



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

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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. This allows us to evaluate if the production of biofuels in a climate-constrained scenario can co-output biomaterials, being also driven by hydrocarbons/carbohydrates liquid streams made available 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. The findings show that bio-based petrochemicals account for 33% of the total petrochemical production in a stringent carbon dioxide mitigation scenario, in 2050. Most of this comes as co-products from facilities that produce advanced fuels as the main product. Moreover, from 2040 mobility electrification leads to the repurpose of ethanol 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.

Keywords Integrated assessment models · Energy transition · Biomass · Petrochemicals

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1 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 (BECCS¹) (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; 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 as a form of CCU² (Junginger et al. 2019; Oliveira et al. 2020a, 2020b).

Most of the studies have dealt with biomass conversion from the perspective of the energy-food dilemma (Bauer et al. 2018; 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. (2014, 2019), 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 or alleviating 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 of 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 emissions³ (Daioglou 2016; Searchinger et al. 2008; Wicke et al. 2015). In addition, hardly any 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.).

Two trajectories of biomass supply are worth considering in deep greenhouse gases (GHG) emissions mitigation scenarios. On the one hand, biomass supply for material production could rise in energy transition scenarios due to a likely increase in urban mobility electrification that might lead to the availability of liquid streams that were previously blended in automotive

¹ Bioenergy with carbon capture and storage.

² Carbon capture and usage.

³ 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).

fuels, including biofuels.⁴ In this case, the use of biomass for chemical production could serve as an alternative market, which would also lead to carbon capture from chemical reactions. Furthermore, the demand for chemicals is expected to grow in energy transition scenarios. For instance, to reduce fuel consumption, plastic-based materials are integrated in vehicles 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 constraints (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 constraints that limit biomass supply for materials production.

Bio-derived materials⁵ refer 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) model.⁶ Materials here are represented by fossil and bio-based petrochemicals.⁷ 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 for the whole period 2010–2050. 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 2018). The model has a plethora of biomass sources defined at regional level and has a detailed technological structure. Moreover, the BLUES model has a vast number of advanced biomass conversion processes, which could be improved to supply feedstock to the chemical industry.

⁴ 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).

⁵ As well as all renewable-derived materials (e.g., from green H₂).

⁶ Previous studies using the BLUES model are Rochedo et al. (2018) and Roelfsema et al. (2020).

⁷ 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.

Therefore, an integrated analysis of energy, land and material systems enables to test if carbon storage in biomaterials would impact the remaining carbon emission budgets⁸ of 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 repurpose hydrocarbons/carbohydrates, from already installed facilities, which 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 2018); 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. As highlighted by Oliveira et al. (2020a), Brazil could be a potential pioneer in large-scale bio-based plastics production due to its well-established sugar and alcohol sector. The Brazilian petrochemical sector is the 8th largest in the world, representing 2% of the global petrochemical production. The sector represents 10% of the industrial GDP and it is the third largest manufacturing sector in the country (Deloitte 2018). Brazil is already well-represented by a highly detailed national IAM, in terms of energy and land-use systems, but without a suitable representation of materials as this study aims to provide.

In Section 2, the technologies included in the model are described as well as the scenarios assumptions and plastic's final disposal options included in the model. The Supplementary Material presents further details on the modified model to incorporate the material module. Section 3 presents the results of the scenario projections highlighting petrochemical demand per technology and its effects on energy and land-use emissions. Section 4 draws conclusions and recommendations for future studies.

2 Methods

Little attention has been given to the non-energy applications of hydrocarbons in IAMs. Table 1 presents the models and their current representation of chemical demand. Among 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 and rubber; 2 have an aggregated non-energy use representation; 1 has a representation for aggregated high value chemicals⁹ (HVC), ammonia, methanol, and refinery products; and 1 has a detailed representation of ethylene, propylene, and ammonia.

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 the Supplementary Material.

⁸ Carbon budget is the cumulative CO₂ emissions associated with achieving certain climate targets with a certain probability (van Vuuren et al. 2016).

⁹ HVC stands for the mixture of ethylene, propylene, butadiene, and aromatics.

Table 1 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	(JGCRJ 2019)
IMAGE-TIMER	Netherlands	HVC, ammonia, methanol, refinery products	(Daloglou 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	(Anandarahaj 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	(Köhler 2018)

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

2.1 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)¹⁰ defined here as main technologies. 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. 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 technology¹¹ that uses naphtha as input. Production of naphtha, in turn, can be achieved by the refining sector, by biomass to liquids (BTL) technology (green naphtha), and by oligomerization technology (fossil or green naphtha depending on the origin of the ethylene). 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.

The Supplementary Material 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 1 presents the flowcharts of the processes included in the BLUES model.

2.2 Scenarios for petrochemicals demand

The model projects one Baseline scenario, which follows a reference case for basic petrochemicals demands, consistent with Brazil's Nationally Determined Contribution (NDC), which follows the petrochemical demand per capita from the Brazilian Association of Chemical Industry (Abiquim)¹²; and a mitigation scenario that assumes cumulative carbon emissions constraints consistent with the "well below 2 °C" targets of the Paris Agreement (WB2 scenario). In this case, a carbon budget of 14 GtCO₂ was established according to the runs of a global IAM developed in parallel with the Brazilian model (called COFFEE model). The COFFEE model was used in different inter-models 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 et al. 2020). Clearly, this carbon budget is uncertain and depends 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

¹⁰ The production chain of liquid fuels in the BLUES model (from biomass, crude oil, and natural gas) produces intermediary streams that will be blended in the pool of the finished products.

¹¹ The model finds as a cost optimal solution what technology or pool of technologies meet energy and material demand between 2010 (base year) and 2050 in 5-year intervals.

¹² It would be better to perform a detailed modeling of the driving forces behind petrochemicals demand in Brazil and even in the world. However, for this to happen, our study would lose its focus on improving the representation of petrochemicals supply in oil and biomass conversion plants (including co-production with fuels). In this case, in our study, we decided to perform a sensitivity analysis on petrochemicals demand.

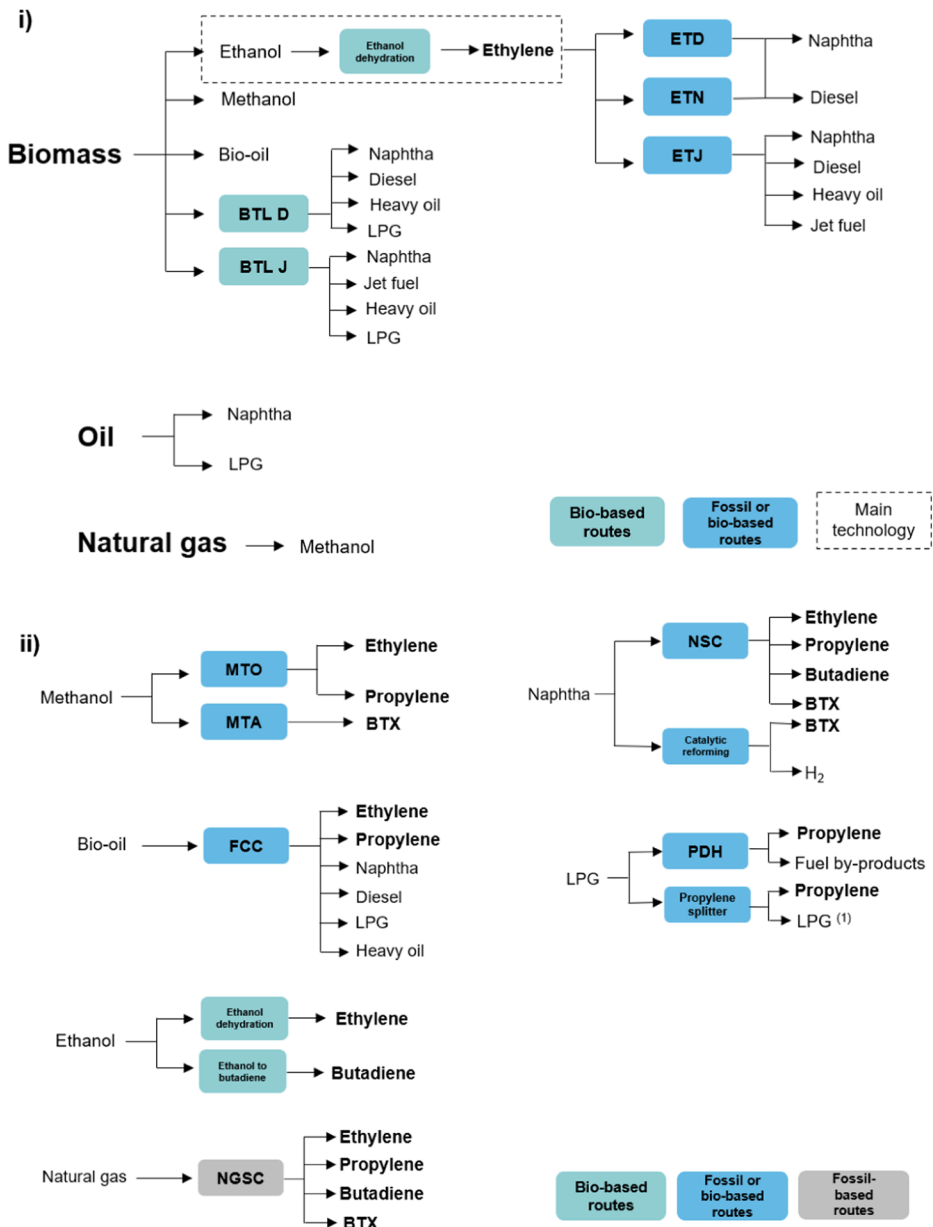


Fig. 1 i Ancillary technologies included in the BLUES model. Despite ethanol dehydration being a main technology, it is represented also here to show the further ethylene oligomerization step to produce intermediary products such as naphtha, diesel, jet fuel, and heavy oil (ETD, ETN, ETJ). ii Main technologies included in the BLUES model. The list of acronyms is presented in the Supplementary Material

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 did we try to make an intermodal comparison exercise to show their contributions and drawbacks (see, for instance, Gambhir et al. 2019a, 2019b; Rogelj et al.

2019; Weyant 2017). Instead, we aimed at developing a material module and identifying the contribution of biomaterials to a stringent GHG mitigation scenario. 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 (for a brief description of COFFEE, see also IAMC Wiki 2019).

In addition, a previous paper (Oliveira et al. 2020b) 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 lifetime material, and 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).¹³

In this case, while the Baseline and WB2 scenarios project the same petrochemical demand, according to IEA (2018), the petrochemical demand of 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).

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. For further details on the material densities, and the assumptions of cement and steel substitution by plastics, please refer to the Supplementary Material and Oliveira et al. (2020b), respectively. 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). 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 can be seen in the Supplementary Material. 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 apply for long lifetime material. Thereby, these scenarios consider the WB2_DemRed as the reference case. The petrochemicals demand for the Baseline, the WB2_DemRed, WB2_CS, and the WB2_SS scenarios can be seen in the Supplementary Material.

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 Supplementary Material shows the price of derivatives¹⁴ considered in the study, which is consistent with a premium or discount relative to the price of oil. In addition, we run a sensitivity analysis for a higher benchmark crude oil price (equal to 75 US\$/bbl)¹⁵ as this higher value can modify the attractiveness of petroleum refineries and the trade

¹³ The carbon budget constraint of the WB2 and its derived scenarios is 14 GtCO₂. The difference between these scenarios is how the carbon budget is allocated between the sectors.

¹⁴ Derivatives from oil and biomass.

¹⁵ We favored simulating a higher oil price, instead of a price lower than 50 US\$/bbl, as higher oil prices will likely affect more the liquid fuel production, by lowering import and favoring exports. In addition, since scenarios with stringent carbon budgets are not expected to find an equilibrium between crude oil demand and supply at higher prices, given the lower crude demand (Huppmann et al. 2018), for the sake of simplicity, we decided to assess the impact of higher oil prices only on the Baseline scenario.

results of liquid products. Again, 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.

2.3 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 3.

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 the Supplementary Material. 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 Eq. 1.

$$NET_i = \frac{n^\circ \text{carbons}_i \times \text{molar mass}_{\text{CO}_2}}{\text{molar mass}_i} \quad (1)$$

where

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

i = bio-based petrochemical;

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

$\text{molar mass}_{\text{CO}_2}$ = 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 of 469 kWh/t plastics (Shonfield 2008), and the Brazilian grid emission factor of 0.58 tCO₂/MWh (MCTIC 2017a).

In the Baseline 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, modeled in MCTIC (2017b). 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 the Supplementary Material.

3 Results and discussion

3.1 Energy system

Primary energy consumption in Brazil increases to 462 and 658 Mtoe/year in 2050 for the Baseline and the WB2 scenarios, respectively. This represents an increase of 56% and 122% for the Baseline and the WB2 scenarios, respectively, when compared to 2019 levels. 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. For further information on the primary energy consumption, please refer to the Supplementary Material.

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.

3.2 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 program.¹⁶ 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 (Fig. 2). For the Baseline scenario, ethanol without CCS (71.5%) and biodiesel (FAME) (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 6469 PJ/year by 2050. Thereby, diesel from BTL technology (green diesel) is the most important biofuel produced, followed by ethanol with CCS and jet fuel from BTL (green jet fuel), 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 account for 14 Mha, 54 Mha, and 8 Mha, respectively. 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 (see Fig. S7 in the Supplementary Material for more information on land use change).

¹⁶ 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).

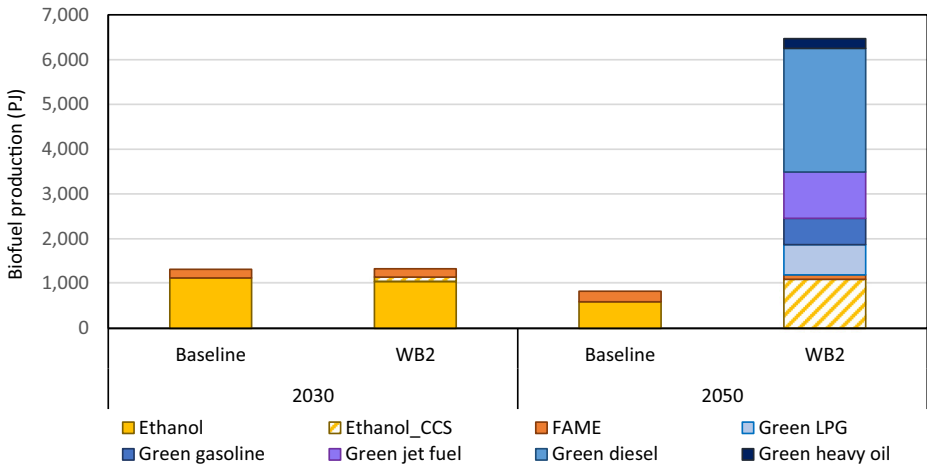


Fig. 2 Biofuel production for all scenarios (PJ/year). The transportation sector drives the demand for biofuel with CCS (BTL technologies with CCS) in 2050 in the WB2 scenario, while, at the same time, produces bio-based feedstock for petrochemical production such as green LPG and green naphtha (represented in the green gasoline pool in this figure)

Therefore, our results show that the higher demand for bio-based materials and fuels in the WB2 scenario does not increase AFOLU emissions (Fig. 3), 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 LPG that are used as feedstock for petrochemical production.

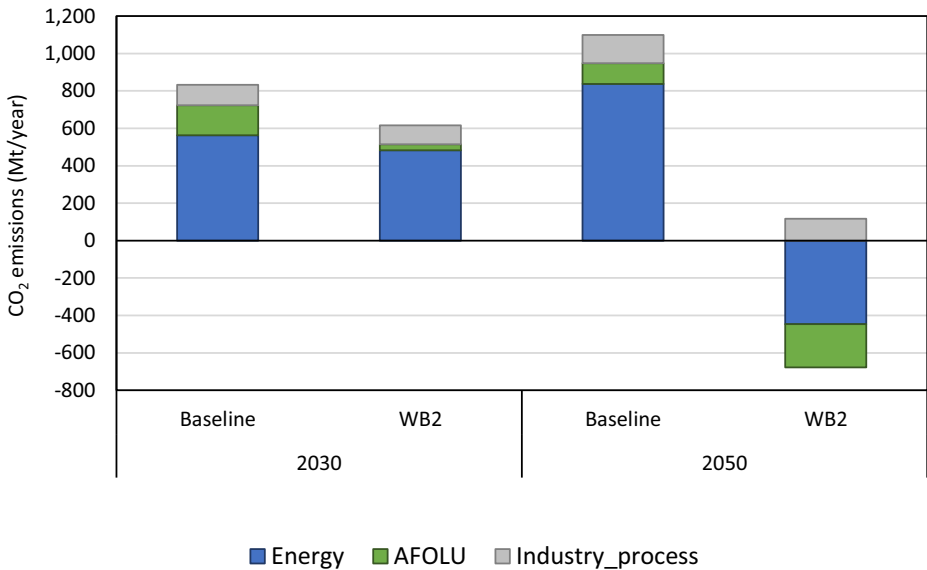


Fig. 3 CO₂ emissions in 2030 and 2050 for the Baseline and WB2 scenarios. Effective climate change mitigation policies in the land-use sector (e.g., forest-protection) lead to decreasing land-use change emissions even though biofuel production increases substantially. CO₂ emissions from AFOLU are negative in 2050 due to afforestation

The results for the sensitivity analysis for a higher benchmark crude oil price (equal to 75 US\$/bbl) in the Baseline scenario shows that biofuel production increased by 20%, driven mostly by ethanol that increased by 15% (mainly for producing jet fuel using the ETJ route). Jet fuel and naphtha imports declined (20% and 15% in 2050). Derivatives exports increased 78% (mainly final gasoline and LPG). Refining utilization factor increased by 2%. All these results were expected, as they revealed that higher oil prices (hence, higher oil product prices) favor exports and undermine imports. This has also implications on materials' findings (see the next section).

3.3 Petrochemical production

Bio-based petrochemical production reaches 33% of total petrochemical production by 2050 for the WB2 scenario (Fig. 4). Naphtha steam cracking (SC) remains the dominant technology to produce ethylene, propylene, BTX and butadiene through the whole period for both scenarios. In 2050, 21.5% of the naphtha used in SC comes from biomass (green naphtha). Ethanol-to-ethylene route is also worthwhile in 2050.

In the WB2 scenario, after 2040, an increase of urban mobility electrification leads to an increasing orientation of liquid streams, hydrocarbons (mostly, naphtha) and carbohydrates (ethanol), to serve as feedstock for material production. They are produced in plants already amortized that were firstly focused only on the production of fuels. Hence, in 2050, ethylene and butadiene produced from ethanol would represent 19% and 20% of the total ethylene and butadiene production, respectively. Still in 2050, MTO technology is used for 7% of the total ethylene production and 10% of the total propylene production. Methanol 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 Baseline 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. In the same scenario, ethanol to butadiene technology increases from 4.5 to 20% of total production. Figure 5 presents ethylene, propylene, BTX, and butadiene productions 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.

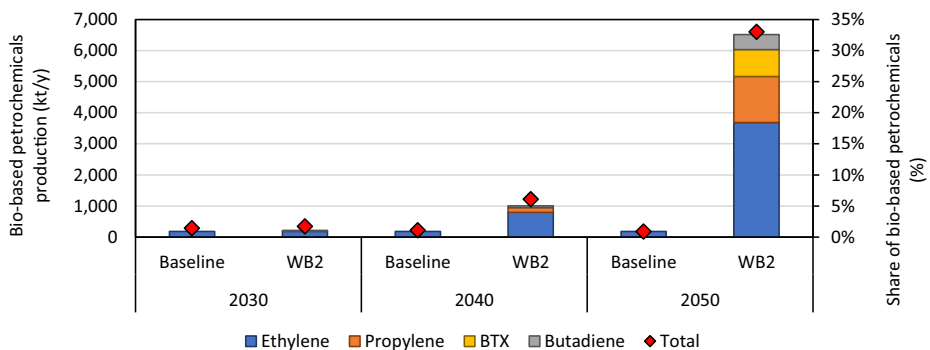


Fig. 4 Bio-based petrochemicals production (left) and share (right). In the WB2 scenario, in 2050, the production of bio-based petrochemicals reaches 33% of total petrochemical production (the remainder derives from petroleum feedstocks)

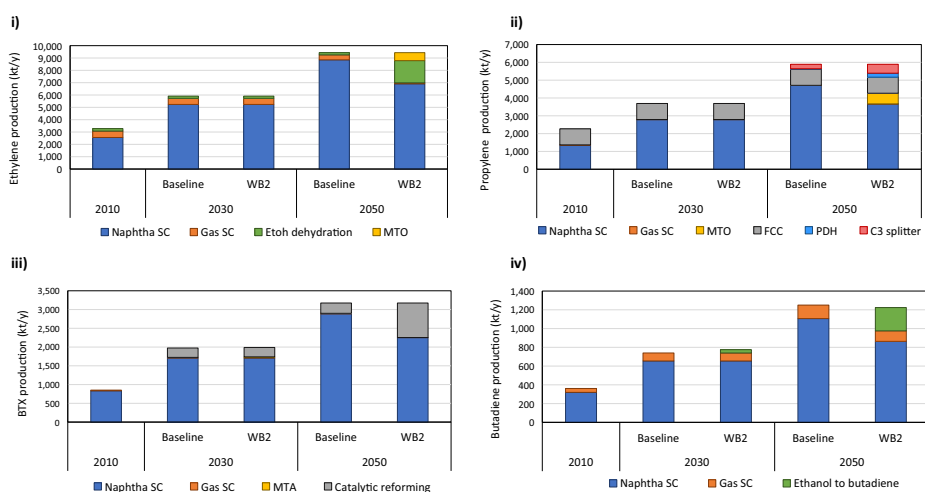


Fig. 5 **i** Ethylene production per technology for all scenarios. **ii** Propylene production per technology for all scenarios. **iii** BTX production per technology for all scenarios. **iv** Butadiene production per technology for all scenarios. For all petrochemicals, SC remains the dominant technology in the WB2 scenario. In 2050, 21.5% of the naphtha used in SC comes from biomass

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.

The results for the sensitivity analysis for a higher benchmark crude oil price (equal to 75 US\$/bbl) in the Baseline scenario shows that due to the decrease of naphtha imports by 15% in 2050, the model increased biomaterials output in almost 10 times (bio-based ethylene, bio-based propylene, and bio-based butadiene). Bio-based ethylene reached 17% of the ethylene market in 2050. Therefore, this higher oil price favored the production of bio-based olefins from consolidated routes, even without implicit carbon prices. This confirms the results of Oliveira et al. (2020a).

3.4 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 factors¹⁷ 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 Mbbbl/day in 2040 was reduced to 0.5 Mbbbl/day 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

¹⁷ 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).

Schaeffer 2007), the avoided emissions in the refinery for not producing 1.3 Mbbbl/day (1.8 – 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 shown previously.

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

The results for the sensitivity analysis for a higher benchmark crude oil price (equal to 75 US\$/bbl) in the Baseline scenario shows that liquid fuels exports increased by 78% (mainly final gasoline and LPG). Raw exports also increased. Imports of jet fuel and naphtha fell by 20% and 15%, respectively, in 2050. The refining utilization factor increased by 2%. All these results were expected, as they revealed that higher oil prices (hence, higher oil product prices) favor exports and undermine imports.

In addition, in order to check the hypothesis that the insertion of the materials module was relevant to change the way the model responded to a deep decarbonization target (the one associated with the WB2 scenario), we simulated the WB2 scenario turning off the materials module that was inserted in BLUES, to compare its main findings with the ones described before. The main results are:

- Biomaterials: As expected, the BLUES version without materials representation reached 97% less biomaterials. BLUES without material detailing was not able to select any biomaterial route, and solely kept running the already existing plant of ethylene from ethanol dehydration, which is owned by the Brazilian company Braskem (200 kt/year). Thus, there is only 2% bio-based ethylene in 2050.
- GHG emissions: Without representing biomaterials, the BLUES model found 91% less accumulated CCU (through biomass feedstock for long lifetime material), and this had to be offset by 1% more of BECCS and 0.5% more of land-based NET options (e.g. afforestation) .
- Biofuel: 2% less in total in 2050, with the swapping of green naphtha for green gasoline. Ethanol production fell 7% in 2050.
- Oil products trade: Without representing biomaterials and not capping naphtha imports, these imports grew 13% in 2045 and 58% in 2050.
- Land use total area: By turning off the material module in the simulation of scenario WB2, we could not find a relevant impact on the price of the food basket and on the use of land area in Brazil. Throughout the period (2010–2050), the maximum variation of the agricultural area (cropland) was 0.6% (about 280,000 hectares) (higher in the simulation without detailed materials representation). In the case of the average food basket price, the maximum variation was just 0.2% (again, we found a higher value without the detailed materials representation in BLUES). This shows that most of the competition happened in the destination of the biorefineries products, instead of in the land demand pressure. At the national level, the food production (and hence the price of the food basket) kept almost unchanged. While in the simulation that better represented petrochemicals (materials module on), the light duty vehicles fleet was increasingly electrified and the green naphtha

was used as feedstock by steam crackers, in the simulation that did not represent petrochemicals in detail (materials module off), the co-produced green naphtha (mostly from BTL plants) had no other use than compose the gasoline pool. In this latter case, naphtha for petrochemicals was imported (which is the current situation in Brazil). It is also worth noting that it is not naphtha that drives the investment in BTL or even in the oligomerization plants (case of the alcohol-to-jet fuel process). What drives investment are the fuels that are needed by the hard-to-abate sectors: jet fuel, diesel (for long-distance road transportation), and marine bunker. This is line with the analysis of Davis et al. (2018).

However, under the WB2 scenario, it is doubtful if there will be sufficient fossil naphtha available to be imported by Brazil in 2050 (only a global IAM could provide this answer). Therefore, we also run a case constraining Brazil's fossil naphtha imports in 2050 at the amount found in the WB2 scenario with biomaterials available (that is, without allowing a huge increase in naphtha imports). In this case, the average petroleum refineries' utilization factor grew from 22 to almost 80% (or close to the Brazilian historical average utilization factor of oil refineries). In sum, this means that turning off the materials module in BLUES resulted in higher naphtha imports or in a much bigger utilization factor of oil refineries (if naphtha imports are limited). In this last situation, petroleum fuels production (consumption and derived GHG emissions) also increased.

3.5 Alternative scenarios for the use and destination of plastics

For all the variations of the WB2 scenario, naphtha SC remains the main route to produce petrochemicals, while 21.5% of the naphtha used is bio-based. Figure 6 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 Baseline scenario projects 150 MtCO₂ process emissions.

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 (1070 MtCO₂) are lower than in the WB2_CS scenario (1102 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.

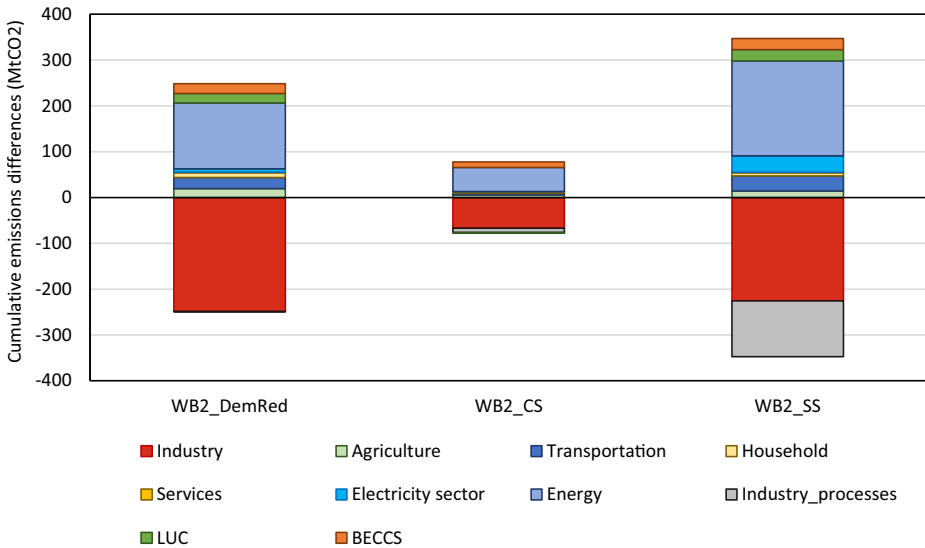


Fig. 6 Cumulative CO₂ emissions differences between the WB2 and their derived scenarios (2010–2050). The positive parts of the bar charts are equal to the negative ones, since the carbon budget (total cumulative emissions) of the WB2 scenarios and its derived scenarios are exactly the same (14 GtCO₂). The difference between them is how the carbon budget is allocated between the sectors. This figure shows how much the emissions in industry decreased in each derived scenario, and what sector could emit more. Because of this balance in the emissions of all the sectors, there are no leakage effects since the carbon budget is the same for the four scenarios

4 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 HVC demand and supply (technological options) in an aggregated manner. Here, we incorporated fossil and bio-based petrochemicals conversion routes to an IAM, in order 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. 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 modeled 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% of the total petrochemical production in the WB2 scenario in Brazil. Naphtha SC 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 finds as an optimal-cost solution to produce diesel from BTL with CCS, and from this solution, it found a co-production of feedstock to materials: particularly green naphtha to steam-crackers, but also green propane to PDH. Hence, by coproducing energy carriers and materials, there was low pressure for land affecting land use GHG emissions. Therefore, the model finds as a cost optimal solution to co-produce energy, fuel, and materials simultaneously, while, at the same time, the exogenous demand for food is maintained. For this, the model has three alternatives: opening of new agricultural areas to increase the production of agricultural commodities and maintain the average productivity of food and energy crops; change agricultural production system to technologies with higher productivity; or a combination of these factors. In most scenarios, a combination of both alternatives is observed, but it will depend on the scenarios' boundaries and restrictions. The soil productivity is maintained for food production. The biomass trilemma, for the level of production required in the scenarios, could be alleviated through biorefinery plants that produce multiple products. Actually, in the WB2 scenarios, by 2050, 22% of the primary energy production is associated with food production, while 22% of the bio-based material production is associated with energy generation. Therefore, the integrated assessment of the trilemma shows the relevance of biorefineries in the bioeconomy, where the biomass competition for food, energy, and material is alleviated since they are co-produced in the same plant. The biorefineries emergence was a minimum cost solution aligned with the targets of deep decarbonization pathways. It is worth noting that the model and the scenarios simulated assume zero illegal deforestation in the Amazon Forest by 2030, as stated in the Brazilian NDC. However, the current weakening of the Brazilian environmental governance (Rajão et al. 2020) is a risk for this strategy and can significantly affect the results of our model exercise.

Moreover, in the WB2 scenario, from 2040 urban mobility electrification leads to the possibility of repurposing liquid streams (e.g., ethanol) 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 the repurposing of liquid fuels (ethanol), from already installed facility, which 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 SC due to the increase of bio-ethylene production negatively affects propylene, BTX and butadiene production. For propylene, C3 splitter, FCC, and MTO compensate for 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%).

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. In order to test if the reduction of petroleum refining utilization factors is a consequence of biomaterial production, we simulated the WB2 scenario turning off the materials module that was inserted in the BLUES. Turning off the material module resulted in higher naphtha imports or in a much bigger utilization factor of oil refineries (if naphtha imports are limited). In this last situation, petroleum fuels production (consumption and derived GHG emissions) also increased.

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 of 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. We also propose the development of a specific material demand module to run in parallel with our IAM to better perform a detailed modeling of the driving forces behind petrochemicals demand in Brazil and even in the world.

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 until 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. Ultimately, 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.

Supplementary Information The online version contains supplementary material available at <https://doi.org/10.1007/s10584-021-03201-1>.

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