials – what we propose here to be framed as a *trilemma*.

Accordingly, a more nuanced understanding on the role of biomass in energy transition scenarios can be developed by considering the volume and type of fossil fuels replaced, land availability, the costs of biomass conversion to energy and/or materials, and the possible direct and indirect LUC emissions²⁷ (Daioglou, 2016; Searchinger et al., 2008;

²⁶ Bioenergy with carbon capture and storage.

²⁷ Direct LUC (dLUC) emissions is a process by which bioenergy/biomaterial production causes direct land use change by converting a previous land use to a bioenergy/biomaterial crop production. Indirect

Wicke et al., 2015). In addition, hardly IAMs represent advanced biomass conversion routes detailing the possibility of co-producing final energy carriers and feedstock to the chemical industry (naphtha, propylene, propane, etc.).

However, two trajectories of biomass supply are worth considering in deep greenhouse gases (GHG) emissions mitigation scenarios. On one hand, biomass supply for material production could rise in energy transition scenarios due to a likely increase of urban mobility electrification that might lead to surpluses of automotive fuels, including biofuels²⁸. In this case, the use of biomass surpluses for chemical production could serve as an alternative market, which would also lead to carbon capture from chemical reactions. Furthermore, the demand of chemicals is expected to grow in energy transition scenarios. For instance, to reduce fuel consumption, plastic-based materials are integrated in vehicle as a strategy to reduce their overall weight. Also, light-weight plastics can help addressing the challenges of making longer turbine blades to increase generation efficiency, while innovative chemical materials can help increase the durability of wind turbines, reducing cost of maintenance (IEA, 2018). On the other hand, biomass supply for material production could decline since alternative uses of biomass can be limited by land availability (Fargione et al., 2010; Plevin, 2017; United Nations University, 2010), water resources constrains (Bonsch et al., 2016; Fargione et al., 2010; Hejazi et al., 2013), biodiversity conservation (Creutzig et al., 2012; Fargione et al., 2010; Visconti et al., 2016), land property issues (Barreiro et al., 2017; Rinaldi et al., 2015) and direct and indirect GHG emissions (Popp et al., 2014; Searchinger et al., 2008; Wicke et al., 2015). For instance, the scenarios run by Daioglou et al. (2019) indicated that biomass supply will represent 8% to 35% of the total primary energy demand by 2050, depending on the stringency of the GHG mitigation ambition - e.g., in scenarios coping with the well below 2°C target, bioenergy makes up 26% to 35% of primary energy demand, or 115 to 180 EJ per year. This biomass supply can be challenging given the various potential constrains that limit biomass supply for materials production.

LUC (iLUC) emissions occurs when bioenergy/biomaterial production indirectly causes land use change by converting forests to cropland somewhere in the globe to meet the demand for commodities displaced by the production of feedstock for bioenergy/biomaterial (Prins et al., 2012).

²⁸ In Brazil and the USA, light vehicles can be fueled 100% with ethanol or gasoline, while gasoline is blended with ethanol (27% in Brazil and 10% in the USA) (EIA, 2019; Petrobras, 2019).

Bio-derived materials²⁹ refers also to a way to pave the full transition from fossil fuels to renewables. Actually, given the technological inflexibility of the hardware of the world petroleum refinery system (within certain limits, it is not possible to alter the yields of petroleum refineries) and the difficult substitution of non-energy petroleum products, the production of petrochemical naphtha in refineries leads to the co-production of petroleum-based fuels (diesel, jet, petrol...), undermining their rapid substitution. Without addressing materials, there is no rapid full transition from fossil fuels, as required by the more stringent climate ambitions.

Our study aims to advance the understanding of how biomass contributes to the long-term evolution of energy and land systems under energy transition scenarios in Brazil. The biomass *trilemma* was implemented through the incorporation of materials routes and demands in the Brazilian Land Use and Energy System (BLUES) model³⁰. Materials here are represented by fossil and bio-based petrochemicals³¹. The new BLUES model version enables to investigate the interactions between biomass demand for energy, food and materials, given land, GHG emissions (from fuel combustion and direct and indirect land use change) and water availability constraints. The BLUES model is currently one of the largest technologically disaggregate national IAMs in the world with a detailed representation of energy and land use modules, which allows the inclusion of a new material module, particularly based on energy-material facilities (facilities that co-output energy carriers and materials) (Köberle et al., 2020; Köberle, 2018b). The model has a plethora of biomass sources defined at space level and has a detailed technological structure. Moreover, the BLUES model has a vast number of advanced biomass conversion process, which could be improved to supply feedstock to the chemical industry.

Therefore, an integrated analysis of energy, land and material systems enables to test if carbon storage in biomaterials would impact the remaining carbon emission budgets ³²of

²⁹ As well as all renewable-derived materials (e.g. from green H₂).

³⁰ Previous studies using the BLUES model are Rochedo et al. (2018) and Roelfsema (2020).

³¹ Clearly other options could have been incorporated to the model, associated with “green” hydrogen and CO₂ from carbon capture (direct or not), but this will be done in further studies, given that the focus of this work is on biomass conversion.

³² Carbon budget is the cumulative CO₂ emissions associated with achieving certain climate targets with a certain probability (Van Vuuren et al., 2016).

other economic sectors; if the production of biofuels in a climate constrained scenario could also generate co-products to produce biomaterials; and if a transition in the energy systems would generate surpluses of hydrocarbons/carbohydrates that could serve as feedstock for material production. It also allows understanding the impacts of biomaterials on the substitution of petroleum products that benefits from captive markets (green naphtha), and because of that, when produced lead to the co-production of other petroleum derivatives.

Brazil is selected as a case study since the country is one of the world's major agricultural producers (MAPA, 2018b); it is the second largest ethanol producer (RFA, 2017); and, along with the USA, it has the lowest ethanol production costs (Gupta and Verma, 2015; RFA, 2017). Brazil's climatic advantages and the large amount of land available to grow sugarcane provide vital opportunities for the production of bio-based petrochemicals (and bio-based plastics) using sugarcane. Therefore, as highlighted by Oliveira et al. (2020b), Brazil could be a potential pioneer in large-scale bio-based plastics production due to its well-established sugar and alcohol sector. Moreover, as mentioned before, Brazil is already well-represented by a highly-detailed national integrated assessment model, in terms of energy and land-use systems, but without a suitable representation of materials as pretended by this study.

In Section 4.3, the technologies included in the model are described as well as the scenarios assumptions and plastic's final disposal options included in the model. Annex B presents further details on the modified model to incorporate the material module. Section 4.4 presents the results of the scenario projections highlighting petrochemical demand per technology and its effects on energy and land-use emissions. Section 4.5 draws conclusion and recommendations for future studies.

4.3. Methods

Little attention has been given to non-energy applications of hydrocarbons in IAMs. Table 25 presents the models and their current representation of chemical demand. Amongst the 12 IAMs selected, 3 have no chemical representation; 4 have an aggregate chemical demand representation; 1 has a detailed representation of chemical fertilizers and plastics

& rubber; 2 have an aggregated non-energy use representation; 1 has a representation for aggregated high value chemicals³³ (HVC), ammonia, methanol, refinery products; and 1 has a detailed representation of ethylene, propylene and ammonia.

Table 25: Representation of chemical demand in IAMs

IAM	Country	Chemical (non-energy use)	References
AIM/CGE	Japan	Aggregate chemical demand	(IAMC Wiki, 2019)
GCAM	USA	no	(JGCRI, 2019)
IMAGE-TIMER	Netherlands	HVC, ammonia, methanol, refinery products	(Daioglou et al., 2014)
MESSAGE-GLOBIOM	Austria	Aggregate non-energy use	(IIASA, 2019)
REMIND	Germany	Aggregate non-energy use	(PIK, 2019)
TIAM - UCL	France	Aggregate petrochemical demand	(Anandarajah et al., 2013)
WITCH	Italy	no	(WITCH, 2019)
EPPA	USA	no	(Chen et al., 2017)
DNE 21+	Japan	Ethylene, propylene and ammonia	(RITE, 2015)
POLES	France	Chemical fertilizers and plastics & rubber	(European Commission, 2017)
COFFEE	Brazil	Aggregate chemical demand	(Rochedo, 2016)
BLUES (version 1.0) ¹	Brazil	Aggregate petrochemical demand	(Köberle, 2018b)

¹Blues version before the implementation of the material module done by this study

Our study models the transition in the use of biomass in the BLUES model, which integrates in an energy and land system the competition between different technologies and energy sources to meet demand for energy service and food. The model aims to minimize costs of the entire Brazilian energy system under emissions constraints. Further details on the BLUES model, techno-economic parameters of technologies and scenario description are available in Annex B.

³³ HVC stands for the mixture of ethylene, propylene, butadiene and aromatics.

4.3.1. Technologies Added to the national IAM

We incorporated in the BLUES model the conversion routes of fossil and bio-based petrochemicals to meet the demand of ethylene, propylene, butadiene and the mixture of benzene, toluene and xylenes (BTX). This research considers only bio-based drop-in petrochemicals, which means that every bio-based petrochemical has a fossil-based reference represented in the model. Only petrochemicals produced at a large-scale were examined, whose bio-based counterpart could significantly reduce CO₂ emissions through NETs. Moreover, we included technologies that produce the required inputs to meet petrochemical demands. Technologies that produce non-petrochemical outputs are defined here as ancillary technologies. For instance, the demand of ethylene could be satisfied by naphtha steam cracking technology³⁴ that uses naphtha as input. Production of naphtha, in turn, can be achieved by the refining sector, by biomass to liquids (BTL) technology, and by oligomerization technology. BTL and oligomerization technologies were incorporated in the model as ancillary technologies to produce naphtha, which, together with the naphtha from the refining sector, will meet the demand to produce ethylene, propylene, butadiene and BTX.

Annex B presents the petrochemical and ancillary technologies included in the BLUES model as well as information on Brazil's technologies capacities, additional capacity, product yields, utilities consumption, capital investment costs (CAPEX) and operation and maintenance (O&M). All costs included in the model were adjusted to US\$₂₀₁₀, according to the Chemical Engineering Plant Cost Index (CEPCI) (Chemical Engineering, 2019). Figure 25 presents the flowchart of the processes included in the BLUES model.

³⁴ The model decides what technology or pool of technologies meet energy and material demand between 2010 (base year) and 2050 in 5-year intervals.

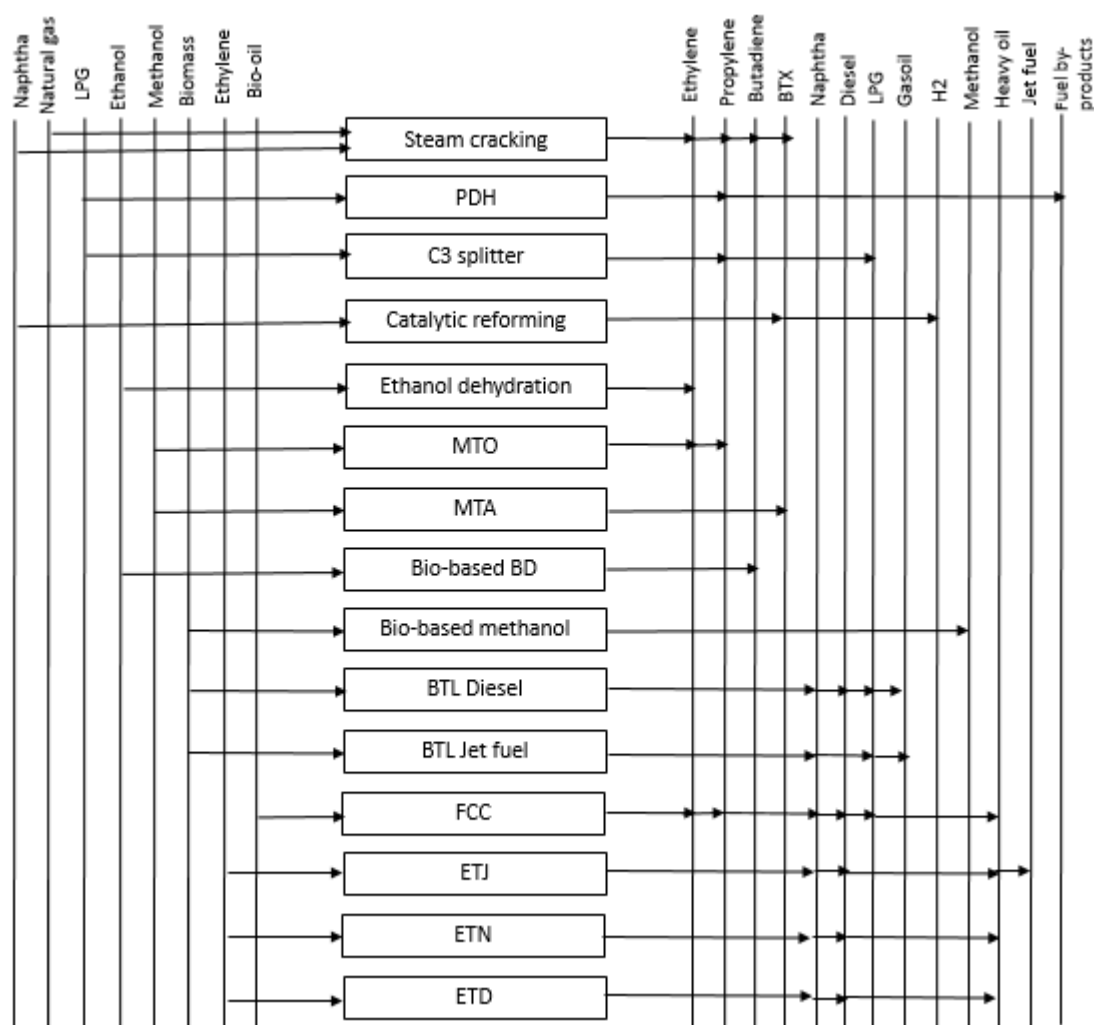


Figure 25: Technologies included in the BLUES model

4.3.2. Scenarios for Petrochemicals demand

The model projects one baseline scenario (Base), which follows a reference case for basic petrochemicals demands, consistent with Brazil's Nationally Determined Contribution (NDC); and a mitigation scenario that assumes cumulative carbon emissions constraints consistent with the "well below 2°C" targets of the Paris Agreement (WB2 scenario), with a carbon budget of 14 GtCO₂. Clearly, these carbon budgets are uncertain and depend on the results of Global Integrated Assessment Models, which are also dependent on their intrinsic assumptions and budget allocation criteria (Alcaraz et al., 2018; Fujimori et al., 2019; Gignac and Matthews, 2015; van den Berg et al., 2019). However, our focus here was not on testing different allocation rules and evaluating the uncertainties associated with global carbon budgets, which are the subject of different types of studies (Ballantyne

et al., 2015; Rogelj et al., 2019). Nor we tried to make an intermodal comparison exercise to show their contributions and drawbacks (see, for instance, Gambhir et al., 2019; Rogelj et al., 2019; Weyant, 2017). Instead, we aim here at developing a material module and identifying the contribution of biomaterials to a stringent GHG mitigation scenario. Therefore, we used Brazil's budgets from a global IAM developed in parallel with the Brazilian model, and used in different intermodels comparison studies, showing results close to the median found by other tools, both for NDC scenarios and WB2 scenarios (CD-LINKS, 2019; Rochedo et al., 2018; Roelfsema, 2020). Further studies could focus on the uncertainties of carbon budgets and on the different findings of IAMs related to that. Here, we will consider the budget mentioned above, derived from the Global IAM COFFEE (see also IAMC Wiki, 2019).

In addition, a previous paper (Oliveira et al., 2020c) indicated the possibility of proposing alternative scenarios for petrochemicals demand, considering the possibility of increasing their use in long-lifetime applications. In this case, the above-mentioned study showed that the use of bio-based plastics in construction brings environmental advantages due to the storage of biogenic carbon in a long life-time material, and also due to demand reduction of energy-intensive construction material such as cement and steel. Here, we incorporate these scenarios in the BLUES model to estimate their impacts on GHG emissions and land use change in an integrated manner. Therefore, we also run three alternative mitigation scenarios derived from the WB2 scenario: demand reduction scenario (WB2_DemRed), cement substitution scenario (WB2_CS), and steel substitution scenario (WB2_SS).

In this case, while Base and WB2 scenarios project the same petrochemical demands, according to IEA (2018), petrochemical demand in the WB2_DemRed scenario is based on the Clean Technology Scenario (CTS) from IEA (2018), which describes an increase in plastic recycling and the phase-out of single-use plastic. This scenario can also grasp the still unclear, yet far-reaching, impacts of Covid-19 on petrochemicals demand (IEA, 2020). Figure 26 presents the petrochemicals demands for the Base and the WB2_DemRed scenarios.

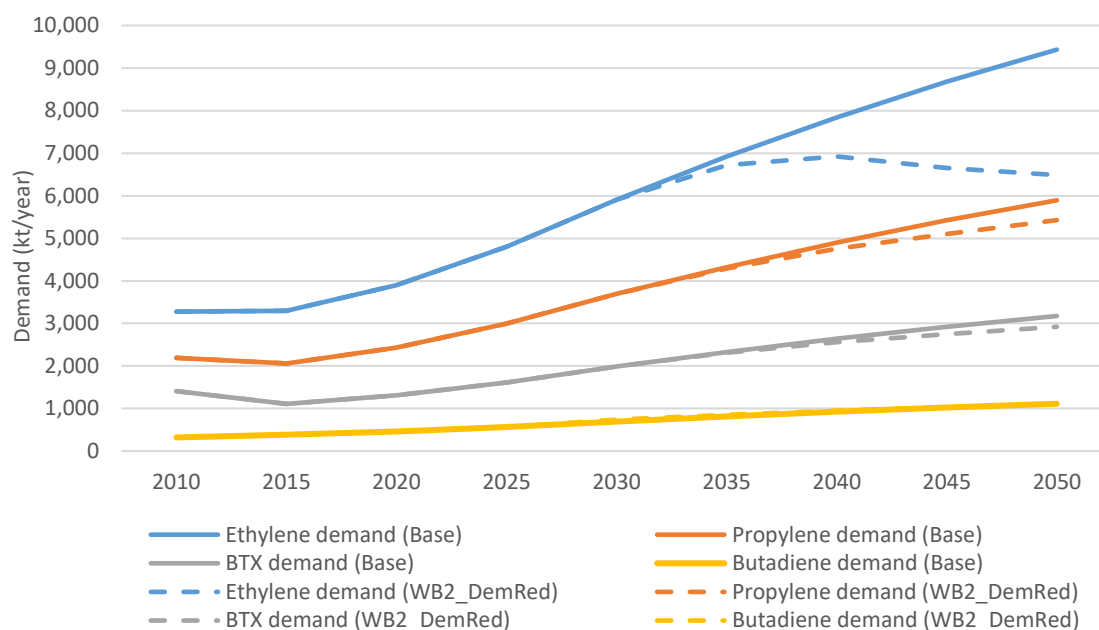


Figure 26: Petrochemicals demands in the Base and the WB2_DemRed scenarios

The WB2_CS and the WB2_SS scenarios consider the substitution of 10% of cement and steel, respectively, by plastics in long lifetime materials (construction sector) in a volume proportion of 1:1 based on the distinct density values of cement and steel (Table 26). For further details on the assumptions of cement and steel substitution by plastics, please refer to Oliveira et al. (2020). The share of plastics used in long lifetime materials was adopted from Geyer et al. (2017) and it was considered constant for the whole period (2010-2050). Table 27 shows the plastics selected in these material substitution scenarios, their share in the construction sector and the mass conversion from the monomers to the final plastics. Butadiene was not considered in these scenarios since its largest use occurs in the production of styrene butadiene rubber (SBR), which is principally used in the manufacture of automobile tires (ICIS, 2010) and therefore does not applies for long lifetime material. Figure 27 Figure 28 present the petrochemicals demand for the WB2_CS and the WB2_SS scenarios, respectively. Thereby, these scenarios consider the WB2_DemRed as the reference case.

Table 26: Material densities

Material	Density (kg/m ³)
Cement	1440
Steel	7850
LDPE ⁽¹⁾	930
HDPE ⁽²⁾	940
PVC ⁽³⁾	1400
PP ⁽⁴⁾	946
EPS ⁽⁵⁾	20
PUR ⁽⁶⁾	100
⁽¹⁾ Low-density polyethylene	
⁽²⁾ High-density polyethylene	
⁽³⁾ Polyvinyl chloride	
⁽⁴⁾ Expanded polystyrene	
⁽⁵⁾ Polyurethane	

Source: Doran, D. & Cather (2014) and The Constructor (2019)

Table 27: Share of polymers in the construction sector, their related monomers and mass conversions applied in the WB2_CS and the WB2_SS scenarios

Polymer	Share in Construction	Related Monomer ⁽¹⁾	Mass conversion
LDPE	1.1%	Ethylene	1.05
HDPE	3.3%	Ethylene	1.05
PVC	8.1%	Ethylene	0.48
PP	1.2%	Propylene	1.02
EPS	2.2%	BTX	0.79
PUR	2.4%	Propylene	0.12

⁽¹⁾ Although some plastics (PVC, EPS and PUR) are made of more than one type of monomer, we have selected the one who has higher mass content in the final polymer.

Source: Geyer et al. (2017) and Platts (2017)

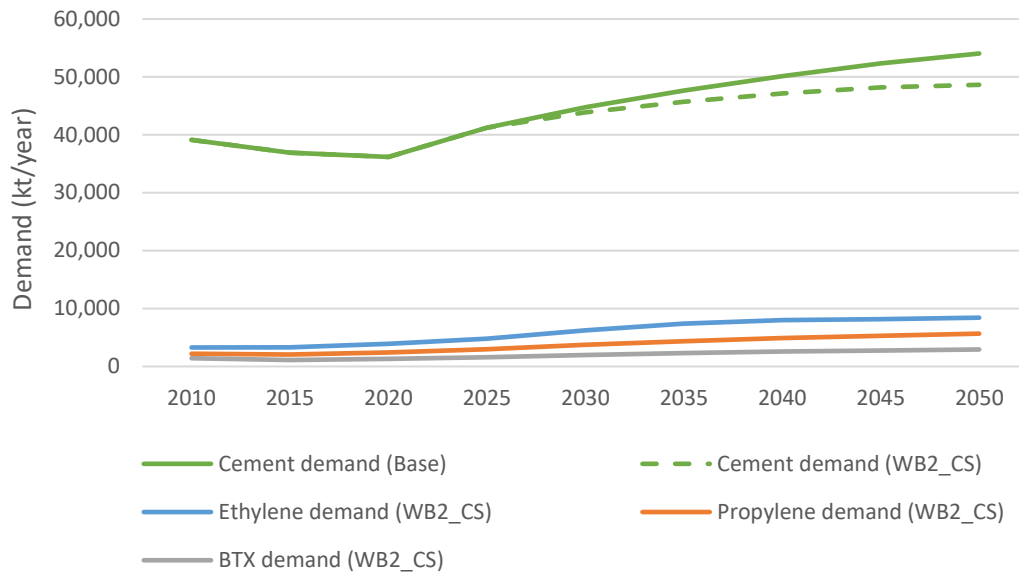


Figure 27: Cement and petrochemicals demands in the WB2_CS scenario

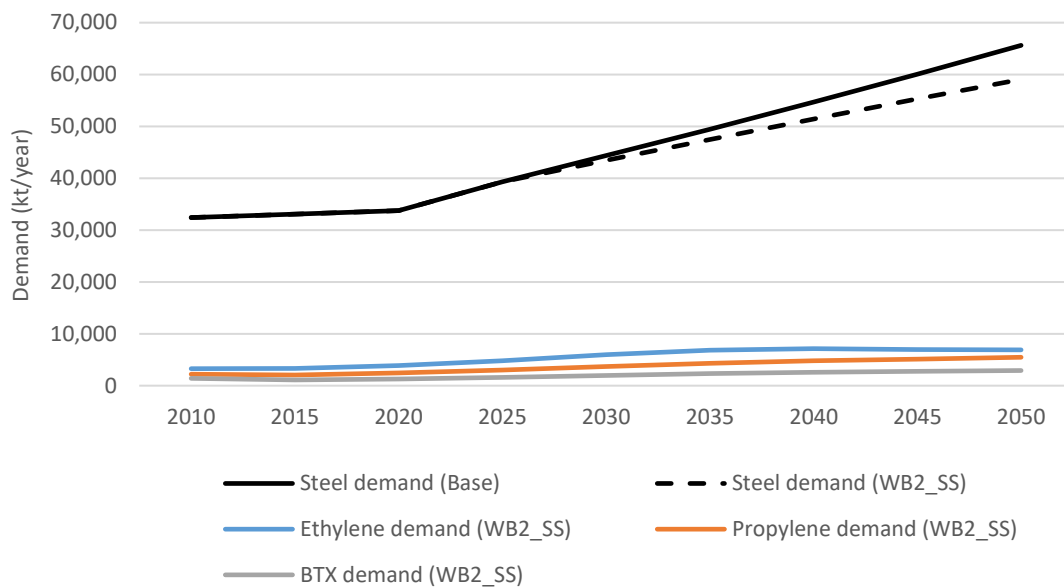


Figure 28: Steel and petrochemicals demands in the WB2_SS scenario

Oil price was assumed as US\$ 50/bbl for the whole period, which is an expected moderate long-term average oil price due to Covid-19 (ADL, 2020). The idea here is not to focus on the uncertainties associated with oil prices. Instead, the idea is to show the advantages of better detailing materials (particularly petrochemicals) in the IAM, under emission constrained scenarios.

4.3.3. Final disposal

In this section, we address direct GHG emissions from fossil and bio-based plastic's final disposal. Indirect GHG emissions from land-use change (LUC) will be assessed after the simulation of the modified IAM and, therefore, will be presented in Section 4.4.

Four final disposal options for fossil and bio-based petrochemicals were incorporated in the IAM: landfill, incineration, recycling and their conversion to long lifetime materials (LM). Emission factors (EF) of final disposal options can be found in Table 28 and Table 29. For ethylene, propylene, BTX and butadiene it was considered the final disposal of HDPE, PP, EPS and SBR, respectively. In terms of GHG emissions, landfill and LM options are the same since they store carbon over a long period of time. It is worth noting that landfill here is defined as a final disposal that stores plastic for decades until its natural decomposition. This disposition includes sanitary landfill, open dumps and littering in the natural environment. When fossil-based petrochemicals are sent to landfill or used in LM, their EF are zero, since there is no carbon release. However, if the petrochemical is bio-based and it is considered that all the carbon embodied in the plastic is biogenic, landfill and LM options would generate NETs. NETs for the selected bio-based petrochemicals were calculated according to Equation 3.

Equation 3:

$$NET_i = \frac{n^o \text{ carbons}_i \times \text{molar mass}_{CO_2}}{\text{molar mass}_i}$$

where,

NET_i = negative emissions of bio-based petrochemical i (t CO₂/t_i);

i = bio-based petrochemical;

$n^o \text{ carbons}_i$ = number of carbons in the bio-based petrochemical i;

molar mass_{CO_2} = molar mass of CO₂ (44 gmol/g);

molar mass_i = molar mass of bio-based petrochemical i (gmol/g).

When plastics are incinerated, they release all their stored carbon, generating net neutral emissions for bio-based petrochemicals. For the recycling process, it was considered electricity consumption of mechanical recycling shown in Table 30, and the Brazilian grid emission factor of 0.58 tCO₂/MWh (MCTIC, 2017a).

Table 28: Final disposal emission factor for fossil-based petrochemicals

Fossil-based petrochemical	EF landfill e LM (tCO₂/ t)	EF incineration (tCO₂/ t)	EF recycling (tCO₂/t)
Ethylene	0.00	3.14	0.29
Propylene	0.00	3.14	0.28
BTX	0.00	3.35	0.35
Butadiene	0.00	3.26	1.51

Source: Oliveira et al. (2020b)

Table 29: Final disposal emission factor for bio-based petrochemicals

Bio-based petrochemical	EF landfill e LM (tCO₂/ t)	EF incineration (tCO₂/ t)	EF recycling (tCO₂/t)
Ethylene	-3.14	0.00	0.29
Propylene	-3.14	0.00	0.28
BTX	-3.35	0.00	0.35
Butadiene	-3.26	0.00	1.51

Source: Oliveira et al. (2020b)

Table 30: Electricity consumption for plastic's mechanical recycling

Recycling step	Electricity consumption (kWh/t plastic)
Shredding	24
Extruders	270
Agglomerators	175
Total	469

Source: Shonfield (2008)

In the Base and the WB2_DemRed scenarios, the share of plastics sent to recycling and incineration is based on the reference scenario and low carbon scenarios, respectively, modelled in (MCTIC, 2017c). It was assumed that the plastics that are not recycled or incinerated are sent to landfill. The share of each polymer (and monomer) recycled derives from PLASTIVIDA (2013) and it is considered constant for the whole period for both scenarios.

In the WB2_CS and the WB2_SS scenarios, the amount of plastics sent to landfill, incineration and recycling is the same as considered in the WB2_DemRed scenario. The amount of the monomers converted into LM in the WB2_CS scenario is the difference between the monomer demand in this scenario and in the WB2_DemRed. The analogous occurs for the amount of monomers converted into LM in the WB2_SS scenario. The projection of plastics' final disposal trend in Brazil can be found in Annex B.

4.4. Results and Discussion

4.4.1. Energy System

As shown in Figure 29, primary energy consumption increases to 462 and 658 Mtoe/year in 2050 for the Baseline and the WB2 scenarios, respectively. In 2010, fossil fuels accounted for 60% of the primary energy use in Brazil. By 2050, this share is projected to change to 62% and 14% for the Baseline and the WB2 scenarios, respectively. Oil production peaks in 2030, dropping by 2050 to 2015 levels in the WB2 scenario. For the WB2 scenario, biomass consumption is expected to grow significantly from 71 Mtoe/year to 504 Mtoe/year.

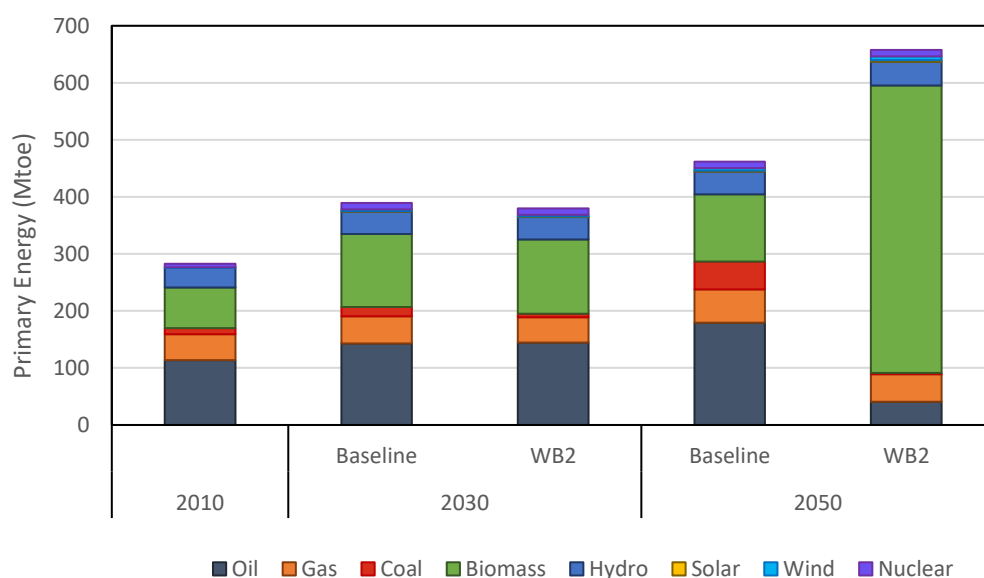


Figure 29: Primary energy consumption in 2030 and 2050 in Base and WB2 scenarios

Electricity generation reaches 898 TWh/year and 941 TWh/year by 2050 for the Baseline and the WB2 scenarios, respectively. For both scenarios, hydropower leads electricity generation (52% by 2050). By 2050, in the Baseline scenario, coal generation, bagasse, wind and distributed generation increase, relative to 2015, by 974%, 197%, 705% and 48%, respectively. When considering the WB2 scenario, coal generation decreases by 66%, while bagasse, wind and distributed generation increase by 496%, 1141% and 77%, respectively, relative to 2015.

4.4.2. Biofuel production, land use change and CO₂ emissions

In the Baseline and WB2 scenarios, ethanol fuel use grows until 2035, which is consistent with the goals established in the Brazilian Renovabio program³⁵. However, particularly in the WB2 scenario, from 2040 onward, ethanol fuel use decreases due to mobility electrification being compensated by the ethanol deployment for petrochemical production.

The increase in the production of biofuels for the WB2 scenario by 2050 is significantly driven by the adoption of BTL technologies with CCS that are used primarily in the transportation sector (

Figure 30). For the Baseline scenario, ethanol without CCS (71.5%) and biodiesel (28.5%) peak in 2035 at 1339 PJ/year and drops to 828 PJ/year in 2050.

In contrast, for the WB2 scenario, biofuel use increases in each period reaching 8146 PJ/year by 2050. Thereby, diesel from BTL technology is the most important biofuel produced, followed by ethanol with CCS and jet fuel from BTL, accounting for 42.7%, 16.9%, and 15.9% of the total biofuel production, respectively. Higher uses of biofuel with CCS by 2050 for the WB2 scenario are combined with higher afforestation, leading to NETs in the energy sector (477 Mt CO₂/year) as well as in the agriculture, forestry and land use (AFOLU) sector (230 Mt CO₂/year). Planted forest to produce biofuels, recuperation of degraded pastures, and integrated livestock-cropland-forest systems

³⁵ The RenovaBio program is the National Biofuels Policy of Brazil designed to support Brazil's COP21 goals. The policy aims to promote the expansion of the production, commercialization and use of biofuels in the national energy mix, by creating a market for carbon decarbonization credits (CBIO) to remunerate the sector for its GHG emissions reduction (Ministério de Minas e Energia, 2020).

account for 14 Mha, 54 Mha, and 8 Mha, respectively (Figure 31). In contrast, the Baseline scenario shows growing deforestation rates, primarily due to degraded pasture which increases from 23 Mha in 2015 to 66 Mha by 2050.

Therefore, our results show that the higher demand for bio-based materials and fuels in the WB2 scenario does not increase AFOLU emissions (Figure 32), as it does not pressure for open areas to dedicated land. Instead, BECCS used in the end of the period triggers bio-based petrochemical production since BTL technology also produces green naphtha and green LPG that are used as feedstock for petrochemical production.

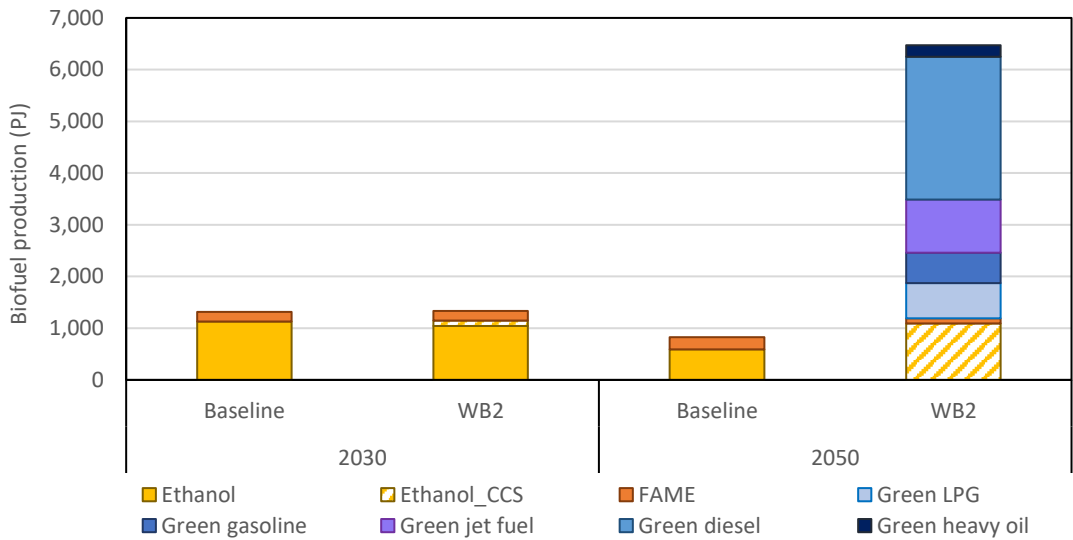


Figure 30: Biofuel production for all scenarios (PJ/year)

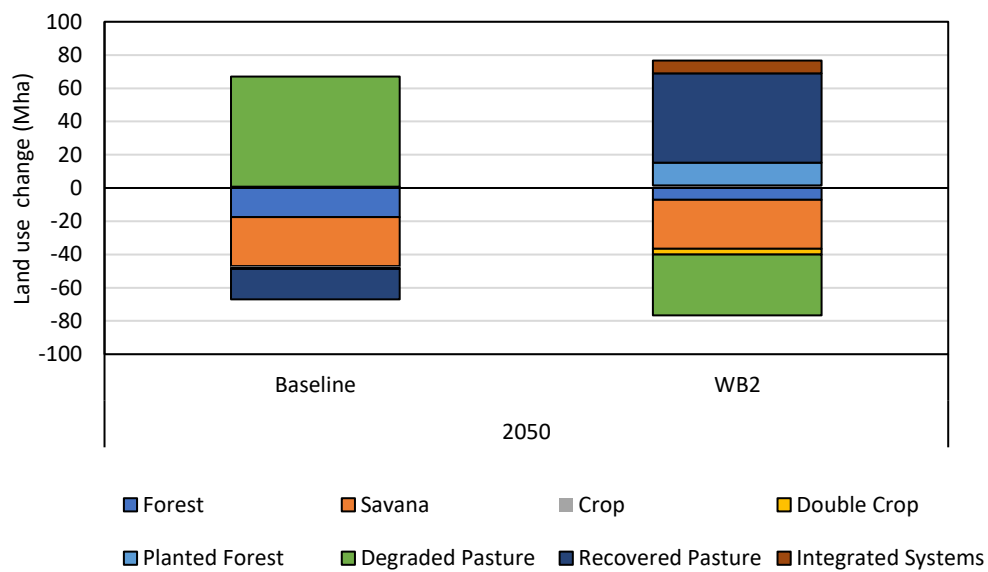


Figure 31: Cumulative land use change (2010 to 2050) for baseline and WB2 scenarios (Mha)

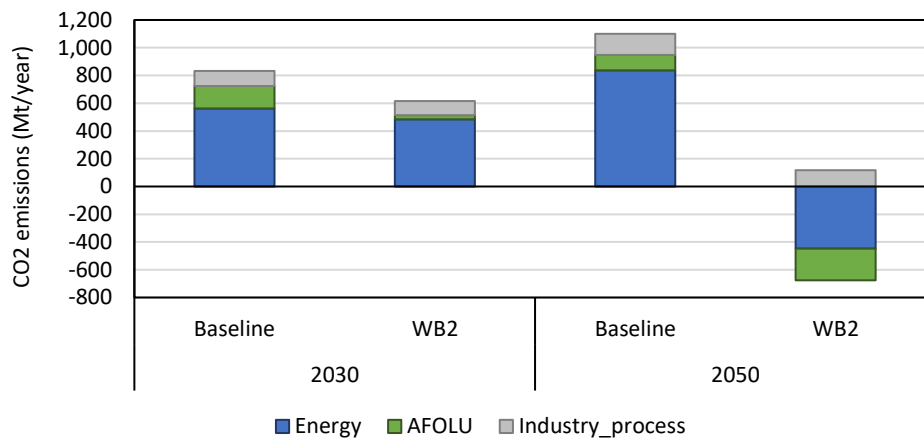


Figure 32: CO₂ emissions in 2030 and 2050 for baseline and WB2 scenarios

4.4.3. Petrochemical production

Bio-based petrochemical production reaches 33% of total petrochemical production by 2050 for the WB2 scenario (Figure 33). Naphtha steam cracking (SC) remains the dominant technology to produce ethylene, propylene, BTX and butadiene through the whole period for both scenarios. In 2050, 21 % of the naphtha used in SC comes from biomass. Ethanol-to-ethylene route is also worthwhile in 2050.

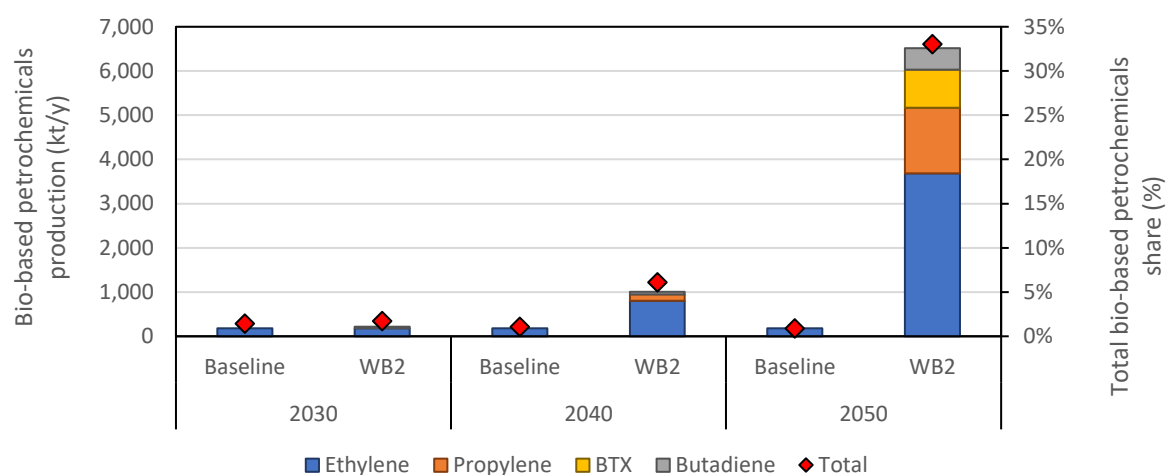


Figure 33: Bio-based petrochemicals production

In the WB2 scenario, after 2040, an increase of urban mobility electrification leads to surpluses of liquid fuels, hydrocarbons (mostly, naphtha) and carbohydrates (ethanol), which could serve as feedstock for material production. In 2050, ethylene and butadiene produced from ethanol would represent 19% (Figure 34) and 20% (Figure 37) of the total ethylene and butadiene production, respectively. Still in 2050, MTO technology is used for 7% of the total ethylene production and 10.0% of the total propylene production (Figure 35). Methanol used in MTO routes is entirely imported for both scenarios throughout the whole period. C3 splitter technology represents, in 2050, 4% and 8.5% of total propylene production in the Base and the WB2 scenarios, respectively. Due to a reduction of naphtha SC technology, BTX production from catalytic reforming reaches 30% of total production in the WB2 scenario (Figure 36). In the same scenario, ethanol to butadiene technology increases from 4.5% to 20% of total production (Figure 37).

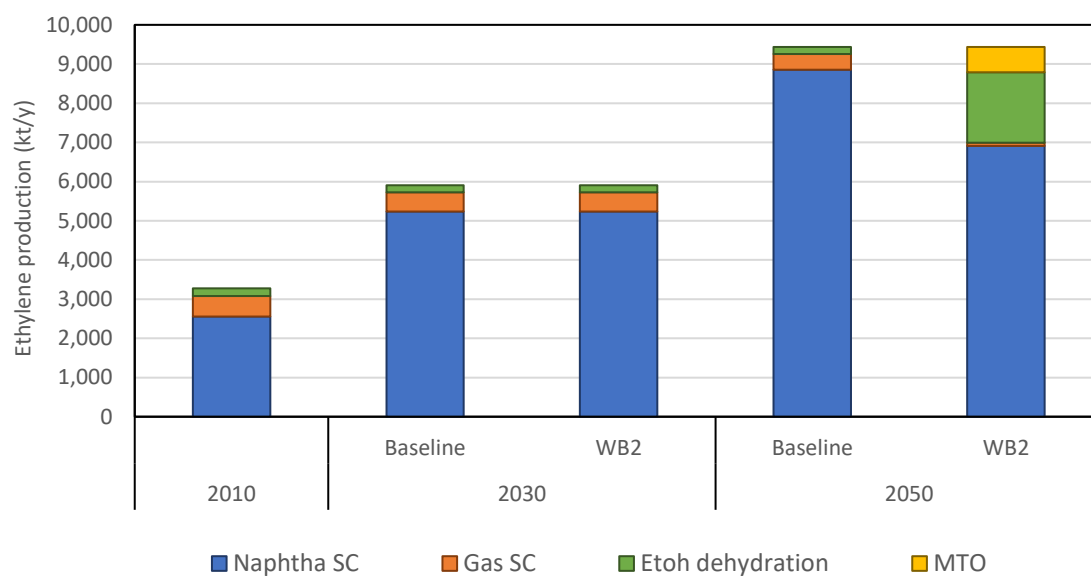


Figure 34: Ethylene production per technology for all scenarios

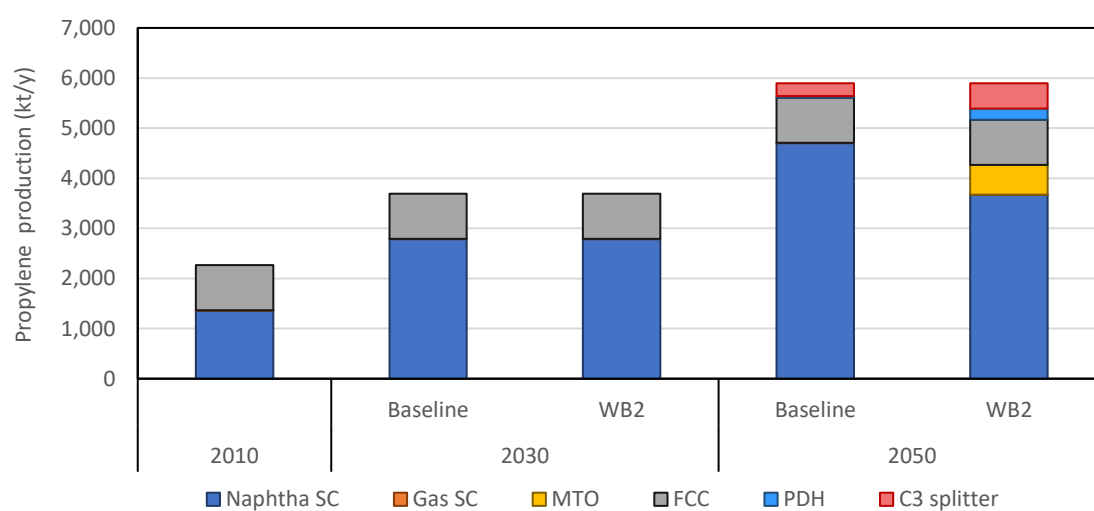


Figure 35: Propylene production per technology for all scenarios

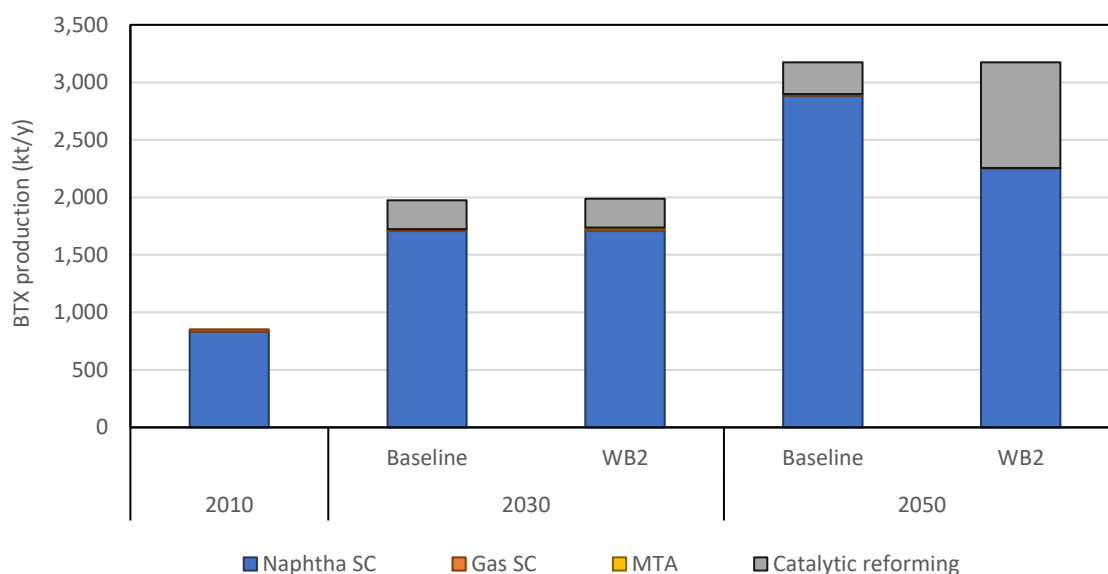


Figure 36: BTX production per technology for all scenarios

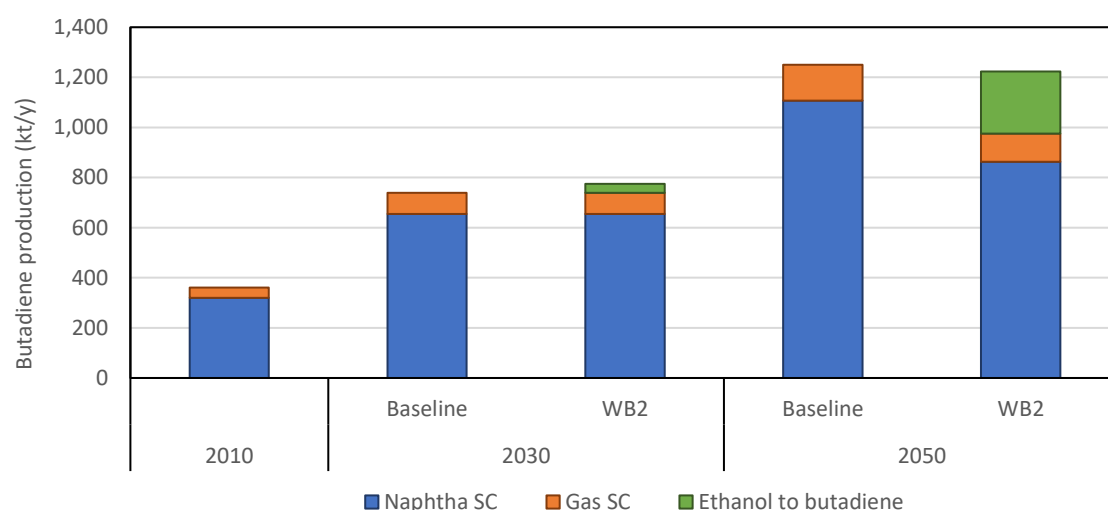


Figure 37: Butadiene production per technology for all scenarios

The WB2 scenario, by increasing the production of petrochemicals and storing carbon on them, was able to directly reduce cumulative CO₂ emissions by 170 Mt CO₂ from 2010 to 2050. This represents 1.7% of NETs achieved in this scenario, including BECCS and AFOLU. It is a small but relevant figure, which can also be better appreciated if we add to it the impacts of replacing fossil naphtha by green naphtha on the petroleum products production.

4.4.4. Side-effects on Petroleum Refineries

The demand reduction of crude oil derived-naphtha for material purposes, both because of green naphtha production in BTL plants and ethylene production from ethanol, affected the refining sector. In this case, simultaneously liquid biofuels replaced fuels from oil refineries, and the green naphtha supply (plus the ethylene production from ethanol) reduced the need for running refineries to produce naphtha for petrochemicals.

As such, in the WB2 scenario, refinery utilization factors³⁶ dropped from 2040 to 2050 from 95% to 13% in the Southeast region and from 87% to 0% in the South region of Brazil. The North and the Northeast regions kept an average refining utilization rate of 85%. Therefore, the country's total refinery throughput that totaled 1.8 Mbbl/d in 2040 reduced to 0.5 Mbbl/d in 2050. As the CO₂ emission factor of Brazilian refineries hovers around 25 MtCO₂/year in the period, both from fuel combustion and hydrogen generation (Guedes, 2019; Szklo and Schaeffer, 2007), the avoided emissions in the refinery for not producing 1.3 Mbbl/d (1.8 minus 0.5) reached 18 MtCO₂ in 2050. In addition, the reduced production of fuel derivatives in refineries also avoided emissions from these liquid fuels combustion, totaling 162 MtCO₂/ year in 2050 of avoided emissions.

Therefore, the production of bio-based petrochemicals in the WB2 scenario avoided around 180 MtCO₂ in 2050. This means that, only in 2050, the impacts of reducing the use of petroleum refineries represented the same amount of avoided CO₂ emissions found for the 2020-2050 period because of CCU from biomaterials, as showed before.

It is a virtuous cycle: by replacing fossil naphtha, the model can use less oil refineries and then produce fewer fuels that can be replaced by renewable fuels, whose production facility can also produce raw materials that replace fossil naphtha.

³⁶ Refinery utilization factor represents the use of the atmospheric crude oil distillation units. The rate is calculated by dividing the gross input to these units by the operable refining capacity of the units (EIA, 2018).

4.4.5. Alternative Scenarios for the use and destination of Plastics

For all the variations of the WB2 scenario, naphtha steam cracking remains the main route to produce petrochemicals, while 21.5% of the naphtha used is bio-based. Figure 38 shows cumulative CO₂ emissions differences between the WB2 scenario and their derived alternative scenarios. Emissions from industry sector decrease for all derived scenarios. For the WB2_CS scenario, this decrease is more moderate since petrochemical demand is higher than in the WB2 scenario. Therefore, emissions increase from petrochemical production is higher than the decrease in emissions from cement demand reduction. By 2050, cement demand is 50 Mt and 45 Mt in the WB2 and the WB2_CS scenarios, respectively. Process emissions from both scenarios are similar: 117 MtCO₂ and 140 MtCO₂ by 2050 for the WB2 and the WB2_CS scenarios, respectively. This is explained by CCS deployment in the cement sector for the WB2 scenario that results in reduced process emission. By 2050, the Base scenario projects 150 MtCO₂ process emissions.

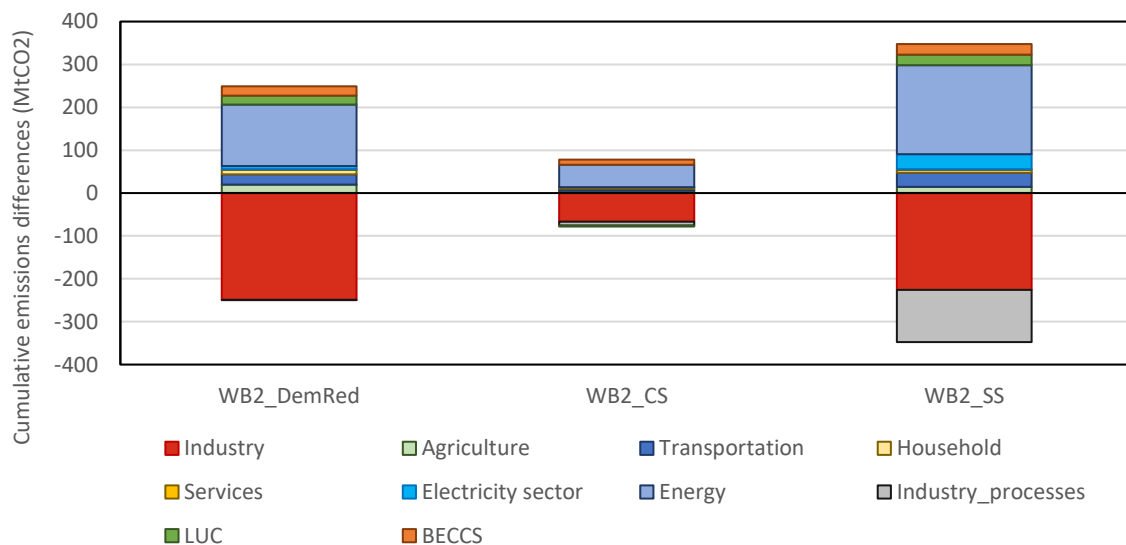


Figure 38: Cumulative CO₂ emissions differences between the WB2 and their derived scenarios

For the WB2_SS scenario, the impact in petrochemical demand is lower, since steel is denser than cement and, therefore, construction requires less plastic to replace steel than cement. Cumulative industrial emissions in this scenario (1,070 MtCO₂) is lower than in the WB2_CS scenario (1,102 MtCO₂). Different from the WB2_CS scenario, here,

emissions from industrial process (108 MtCO₂ by 2050) are even lower when compared to the WB2 scenario (117 MtCO₂ by 2050), since the model does not project CCS in the steel industry for the WB2 scenario up to 2050. Therefore, the reduction in steel demand due to plastic substitution impacts the overall industrial process emissions.

The WB2_CS and WB2_SS scenarios did not lead to higher NETs than in the WB2 scenario. NETs achieved 566 MtCO₂, 578 MtCO₂ and 559 MtCO₂ in the WB2_CS, WB2_SS, and WB2 scenarios, respectively, in 2050. Although these mitigation measures do not increase NETs when compared to the WB2 scenario, they lead to co-benefits in cumulative emissions reductions due to drops in industrial emissions from cement (by 70 MtCO₂) and steel (by 225 MtCO₂) sectors.

4.5. Conclusion

This study aimed to contribute to the evaluation of the non-energy use of biomass in the bio-based economy and to assess how bio-based materials can help to mitigate climate change. To achieve this, we included a petrochemical module in the Brazilian Land Use and Energy System (BLUES) model. Very few IAMs have material representation and those exceptions present the petrochemical demand and supply (technological options) in an aggregated manner. Here, we incorporated in an IAM fossil and bio-based petrochemicals conversion routes to meet the demand of ethylene, propylene, BTX and butadiene. We have considered petrochemicals produced at a large-scale whose bio-based counterpart could significantly reduce CO₂ emissions through NETs. Besides petrochemical routes and demands, we included in the model ancillary technologies that produce the required feedstock to meet petrochemical demands such as BTL (co-producing naphtha and LPG), oligomerization (the same) and FCC technologies (co-producing LPG and olefins). We modelled a baseline scenario and a mitigation scenario that assumes cumulative carbon emissions constraints consistent with the well-below 2°C targets of the Paris Agreement (WB2 scenario). We also run three alternative mitigation scenarios derived from the WB2 scenario: demand reduction scenario (WB2_DemRed), cement substitution scenario (WB2_CS), and steel substitution scenario (WB2_SS). The two latter scenarios enable to assess the potential of bio-based materials in creating NETs through carbon storage in long lifetime materials.

Our results indicate that bio-based petrochemical accounts for 33.0% of the total petrochemical production in the WB2 scenario in Brazil. Naphtha steam cracking remains the dominant technology to produce basic petrochemicals for all the scenarios, but in the case of WB2 scenarios, 21.5 % of this feedstock comes from biomass instead of from crude oil, in 2050. Interestingly, this green naphtha is co-produced by BTL technologies dedicated to produce advanced diesel as their main product. This means that the Brazilian IAM model decided to produce diesel from BTL with CCS, and from this decision, it found a co-production of feedstock to materials: particularly green naphtha to steam-crackers, but also greenpropane to PDH. Hence, by coproducing energy carriers and materials, there was no competition for land affecting land use GHG emissions.

Moreover, in the WB2 scenario, from 2040 urban mobility electrification leads to a surplus of ethanol, which, in turn, is repurposed for material production, compensating for the fuel market loss. In this scenario, ethylene and butadiene produced from ethanol would represent 19% and 20% of the total ethylene and butadiene production, respectively, in 2050. This finding confirms our hypothesis that a transition in the energy system would generate surpluses of liquid fuels (ethanol) that could serve as feedstock for material production. By 2050, 61% of ethanol supply would be used for petrochemical production. Besides, the ethanol produced in the WB2 scenario, from 2040 onward, is combined with CCS. This shows that the increased supply of ethanol as a fuel from 2010 to 2040 does not generate lock-in effects, but instead pave the way afterwards for adding CCS to ethanol producing facilities and repurposing them partially towards the material industry.

However, in the WB2 scenario, the reduction of naphtha steam cracking due to the increase of bio-ethylene production negatively affects propylene, BTX and butadiene production. For the first petrochemical, C3 splitter, FCC and MTO compensate the reduction of naphtha SC. Methanol used to meet the demand of ethylene and propylene comes entirely from imports. BTX production is met by an increase of catalytic reforming using naphtha. Finally, butadiene starts to be produced from ethanol in 2030 (5%) increasing its share by 2050 (20%).

At the end, by producing and using ethanol as feedstock to materials and co-producing green naphtha and green LPG in BTL plants (all these facilities equipped with CCS), the

WB2 scenario led to 677 Mt of negative CO₂ emissions. In the case of also replacing cement and steel partially by plastics, cumulative emissions reductions due to drops in industrial emissions from cement and steel sectors reached 70 MtCO₂ and 225 MtCO₂, respectively.

In addition, the emergence of biorefineries to provide bio-based energy and feedstock led to the reduction of petroleum refining utilization rates, which also affects the production of oil derivatives for energy purposes, and, hence, the GHG emissions associated with their production and combustion. For example, this led to a reduction of 180 MtCO₂ in 2050, both by lowering the utilization factor of oil refineries and, hence, their emissions, and by lowering the output of oil products. Interestingly, only in 2050, the impacts of reducing the use of petroleum refineries represented the same amount of avoided CO₂ emissions found for the 2020-2050 period because of CCU from biomaterials.

In other words, materials substitution has spillover effects on the energy transition, by lowering the production of gasoline, diesel, jet and bunker fuels, which were produced along with petrochemical naphtha. Further studies could assess which refineries could repurpose (and how) to process biomass and increase their yields in materials. This would both reduce the cost for implementing bioplatfroms and the stranded assets associated with the petroleum industry under a stringent mitigation ambition.

Finally, this study was a first attempt to understand how better representing materials in IAMs can improve the evaluation of deep decarbonization pathways. The analysis focused on a national IAM, as it allowed detailing material, energy and land use in the same tool. However, results are clearly dependent on the Brazilian context, where the biofuel industry stands out and there is an already operating ethylene-from-ethanol plant. Other national IAMs could benefit from the approach here undertaken but highlight other technological routes. Even in the case of our study, it would be recommendable to add to our national model other petrochemicals routes based on the chemical reaction of “green” hydrogen (from electrolysis and thermolysis, or from gasification and steam reform) and CO₂ (two steps, using reverse water gas shift, or one step). This will be the focus of further improvements of the IAM Blues.

Another study could well focus on adding materials representation (supply and demand and nexus with to the energy and land use systems) to global IAMs. This could better

appraise the total contribution of renewable raw materials to deep decarbonization scenarios, at a global level, also revealing the competitive advantages of each world region in terms of resources, raw materials, etc.

This study also did not focus on stressing the sources of uncertainties of the scenarios run. For instance, the oil price assumed (US\$50/bbl) throughout the whole period is a conservative assumption. Finally, the simplification made for defining the substitution rate of cement and steel by plastics in the construction sector is also a weakness of our study. However, the assumptions made here indicate that using plastics in long lifetime materials is an attractive strategy for the plastic industry since it leads to NETs. Further studies should better evaluate which type of plastics have a real potential to substitute traditional construction materials and at which rates this substitution could occur. Another weakness of our model also stems from the assumption that the use of plastics in long lifetime material is a final step of plastic final disposal. Plastic in construction has an average lifetime of 35 years, what assures carbon storage till the end of the period analyzed in the model, contributing to the global effort to achieve net zero CO₂ emissions by 2050. Appropriate regulatory framework should be designed to ensure that the carbon photosynthetically captured will be stored in long lifetime material for several decades, before being correctly reused or disposed. At the end, the concept of material transition has the potential to introduce a plethora of new research lines, to bring the real complexity of renewable raw materials to a level of informed policy debate.

5. Conclusions

A low carbon economy that is based on biomass should consider not only the energy uses of this primary energy option, but also its conversion to chemical, particularly to materials, under the concept of the bio-based economy BBE. To guarantee the benefits of biomass use in terms of GHG emissions reduction, the production of biomass has to be managed in order to meet the demand for food, bioenergy and biomaterials production, while maintaining soil fertility and dealing with water availability and chemical inputs as fertilisers and pesticides. Under other conditions, biomass production may cause rebound effects in carbon emissions due to land-use (LUC), deforestation and biodiversity loss. Therefore, to have a clear understanding on the role of biomass in the global energy system and for curbing GHG emissions, scientists use integrated assessment models (IAMs) to analyze mitigation scenarios considering biomass use competition and land availability. This integrated manner to evaluate mitigation scenarios looking simultaneously at energy, land and climate systems helps policymakers to explore the feedbacks and tradeoffs between choices during decision making process.

To keep global warming below 1.5°C, most IAMs highlight that a large-scale deployment of negative emissions technologies (NETs) is needed. Biomass captures CO₂ during its cultivation and, depending on the biomass application, this CO₂ is released back to the atmosphere, or is stored generating NETs. Biomass can achieve NETs through two applications: when it is converted into energy (bioenergy) with carbon capture and storage (BECCS); and when it is converted into long-life time materials, defined in this thesis as biomass with carbon capture utilization and storage (BIOCCUS). Both biomass applications differ between energy use, when biomass is consumed as a (bio-based) fuel, and non-energy use, when biomass is used as a feedstock for material production. While the energy use of biomass as well as the potential capacity of biomass to generate BECCS are well assessed in the literature, the evaluation of biomass conversion into materials as a NET option is poorly represented.

Interestingly enough, bio-derived materials³⁷ refers to materials not only as NET, but also as a way to pave the *full* transition from fossil fuels to renewables. Actually, given the

³⁷ As well as all renewable-derived materials (e.g. from green H₂).

technological inflexibility of the hardware of the world petroleum refinery system (within certain limits, it is not possible to alter the yields of petroleum refineries) and the difficult substitution of non-energy petroleum products, the production of petrochemical naphtha in refineries leads to the co-production of petroleum-based fuels (diesel, jet, petrol...), undermining their rapid substitution. Without addressing materials, there is no *full* transition from fossil fuels, as required by the more stringent climate ambitions.

This thesis therefore aims to fill this gap in the scientific literature, providing a valuable contribution to the non-energy use of biomass in energy transition scenarios, using an integrated assessment analysis, where the different direct purposes of biomass for the society are consistently assessed (food, energy and materials³⁸).

All the case studies here presented are conducted in Brazil, due to the country's vast production of biomass such as sugarcane, and due to its edaphoclimatic conditions that support different food and energy crops, being the largest sugar, meal and cake exporter and the second largest maize exporter in the world (FAO, 2019). Moreover, the BLUES model is currently one of the largest technologically disaggregate national IAMs in the world with a detailed representation of energy and land use modules, which allows the inclusion of a new material module, particularly based on energy-material facilities (facilities that co-output energy carriers and materials). The model has a plethora of biomass sources defined at space level and has a detailed technological structure. Moreover, the BLUES model has a vast number of advanced biomass conversion process which could be improved to supply feedstock to the chemical industry.

Herein, three papers present evaluations on the potential role of biomass in the BBE of Brazil. The focus of the three studies was on petrochemicals, given their scale and importance to manufacturing and the needed materials for energy transition, and the possible competition between biomass and petroleum to provide them. The first paper develops a detailed life-cycle analysis (LCA) with conversion process. The second one presents the detail of the waste disposal. Finally, in the third paper, the outputs created in the previous studies are inputs to the IAM, which needs to be improved to incorporate

³⁸ Most of the IAMS do not incorporate explicitly the biomass ecosystem services that can benefit societies.

hydrocarbon pools that derives from biomass conversion processes, such as propylene, butadiene and C5+³⁹.

The first paper, co-authored by Oliveira et al. (2020b), presented in Chapter 2, compares four ethylene production routes according to their estimated cost of production in Brazil under a simplified LCA: sugar-cane-derived ethanol to ethylene (with and without CO₂ capture and storage – BECCS); bio-methanol to olefin; and conventional steam cracking of naphtha. Findings show that bio-based ethylene from sugarcane could become competitive with naphtha-based derived ethylene for a CO_{2e} price range of around 75–150 US\$/tCO_{2e}, depending on whether the ethylene is converted into long lifetime products and on the costs of pioneer plants. This range of prices agrees with the results of different studies that refer to scenarios associated with a global temperature increase capped to 2°C. Therefore, under a strong global climate governance expressed by relevant CO₂ prices, Brazil could be a potential pioneer in large-scale bio-based ethylene production due to its well-established sugar and alcohol sector. A carbon mechanism should be applied in the Brazilian economy to boost the decarbonization of the chemical sector and to favor an industry in a severe crisis. Nonetheless, this paper, due to its focus, did not detail the final disposal of the chemical products, nor whether the emissions from BIOCCUS would be lost by AFOLU indirect emissions or even by the lower supply of ethanol for energy use.

The second paper, co-authored by Oliveira et al. (2020), presented in Chapter 3, deepens the analysis on the benefits of converting bioplastics into long lifetime material. Here, GHG life-cycle emissions of ethylene were expanded through further steps: the conversion of ethylene into final products (plastics) and their final disposals. The plastics studied are high-density polyethylene (HDPE), polyvinyl chloride (PVC), polyethylene terephthalate (PET) and polystyrene (PS), which accounts for 13.6%, 13.6%, 8.1% and 6.5% of the total plastics produced in Brazil, respectively. For final disposal option, the study considered incineration, incineration with energy recovery (plastic to energy, P2E) and recycling. Moreover, it was assessed the use of plastics for long-term applications (construction & infrastructure). Findings showed that using plastics as long life-time material could lead to NETs, depending on the feedstock, the polymer and the strategy

³⁹ Mixture of hydrocarbons that consists mostly of pentanes (five-carbon chain) and higher carbon number hydrocarbons.

for its final disposal. Fossil-based plastics could also mitigate GHG emissions when credits are accounted for material substitution in the construction sector. Therefore, the final disposal of the polymer is more relevant than its feedstock when emissions reduction in plastic life-cycle is desired. Particularly, in times of climate emergency and plastic pollution, an opportunity arises in producing plastics for long-term applications to reduce both the carbon footprint and the plastic waste generation that may enter the marine environment. Hence, for the plastic industry adhere to the agenda of climate emergency and plastic pollution by changing its feedstock and purpose, it must become a NET and little-waste-generating industry. This, in turn, would represent a technology that provides both private – housing, insulation, lower cost – and collective, social – climate alleviation and waste reduction - benefits. A shift to construction & IF could provide an attractive opportunity to the plastics industry. To assess this opportunity in more detail the material substitution needs to be further researched. This paper showed that the BBE associated with sustainability goals must consider not only the conversion processes, but also the final disposal of the final products. Nonetheless, this study did not allow the investigation of direct and indirect impacts of biomass use on the energy-food-materials competition.

Chapter 4 presents the third paper (Oliveira et al., 2020a) produced during the PhD research, which aims to advance the understanding of the role of biomass under energy transition scenarios in Brazil and to investigate how bio-based materials can help to mitigate climate change. To achieve this, we incorporated a biomass *trilemma* (instead of the usual *dilemma* food-energy) in the Brazilian Land Use and Energy System (BLUES) model, which represents biomass competition between energy, food and materials, given land, GHG emissions (from fuel combustion and direct and indirect land use change) and water availability constrains. Very few IAMs have material representation and those exceptions usually present the petrochemical demand in an aggregated manner, although the petroleum revolution of the last century comprehended energy and food, but also materials (Smil, 2004). In addition, hardly IAMs represent advanced biomass conversion routes detailing the possibility of co-producing final energy carriers and feedstock (naphtha, propylene, propane, etc.) to the chemical industry.

As defined before, this integrated analysis of energy, land and material systems enabled to test if carbon storage in biomaterials would impact the remaining carbon emission budgets of other economic sectors; if the production of biofuels in a climate constrained

scenario could also generate co-products to produce biomaterials; or if a transition in the energy systems would generate surpluses of hydrocarbons/carbohydrates that could serve as feedstock for material production. It also allows understanding the impacts of biomaterials on the substitution of petroleum products that benefits from niche markets (green naphtha), and because of that, when produced lead to the co-production of other petroleum derivatives.

For that, we have considered the first-generation petrochemicals produced at a large-scale (ethylene, propylene, BTX and butadiene) whose bio-based counterpart could significantly reduce CO₂ emissions⁴⁰. Moreover, two major scenarios were modeled: baseline (BAU scenario) and a mitigation scenario (WB2 scenario), which assumes cumulative carbon emissions constraints consistent with the 1.5°C targets of the Paris Agreement.

Our results show that a transition in the energy system, for example, the increasing urban mobility electrification after 2040, under the WB2 scenario, would generate surpluses of hydrocarbons (mostly, naphtha)/carbohydrates (ethanol) that could serve as feedstock for material production (e.g. ethylene). Actually, in this scenario, ethylene and butadiene produced from ethanol would represent 19.0% and 20.3% of the total ethylene and butadiene production, respectively, in 2050. In both scenarios, ethanol use grows until 2035, which is consistent with the goals established in the Brazilian Renovabio program. However, from 2040 onward, ethanol use would decrease due to mobility electrification, if not deployed for petrochemical production. By 2050, 60.8% of ethanol supply would be used for petrochemical production.

Besides, the stringent mitigation scenario also led to an increase in liquid advanced biofuel production through technologies that also co-produce bio-based feedstock for material production. Diesel from BTL technology is the most important biofuel produced by 2050 for the WB2 scenario, followed by ethanol with CCS and jet fuel from BTL,

⁴⁰ The main derivatives of these resins are polypropylene (PP), low-density polyethylene (LDPE), high-density polyethylene (HDPE), polyvinyl chloride (PVC), *polyethylene* terephthalate (PET), polyurethane (PUR) and polystyrene (PS), which accounts for 21.0%, 20.0%, 16.3%, 11.8%, 10.2%, 8.2%, 7.6% of the total plastics produced globally (Geyer et al., 2017b), respectively. In Brazil, the main polymers consumed are PP (21.6%), LDPE (18.3%), HDPE (13.6%), PVC (13.6%), PET (8.1%), and PS (6.5%) (ABIPLAST, 2017b).

accounting for 42.7%, 16.9%, and 15.9% of the total biofuel production, respectively. Due to the necessity of decarbonisation associated with oil derivatives with low elasticity, advanced biomass processes with CCS (BECCS) are chosen by the model. However, by producing jet and diesel, these routes also co-output naphtha from biomass (as well as other energy carriers), which was called as “bionaphtha”. As such, under the WB2 scenario, 21.5% of the total naphtha use is bio-based by 2050. This finding shows that the production of biofuels in a climate-constrained scenario could also generate co-products, particularly naphtha to steam-crackers, but also propane to PDH, to produce bio-based materials. Interesting enough, by coproducing energy carriers and materials, the scenario was able to overcome the biomass *trilemma*. Indeed, biomass competition between energy, food and materials did not affect land use (LUC) emissions. Biomass used to produce energy enabled the co-production of bio-based materials.

In addition, given the basic lessons from paper 2, previously detailed here, paper 3 also assessed the potential of bio-based materials as NETs through carbon storage in long lifetime materials. Therefore, it modeled three mitigation scenarios derived from the WB2 scenario: demand reduction scenario (WB2_DemRed), cement substitution scenario (WB2_CS), and steel substitution scenario (WB2_SS). Our results showed that by replacing carbon-intensive materials, these scenarios reduced the needed adoption of NET. These mitigation measures led to co-benefits in cumulative emissions reductions due to drops in industrial emissions from cement (by 70.00 MtCO₂) and steel (by 225.50 MtCO₂) sectors.

NETs from carbon storage in biomaterials led to a marginally higher carbon emission budget allowed to the transport and power sectors and a higher one in the energy sector, when we considered the substitution of steel by biomaterials in construction (WB2_SS scenario). Cumulative carbon emissions in the transport sector rise from 1,400.00 Mt CO₂ in the WB2 scenario to 1,405.66 Mt CO₂ to the WB2_SS scenario; in the power sector, from 207.73 Mt CO₂ to 214.85 Mt CO₂; and in the energy sector, from 39.18 Mt CO₂ to 74.17 Mt CO₂. This higher emission budget in the energy sector is explained by the reduced demand of BECCS through BTL and ethanol production in the WB2_SS scenario. Up to 2035, carbon emissions from the energy sector in the WB2 scenario and in the WB2_SS scenarios are mostly the same. From 2040 onward, these emissions started to decouple, leading to less NETs in the WB2_SS scenario (-479.28 Mt CO₂) than in the

WB2 scenario (- 484.91 Mt CO₂) by 2050. Contrasting to the substitution of steel by biomaterials, the WB2_CS scenario did not impact the emission budget of other sectors since this scenario led to less NETs than in the WB2 scenario. This is because in the WB2 scenario CCS in the cement sector was applied, what led to an industrial emission reduction of 96.00%, when compared to the BAU scenario. Overall, the NETs achieved in the WB2_CS scenario are lower than in the WB2_SS scenario, since the reduction of steel demand had a greater impact on industrial emissions than the reduction of cement demand, which already had lower emissions due to CCS deployment.

Even though BIOCCUS in the WB2_CS and WB2_SS did not lead to higher NETs than in the WB2 scenario, the demand reduction of petroleum-derived naphtha for material purposes could impact significantly the emissions from the petroleum sector. From our results, as a significant share of the petrochemical demand could be met by bio-based feedstock such as green naphtha, green LPG and ethanol, the refinery utilization rates dropped from 2040 onwards from 95% to 13% in the Southeast region and from 87% to 0% in the South region of Brazil. The North and the Northeast regions kept an average refining utilization rate of 85%. It means that, considering the oil price assumed in the model (US\$50/ bbl), the emergence of biorefineries to provide bio-based energy and feedstock led to the reduction of refining utilization rates, which also impacts the production of oil derivatives for energy purposes, and, hence, the GHG emissions associated with their combustion. In other words, materials substitution has spillover effects on the energy transition, by lowering the production of gasoline, diesel, jet and bunker fuels, which were produced along with naphtha.

At the end, this thesis highlights the privileged position Brazil has when considering the high revenues generated from carbon credits and the attraction of investors searching for regions with available, cheap, and renewable feedstock, and already installed large-scale chemical and biofuel industries, with also qualified skilled labour to undertake the transition to the BBE. In the last years, Brazil has suffered from a deep economic recession, losing competitiveness in the international market and relying on dependence on imported chemicals. The comparative advantage of the country in biomass could be strategically used to boost the competitiveness of the chemical industry as a global player and to accelerate the decarbonisation of the sector. The concept of the biomass *trilemma* has the potential to introduce a plethora of new research lines, to bring the real complexity

of biomass use to a level of informed policy debate, and to bring attention to the importance of climate policies and carbon market mechanisms to support Brazilian chemical industry competitiveness retake.

In order to increase the robustness of our results and to expand research lines, we propose the following further researches:

- Evaluate other feedstock for the production of ethylene. Further studies could assess the hydrocarbon (e.g. naphtha) and carbohydrate production (e.g. methanol) from the hydrogenation of CO₂ with H₂ being produced through water electrolysis;
- Evaluate life-cycle GHG emissions for other plastics, such as those derived from propylene and aromatics, as well as for other routes of ethylene production;
- Apply the methodology of the second paper to other countries with different grid emission factors, chemical industry and biomass feedstock;
- Expand material representation in IAM, including other technology routes, feedstock and novel functionality of bio-based chemicals;
- Include the material module in a global IAM to assess biomass' and other feedstock's trade between regions and how it affects land use emissions and countries' carbon budges.
- Develop a material demand module in the IAM in order to consider the linkages between the energy transition, the food supply and the demand for materials.

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6. Annex A – Achieving negative emissions in plastics life-cycle through the conversion of biomass feedstock

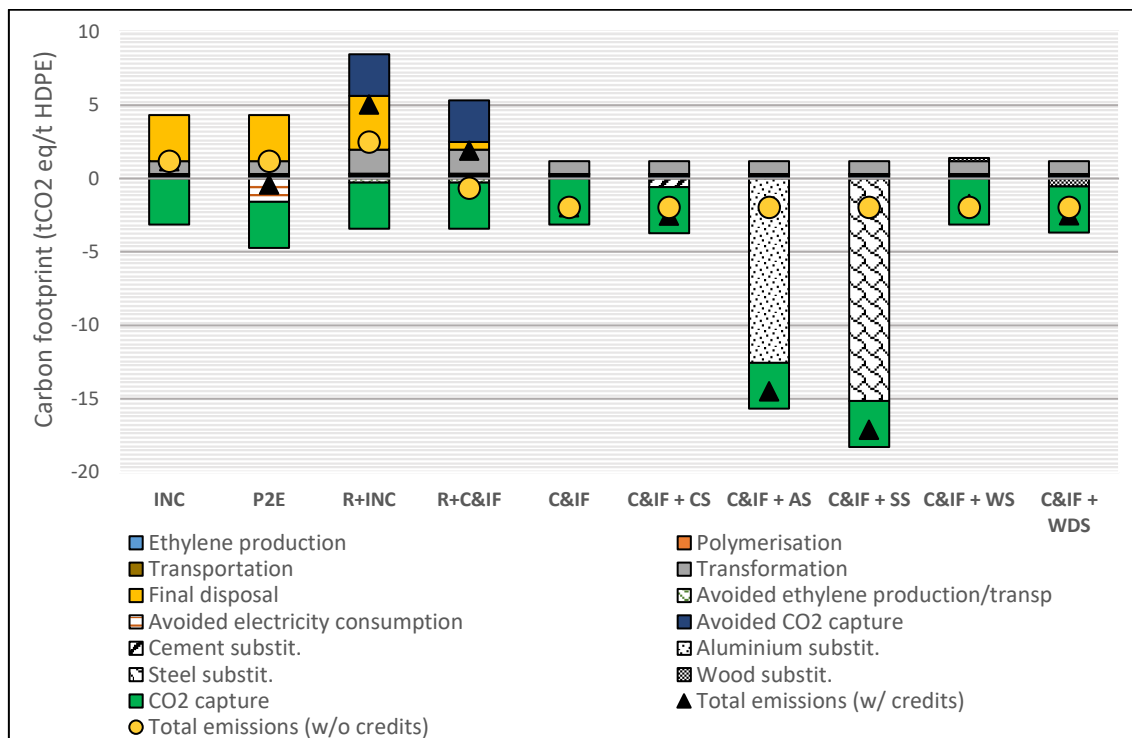


Figure 39: Carbon footprint for HDPE (ethanol to ethylene without BECCS)

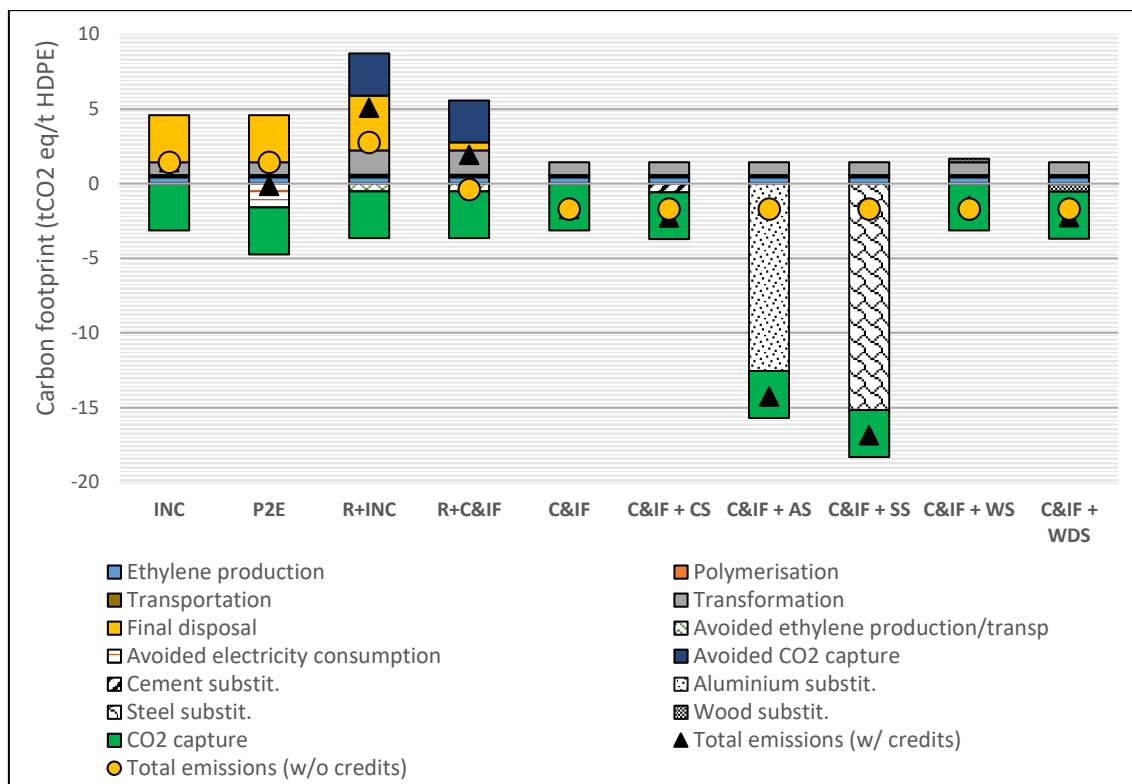


Figure 40: Carbon footprint for HDPE (bio-methanol to olefins)

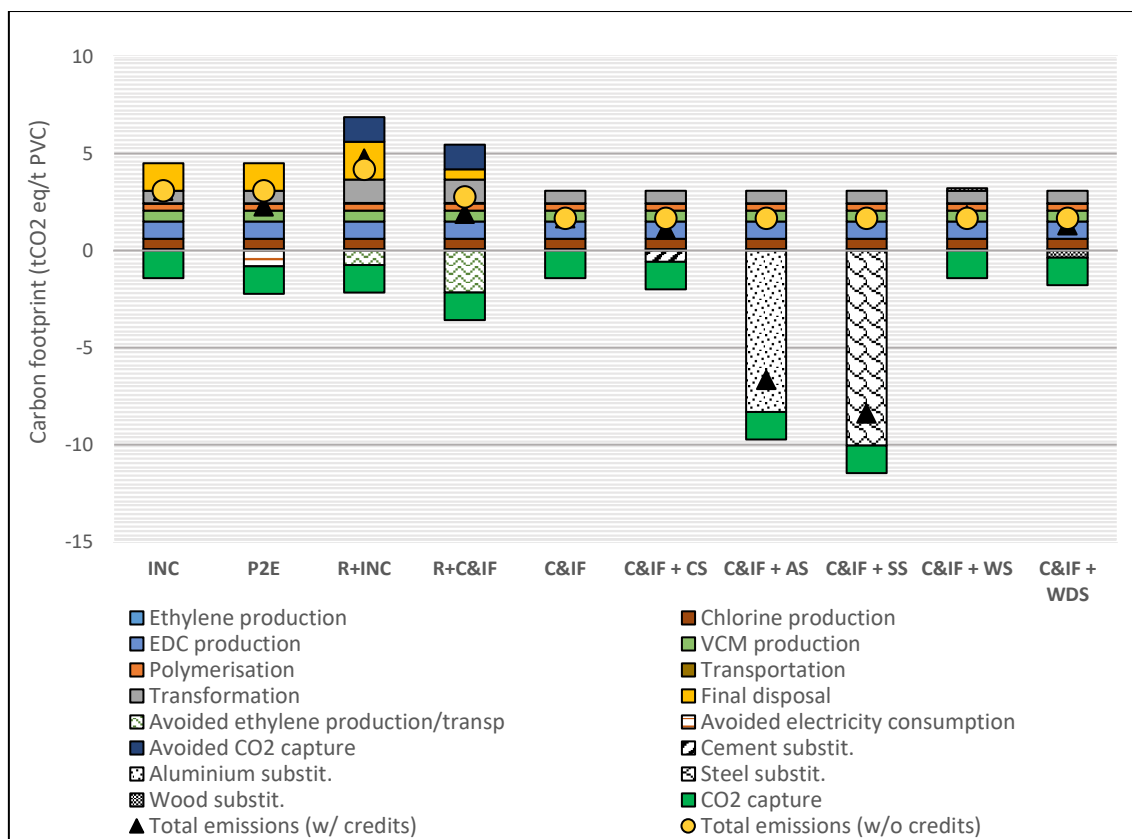


Figure 41: Carbon footprint for PVC (ethanol to ethylene without BECCS)

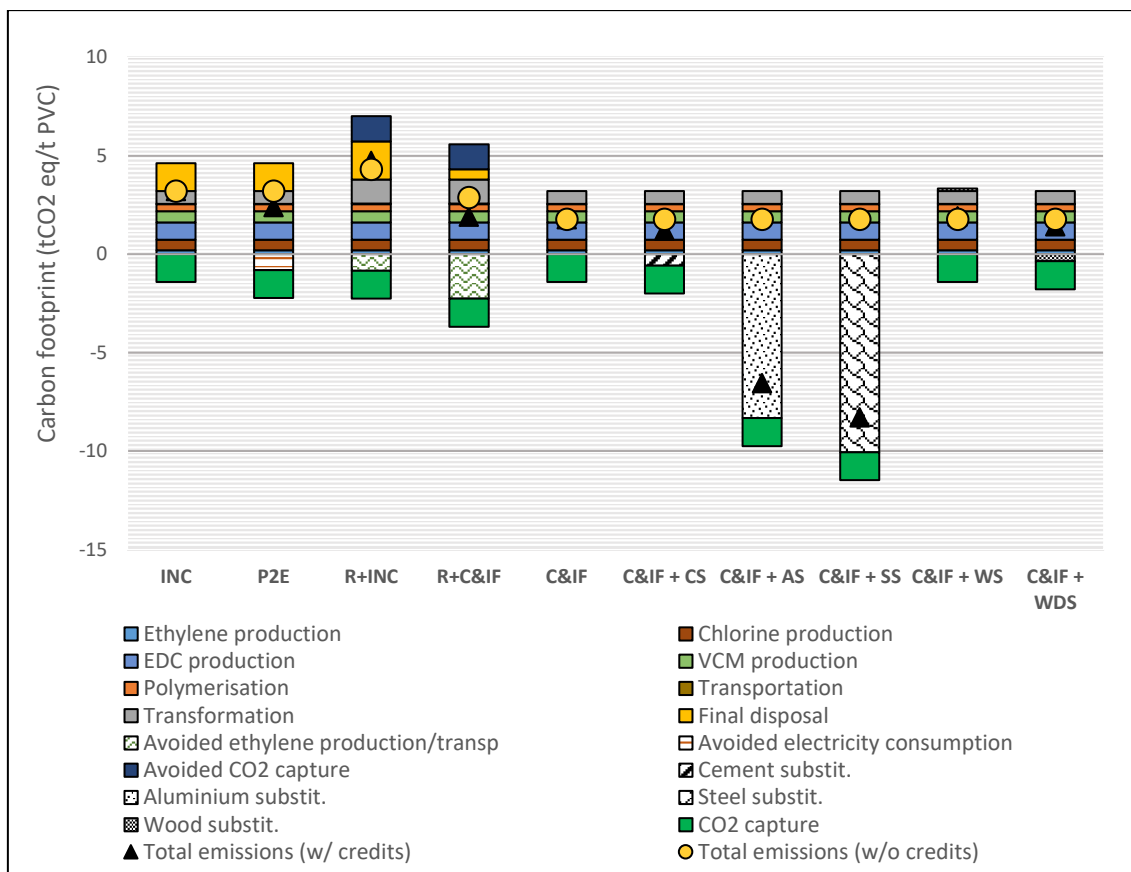


Figure 42: Carbon footprint for PVC (bio-methanol to olefins)

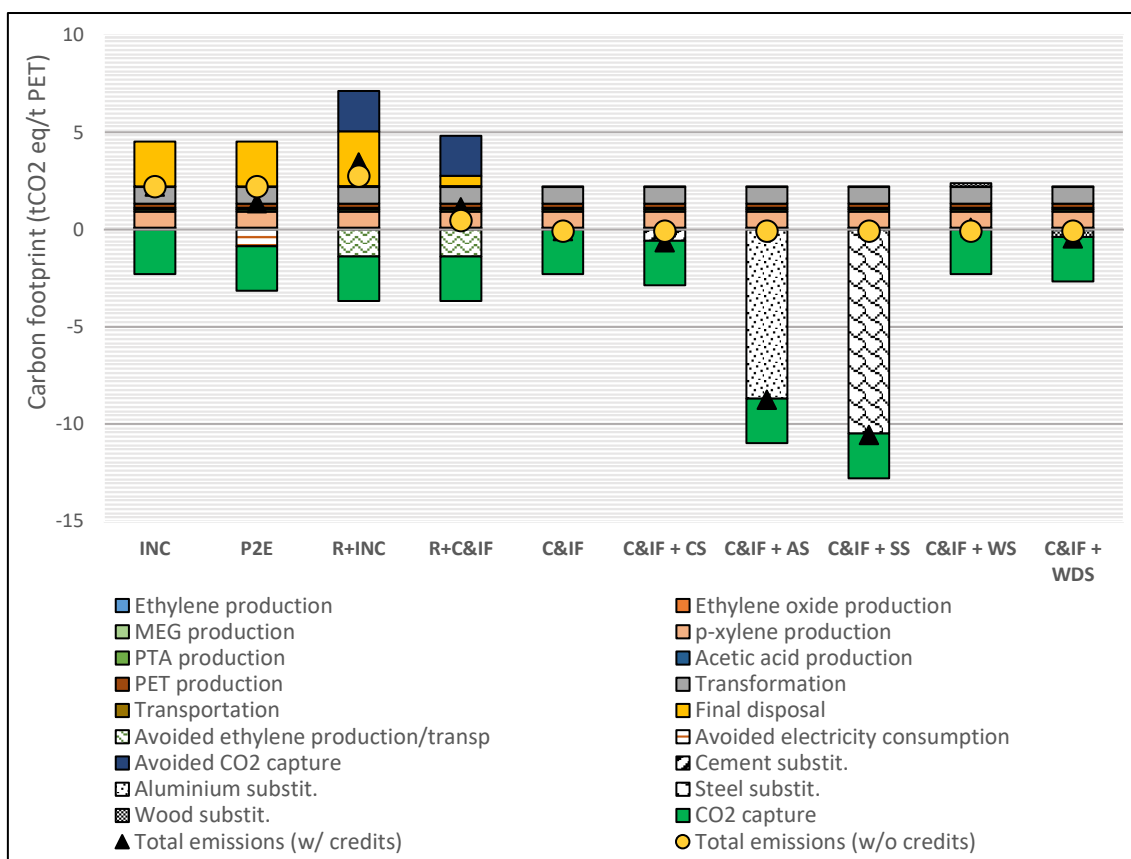


Figure 43: Carbon footprint for PET (ethanol to ethylene without BECCS)

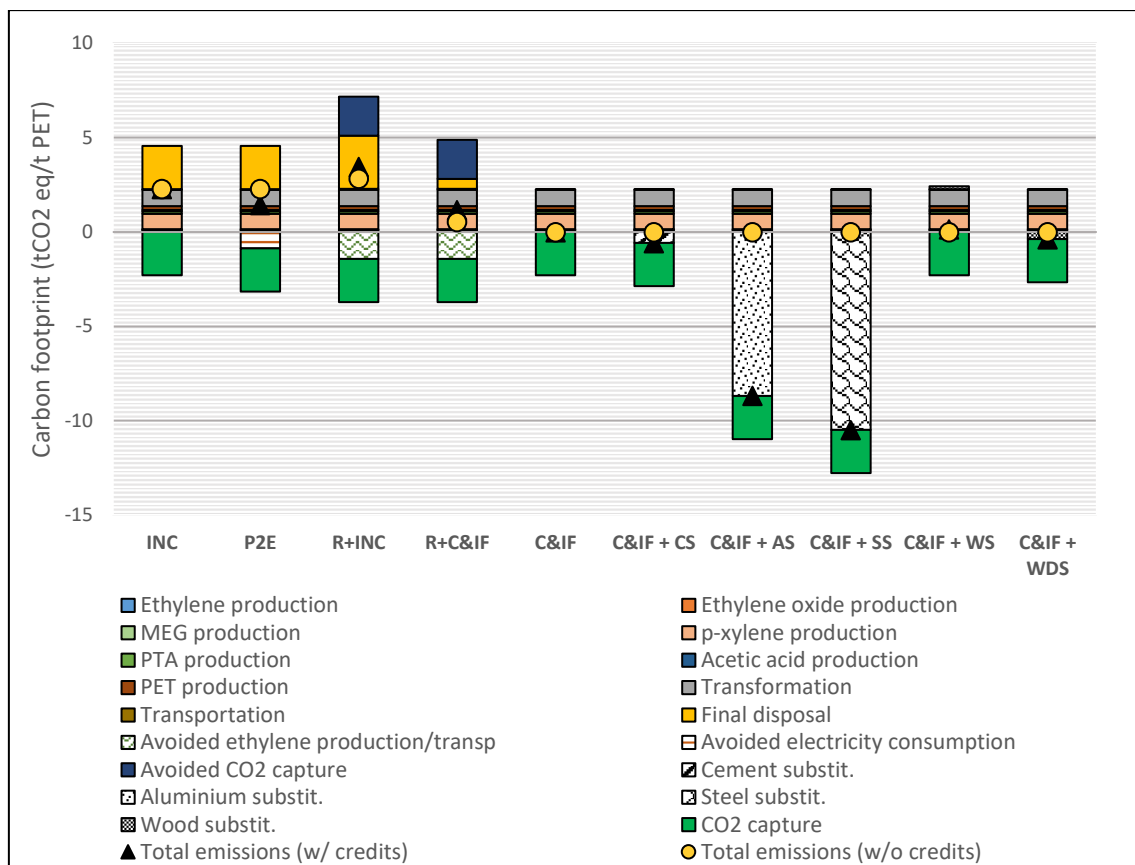


Figure 44: Carbon footprint for PET (bio-methanol to olefins)

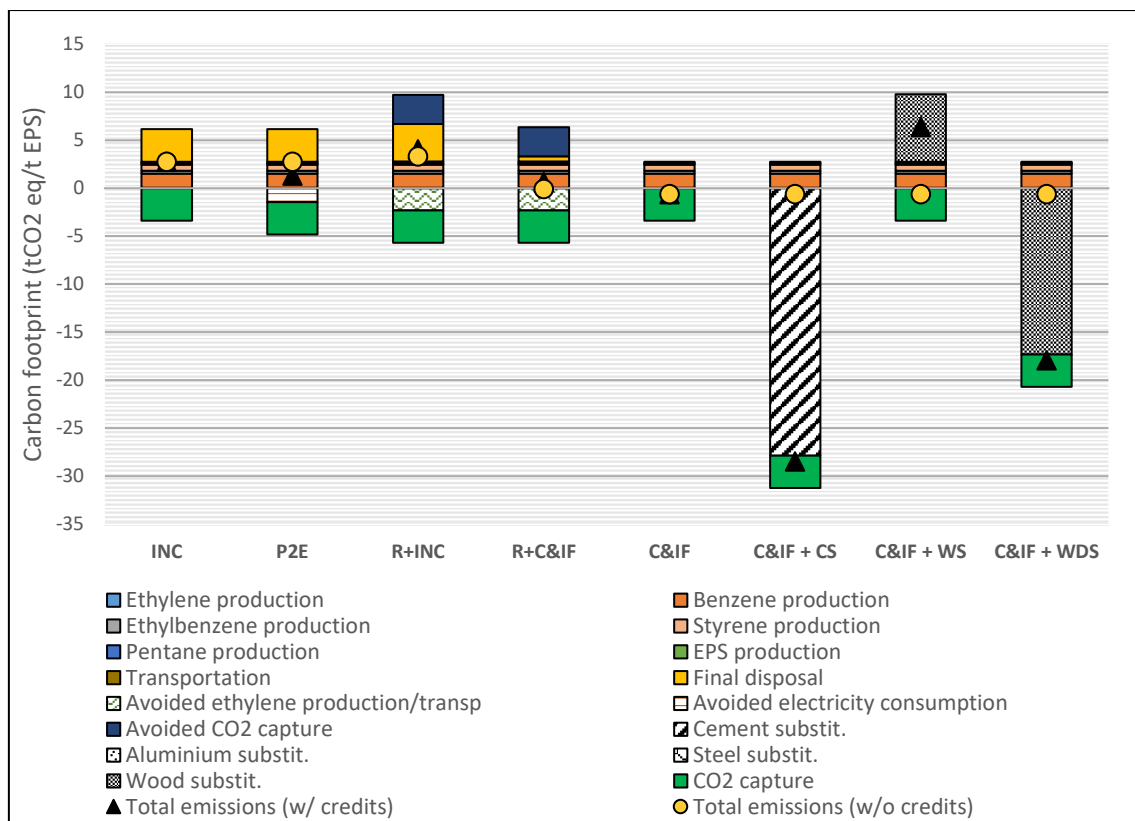


Figure 45: Carbon footprint for EPS (ethanol to ethylene without BECCS)

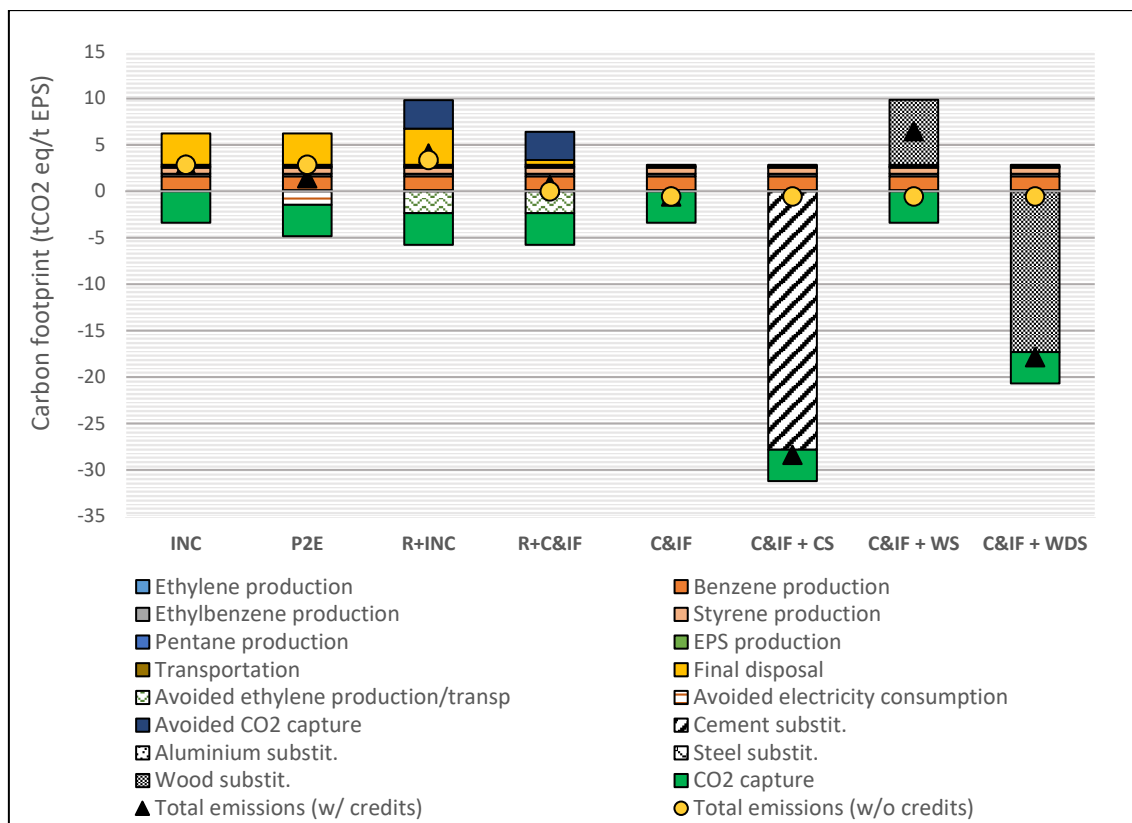


Figure 46: Carbon footprint for EPS (bio-methanol to olefins)

7. Annex B – The role of biomaterials for the energy transition from the lens of a national integrated assessment model

The Brazilian Land Use and Energy System (BLUES) model is a Brazilian integrated assessment model (IAM) built on the MESSAGE⁴¹ (Model for Energy Supply Strategy Alternatives and Their General Environmental Impacts) model generator platform. The model simulates the competition between technologies and energy sources to meet the demand for energy services and food with the objective of minimizing costs of the entire energy system, which includes: electricity generation, industry, transport, building sectors and agriculture. BLUES has around 8,000 technologies for the energy system and 20,000 for the land system.

Using the BLUES model, Rochedo et al. (2018) found that for Brazil to achieve its pledges to the Paris Agreement, the country would rely on advanced technologies, implying a large cost for the domestic economy. The authors argue that reducing deforestation is, by far, the lowest-cost option for Brazil to achieve its nationally determined contributions (NDC). More information on the BLUES model can be seen in Rochedo et al. (2018).

Our study incorporates non-energy conversion routes of oil and biomass to the BLUES model to expand the competing applications of biomass. This serves to gain insight into how biomass can contribute to the long-term Brazilian petrochemical demand under energy transition scenarios. In sum, the new BLUES model version enables to test if and how hydrocarbons currently used for the transportation sector may have their conversion chain modified for the production of materials.

BLUES optimizes the energy system between 2010 (base year) and 2050 in 5-year intervals. All costs included in the model were adjusted to US\$₂₀₁₀, according to the Chemical Engineering Plant Cost Index (CEPCI) (Chemical Engineering, 2019).

Steam cracking

⁴¹ For further details on the MESSAGE software, please refer to IAEA (2009), and Gritsevskiy and Nakićenović (2000).

Steam cracking (SC) technologies have (fossil or bio-based) naphtha or natural gas as inputs, ethylene as main output, and propylene, butadiene and the mixture of benzene, toluene and xylene (BTX) as secondary outputs. SC capital investment costs (CAPEX) and operation and maintenance costs (O&M) were calculated assuming a 500 kt ethylene/year capacity, which is the average capacity of naphtha steam crackers in Brazil (OGJ, 2015).

Table 31: SC product yields and utilities consumption

Feedstock	Yield (t ethylene/ t feedstock)	Yield (t propylene/ t feedstock)	Yield (t butadiene/ t feedstock)	Yield (t BTX/ t feedstock)	Fuel (GJ/t HVC ¹)	Steam (GJ/t HVC ¹)	Electricity (GJ/t HVC ¹)
Naphtha	0.32	0.17	0.04	0.10	14.60	-0.30	0.90
Natural gas	0.84	0.02	0.01	0.03	17.10	-0.10	0.80

⁽¹⁾ High-value chemicals (HVC) stands for ethylene, propylene, butadiene and BTX.

Source: Ren et al. (2006) and IEA (2018)

Table 32: Steam cracking cost data

Feedstock	CAPEX (\$/tpy ¹ ethylene)	OPEX (\$/t ethylene)
Naphtha	2,718	109
Natural gas	1,681	67

¹ tonnes per year

Source: TNO (2018) and Seddon (2015)

Table 33: Brazil's steam cracking capacity

Brazilian State	Feedstock	Capacity (kt ethylene/ year)
Bahia	Naphtha	600
Bahia	Naphtha	680
Rio de Janeiro	Natural gas	520
São Paulo	Naphtha	500
Rio Grande do Sul	Naphtha	700
Rio Grande do Sul	Naphtha	500

Source: OGJ (2015)

Table 34: Steam cracking additional capacities

Feedstock	Additional capacity (kt ethylene/year)				
	2010	2020	2030	2040	2050
Naphtha	200	200	200	200	200
Natural gas	100	100	150	150	150

Ethanol dehydration

Ethanol dehydration technology takes ethanol as input and ethylene as output.

Table 35: Ethanol dehydration product yield and utilities consumption

Feedstock	Yield (t ethylene/ t ethanol)	Fuel (GJ/ t ethylene)	Steam (GJ/ t ethylene)	Electricity (GJ/ t ethylene)
Ethanol	0.57	1.60	1.40	1.90

Source: Dechema (2017) and IEA (2018)

CAPEX and O&M cost for a 200 kt ethylene/ year plant capacity⁴² were obtained from SECCHI et al. (2018)

Table 36: Ethanol dehydration cost data

CAPEX (\$/tpy¹ ethylene)	OPEX (\$/t ethylene)
1,189	167

¹ tonnes per year

Source: SECCHI et al. (2018)

Table 37: Ethanol dehydration plant capacity in Brazil

Brazilian State	Feedstock	Capacity (kt ethylene/ year)
Rio Grande do Sul	Ethylene	200

Source: OGJ (2015)

Table 38: Ethanol dehydration plant additional capacities

Feedstock	Additional capacity (kt ethylene/year)				
	2010	2020	2030	2040	2050
Ethanol	0	0	40	80	120

Methanol to olefins

Methanol to olefins (MTO) technology takes (fossil or bio-based) methanol as input, ethylene as main output, and propylene as secondary output.

⁴² Brazilian ethanol-to-ethylene plant capacity based in Rio Grande do Sul.

Table 39: MTO product yields and utilities consumption

Feedstock	Yield (t ethylene/ t methanol)	Yield (t propylene/ t methanol)	Fuel (GJ/ t product ¹)	Steam (GJ/ t product ¹)	Electricity (GJ/ t product ¹)
Methanol	0.19	0.18	11.40	-2.10	0.20

(1) Product refers to the production of ethylene and propylene.

Source: TNO (2018) and IEA (2018)

CAPEX and O&M cost for a 500 kt ethylene/ year plant capacity were obtained from TNO (2018)

Table 40: MTO cost data

CAPEX (\$/tpy ¹)	OPEX (\$/t ethylene)
1,340	33

¹ tonnes per year

Source: TNO (2018)

Table 41: MTO plant additional capacities

Feedstock	Additional capacity (kt ethylene/year)				
	2010	2020	2030	2040	2050
Methanol	0	0	20	40	60

Methanol to aromatics

Methanol to aromatics (MTA) technology takes (fossil or bio-based) methanol as input, and aromatics (BTX) as output.

Table 42: MTA product yield and utilities consumption

Feedstock	Yield (t BTX/ t methanol)	Fuel (GJ/ t BTX)	Steam (GJ/ t BTX)	Electricity (GJ/ t BTX)
Methanol	0.23	11.4	-2.1	0.2

Source: Dechema (2017) and IEA (2018)

According to IEA (2018), MTA and MTO plants present analogous CAPEX and O&M cost. To calculate the costs, it was considered a 500 kt BTX/ year plant capacity.

Table 43: MTA cost data

CAPEX (\$/tpy ¹ BTX)	OPEX (\$/t BTX)
1,380	34

¹ tonnes per year

Source: TNO (2018) and IEA (2018)

Ethanol to butadiene

Ethanol to butadiene technology takes ethanol as input, and butadiene as output.

Table 44: Ethanol to butadiene product yield and utilities consumption

Feedstock	Yield (t butadiene/ t ethanol)	Heating (GJ/ t butadiene)	Cooling (GJ/ t butadiene)	Electricity (GJ/ t butadiene)
Ethanol	0.28	99.76	83.30	3.57

Source: Farzad et al. (2018)

CAPEX and O&M cost for a 29,8 kt butadiene/ year plant capacity were also obtained from Farzad et al. (2018).

Table 45: Ethanol to butadiene cost data

CAPEX (\$/tpy ¹ butadiene)	OPEX (\$/t butadiene)
7,005,002	717

¹ tonnes per year

Source: Farzad et al. (2018)

Propane Dehydrogenation

Propane dehydrogenation (PDH) technology takes (fossil or bio-based) LPG as input, propylene as main output and fuel by-products as secondary output. Costs were obtained from Meyers (2003) for a 350 kt propylene/year capacity.

Table 46: PDH product yields and utilities consumption

Feedstock	Yield (t propylene/ t LPG)	Yield (t fuel by-products/ t LPG)	Electricity (kWh/ t propylene)	Fuel gas (GJ/t propylene)
LPG	0.75	0.19	130.15	10.97

Source: Meyers (2003)

Table 47: PDH cost data

CAPEX (\$/tpy ¹ propylene)	O&M (\$/t propylene)
855	46

¹ tonnes per year

Source: Meyers (2003)

Propylene splitter

Propylene splitter technology has (fossil or bio-based) LPG as input, propylene as main output and LPG (without propylene concentration) as secondary output. Costs were obtained from Mustang Engineers and Constructors (2014) for a 118 kt propylene/year capacity.

Table 48: Propylene splitter product yields and utilities consumption

Feedstock	Yield (t propylene/ t LPG)	Yield (t LPG/ t LPG)	Heat (GJ/t propylene)
LPG	0.28	0.71	5.44E-06

Source: Petrobras (2005) and Umo and Bassey (2017)

Table 49: Propylene splitter cost data

CAPEX (\$/tpy ¹ propylene)	O&M (\$/t propylene)
577	46

¹ tonnes per year

Source: Mustang Engineers and Constructors (2014)

Bio-oil fluid catalytic cracking

Bio-oil fluid catalytic cracking (Bio-oil FCC) technology takes bio-oil as input, liquefied petroleum gas (LPG) as main output, and ethylene, naphtha, light cycle oil and clarified slurry oil as secondary outputs.

Table 50: Bio-oil FCC product yields and utilities consumption

Feedstock	Yield (t LPG/ t bio-oil)	Yield (t ethylene/ t bio-oil)	Yield (t propylene/ t bio-oil)	Yield (t naphtha/ t bio-oil)	Yield (t diesel/ t bio-oil)	Yield (t heavy oil/ t bio- oil)	Steam (MJ/t bio-oil)	Electricity (kWh/t bio-oil)	Fuel (MJ/t bio- oil)
Bio-oil	0.07	0.02	0.05	0.45	0.11	0.13	4.61	64.71	2,705.88

Source: UOP (2005) and Meyers (2003)

CAPEX for bio-oil FCC was assumed analogous to conventional FCCs including a contingency factor of 0.3 (NETL, 2010). CAPEX and O&M cost were obtained from Lantz et al. (2012).

Table 51: Bio-oil FCC cost data

CAPEX (\$/tpy ¹ LPG)	O&M (\$/t LPG)
3,291	102

¹ tonnes per year

Source: Lantz et al. (2012)

Table 52: Bio-oil FCC plant capacity per Brazilian region⁽¹⁾

Regions	North	Northeast	South	Southeast
Existing capacity bio-oil FCC (t bio-oil/year)	20,000	198,000	476,000	1,794,000

⁽¹⁾ Existing regional capacity of bio-oil FCC was assumed as 10%(U.S. Department of Energy, 2019) of existing conventional FCC in Brazil

Source: ANP (2018) and U.S. Department of Energy (2019)

Catalytic reforming

Catalytic reforming technology has (fossil or bio-based) naphtha as input, BTX as main output, and hydrogen as secondary output. Costs were obtained from Meyers (2003) for a 804 kt BTX/year capacity.

Table 53: Catalytic reforming product yields and utilities consumption

Feedstock	Yield (t BTX/ t naphtha)	Yield (t H ₂ / t naphtha)	Electricity (kWh/t BTX)	Fuel fired (GJ/t BTX)
Naphtha	0.88	0.03	83.37	3.18

Source: Meyers (2003)

Table 54: Catalytic reforming cost data

CAPEX (\$/tpy ¹ BTX)	O&M (\$/t BTX)
84	16

¹ tonnes per year

Source: Meyers (2003)

The ancillary technologies included in the BLUES model are following:

Biomass to liquids

Two biomass to liquids (BTL) technologies were incorporated in the model: one has diesel as main output (BTL D), and naphtha, LPG, gasoil as secondary outputs; and the other one has jet fuel (BTL J) as main output and naphtha, LPG and gasoil as secondary outputs. Product yields by mass and utilities consumption were derived from Tagomori (2017) and Carvalho (2017) for BTL D and BTL J technologies, respectively. It was considered a BTL plant with and without CO₂ capture. Costs were obtained from Tagomori (2017) for a 290 kt naphtha/ year plant capacity.

Table 55: BTL product yields and utilities consumption

Tech nol.	Input	Yield (GJ diesel/ GJ bioma ss)	Yield (GJ jet fuel/ GJ biomas s)	Yield (GJ naphtha/ GJ biomass)	Yield (GJ LPG/ GJ biomass)	Yield (GJ gasoil/ GJ biomass)	Electricity w/o capture (MWh/ main output)	Electricity w/ capture (MWh/ main output)
BTL D	Biom ass	0.32	-	0.13	0.11	0.03	0.30	0.30
BTL J	Biom ass	-	0.3 1	0.11	0.11	0.03	0.30	0.30

Source: Tagomori (2017) and Carvalho (2017)

Table 56: BTL cost data

Technol.	CAPEX w/o capture (\$/GJ main output)	CAPEX w/ capture (\$/GJ main output)	OPEX w/o capture (\$/GJ main output)	OPEX w/capture (\$/GJ main output)
BTL D	266	269	10	11
BTL J	266	269	10	11

Source: Tagomori (2017)

Biomass to methanol

Biomass to methanol technology has biomass as input and methanol as output. CAPEX and O&M cost were obtained from IEA (2018).

Table 57: Biomass to methanol product yield and utilities consumption

Feedstock	Yield (t methanol/ t biomass)	Fuel (GJ/ t methanol)	Steam (GJ/ t methanol)	Electricity (GJ/ t methanol)
Biomass	0.30	28.00	-5.90	5.00

Source: Renó et al. (2011) and IEA (2018)

Table 58: Biomass to methanol cost data

CAPEX (\$/tpy ¹ methanol)	O&M (\$/t methanol)
4,900	245

¹ tonnes per year

Source: IEA (2018)

Oligomerization

Oligomerization technologies have ethylene as main input and they are categorized into three sub-technologies regarding their main outputs: ethylene to jet fuel (ETJ) has jet fuel as main output and diesel, naphtha and heavy oil as secondary outputs; ethylene to diesel (ETD) has diesel as main output and naphtha as secondary output; and ethylene to naphtha (ETN) has naphtha as main output and diesel as secondary output. Costs were obtained from Diederichs (2015) for a 75 kt jet fuel/year capacity.

Table 59: Oligomerization product yields and utilities consumption

Technology	Feedstock	Yield (t naphtha/t ethylene)	Yield (t jet fuel/t ethylene)	Yield (t diesel/t ethylene)	Yield (t heavy oil/t ethylene)	H ₂ consumption (t H ₂ / t main output)	Electricity use (kWh/t main output)	Water use (l/t main output)
ETJ	Ethylene	0.10	0.33	0.09	0.02	0.01	9.31	2,436.57
ETD	Ethylene	0.12	-	0.42	-	0.01	7.24	1,906.88
ETN	Ethylene	0.49	-	0.05	-	0.01	6.50	1,624.38

Source: BYOGY (2017)

Table 60: Oligomerization cost data

Technology	CAPEX (\$/tpy ¹ main output)	O&M (\$/t main output)
ETJ	596	14
ETD	466	11
ETN	416	10

Source: Diederichs (2015)

Table 61: Projection of plastics' final disposal in *BAU scenario*

Final disposal (BAU)	2010	2015	2020	2025	2030	2035	2040	2045	2050
Landfill (%)	81.73%	81.73%	80.00%	79.50%	79.50%	79.50%	79.00%	79.00%	79.00%
Ethylene	76.29%	76.29%	73.02%	72.52%	72.52%	72.52%	72.02%	72.02%	72.02%
Propylene	85.31%	85.31%	83.29%	83.04%	83.04%	83.04%	82.80%	82.80%	82.80%
BTX	91.41%	91.41%	90.23%	90.16%	90.16%	90.16%	90.09%	90.09%	90.09%
Butadiene	81.31%	81.31%	92.54%	92.53%	92.53%	92.53%	92.52%	92.52%	92.52%
Incineration (%)	0.00%	0.00%	0.00%	0.50%	0.50%	0.50%	1.00%	1.00%	1.00%
Ethylene	0.00%	0.00%	0.00%	0.50%	0.50%	0.50%	1.00%	1.00%	1.00%
Propylene	0.00%	0.00%	0.00%	0.24%	0.24%	0.24%	0.48%	0.48%	0.48%
BTX	0.00%	0.00%	0.00%	0.07%	0.07%	0.07%	0.14%	0.14%	0.14%
Butadiene	0.00%	0.00%	0.00%	0.01%	0.01%	0.01%	0.02%	0.02%	0.02%
Recycling (%)	18.27%	18.27%	20.00%	20.00%	20.00%	20.00%	20.00%	20.00%	20.00%
Ethylene	23.71%	23.71%	26.98%	26.98%	26.98%	26.98%	26.98%	26.98%	26.98%
Propylene	14.69%	14.69%	16.71%	16.71%	16.71%	16.71%	16.71%	16.71%	16.71%
BTX	8.59%	8.59%	9.77%	9.77%	9.77%	9.77%	9.77%	9.77%	9.77%
Butadiene	6.56%	6.56%	7.46%	7.46%	7.46%	7.46%	7.46%	7.46%	7.46%
Total	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

Table 62: Projection of plastics' final disposal in *WB2_DemRed* scenario

Final disposal (WB2_DemRed)	2010	2015	2020	2025	2030	2035	2040	2045	2050
Landfill (%)	81.73%	81.73%	75.14%	67.72%	64.89%	62.73%	60.58%	59.41%	58.71%
Ethylene	76.29%	76.29%	66.47%	56.64%	52.65%	49.18%	44.31%	38.97%	34.68%
Propylene	85.31%	85.31%	79.22%	73.20%	70.73%	69.27%	68.75%	69.37%	69.93%
BTX	91.41%	91.41%	87.86%	84.41%	82.96%	82.11%	81.87%	82.23%	82.56%
Butadiene	81.31%	81.31%	90.73%	88.14%	87.80%	87.03%	86.99%	87.38%	87.75%
Incineration(%)	0.00%	0.00%	0.00%	0.50%	0.50%	0.51%	1.07%	1.16%	1.23%
Ethylene	0.00%	0.00%	0.00%	0.50%	0.50%	0.52%	1.13%	1.31%	1.45%
Propylene	0.00%	0.00%	0.00%	0.24%	0.24%	0.24%	0.50%	0.51%	0.52%
BTX	0.00%	0.00%	0.00%	0.07%	0.07%	0.07%	0.15%	0.15%	0.16%
Butadiene	0.00%	0.00%	0.00%	0.01%	0.01%	0.01%	0.02%	0.02%	0.02%
Recycling (%)	18.27%	18.27%	24.86%	31.78%	34.61%	36.77%	38.35%	39.43%	40.06%
Ethylene	23.71%	23.71%	33.53%	42.86%	46.85%	50.31%	54.56%	59.73%	63.87%
Propylene	14.69%	14.69%	20.78%	26.56%	29.03%	30.49%	30.76%	30.12%	29.54%
BTX	8.59%	8.59%	12.14%	15.52%	16.97%	17.82%	17.98%	17.61%	17.28%
Butadiene	6.56%	6.56%	9.27%	11.85%	12.19%	12.96%	12.99%	12.60%	12.23%
Total	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

Table 63: Projection of plastics' final disposal in WB2_CS scenario

Final disposal (WB2_CS)	2010	2015	2020	2025	2030	2035	2040	2045	2050
Landfill (%)	81.73%	81.73%	75.14%	67.89%	63.21%	59.66%	56.44%	53.94%	52.01%
Ethylene	76.29%	76.29%	66.47%	56.64%	49.94%	44.63%	38.33%	31.78%	26.70%
Propylene	85.31%	85.31%	79.22%	73.20%	69.98%	67.94%	66.88%	66.94%	66.99%
BTX	91.41%	91.41%	87.86%	84.41%	82.91%	82.02%	81.74%	82.07%	82.36%
Butadiene	93.44%	81.31%	90.73%	88.14%	87.80%	87.03%	86.99%	87.38%	87.75%
Incineration (%)	0.00%	0.00%	0.00%	0.50%	0.48%	0.48%	0.99%	1.05%	1.08%
Ethylene	0.00%	0.00%	0.00%	0.50%	0.47%	0.47%	0.98%	1.07%	1.12%
Propylene	0.00%	0.00%	0.00%	0.24%	0.24%	0.24%	0.48%	0.49%	0.50%
BTX	0.00%	0.00%	0.00%	0.07%	0.07%	0.07%	0.15%	0.15%	0.16%
Butadiene	0.00%	0.00%	0.00%	0.01%	0.01%	0.01%	0.02%	0.02%	0.02%
Recycling (%)	18.27%	18.58%	24.86%	31.78%	33.63%	34.87%	35.50%	35.55%	35.23%
Ethylene	23.71%	23.71%	33.53%	42.86%	44.43%	45.66%	47.21%	48.72%	49.17%
Propylene	14.69%	14.69%	20.78%	26.56%	28.72%	29.90%	29.92%	29.07%	28.30%
BTX	8.59%	8.59%	12.14%	15.52%	16.96%	17.80%	17.95%	17.58%	17.24%
Butadiene	6.56%	6.56%	9.27%	11.85%	12.19%	12.96%	12.99%	12.60%	12.23%
Long lifetime material (%)	0.00%	0.00%	0.00%	0.00%	2.85%	5.16%	7.41%	9.83%	12.05%
Ethylene	0.00%	0.00%	0.00%	0.00%	5.16%	9.24%	13.48%	18.43%	23.01%
Propylene	0.00%	0.00%	0.00%	0.00%	1.06%	1.92%	2.72%	3.50%	4.21%
BTX	0.00%	0.00%	0.00%	0.00%	0.06%	0.11%	0.15%	0.20%	0.24%
Butadiene	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Total	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00

Table 64: Projection of plastics' final disposal in WB2_SS scenario

Final disposal (WB2_SS)	2010	2015	2020	2025	2030	2035	2040	2045	2050
Landfill (%)	81.73%	81.73%	75.14%	67.89%	64.72%	62.26%	59.99%	58.48%	57.39%
Ethylene	76.29%	76.29%	66.47%	56.64%	52.14%	48.24%	42.97%	37.20%	32.51%
Propylene	85.31%	85.31%	79.22%	73.20%	70.59%	69.01%	68.36%	68.84%	69.25%
BTX	91.41%	91.41%	87.86%	84.41%	82.95%	82.09%	81.84%	82.20%	82.52%
Butadiene	93.44%	81.31%	90.73%	88.14%	87.80%	87.03%	86.99%	87.38%	87.75%
Incineration (%)	0.00%	0.00%	0.00%	0.50%	0.50%	0.50%	1.06%	1.14%	1.19%
Ethylene	0.00%	0.00%	0.00%	0.50%	0.50%	0.51%	1.10%	1.25%	1.36%
Propylene	0.00%	0.00%	0.00%	0.24%	0.24%	0.24%	0.49%	0.51%	0.52%
BTX	0.00%	0.00%	0.00%	0.07%	0.07%	0.07%	0.15%	0.15%	0.16%
Butadiene	0.00%	0.00%	0.00%	0.01%	0.01%	0.01%	0.02%	0.02%	0.02%
Recycling (%)	18.27%	18.58%	24.86%	31.78%	34.43%	36.39%	37.74%	38.54%	38.87%
Ethylene	23.71%	23.71%	33.53%	42.86%	46.39%	49.35%	52.91%	57.02%	59.88%
Propylene	14.69%	14.69%	20.78%	26.56%	28.97%	30.37%	30.59%	29.90%	29.26%
BTX	8.59%	8.59%	12.14%	15.52%	16.96%	17.81%	17.98%	17.61%	17.27%
Butadiene	6.56%	6.56%	9.27%	11.85%	12.19%	12.96%	12.99%	12.60%	12.23%
Long lifetime material (%)	0.00%	0.00%	0.00%	0.00%	0.53%	1.02%	1.58%	2.24%	2.96%
Ethylene	0.00%	0.00%	0.00%	0.00%	0.98%	1.90%	3.02%	4.54%	6.24%
Propylene	0.00%	0.00%	0.00%	0.00%	0.19%	0.37%	0.56%	0.76%	0.97%
BTX	0.00%	0.00%	0.00%	0.00%	0.01%	0.02%	0.03%	0.04%	0.05%
Butadiene	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%	0.00%
Total	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00	1.00