nature communications

Article

https://doi.org/10.1038/s41467-024-53201-9

Sustainability synergies and trade-offs considering circularity and land availability for bioplastics production in Brazil

Received: 12 January 2024

Accepted: 4 October 2024

Published online: 13 October 2024

Check for updates

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Alongside the concerns of waste management, plastic production represents a future problem for managing greenhouse gas emissions. Advanced recycling and bio-based production are paramount to face this challenge. The sustainability of bio-based polyethylene (bioPE) depends on the feedstock, avoiding stress on natural resources. This work discusses Brazil's potential to meet future global bioPE demand by 2050, using sugarcane as feedstock and considering environmental sustainability for production expansion. From the assessed 35.6 Mha, 3.55 Mha would be exempt from trade-offs related to land use change (dLUC), biodiversity, and water availability. The scenario with the highest circularity efficiency would require 22.2 Mha to meet the global demand, which can be accommodated in areas with positive impacts in carbon stocks, neutral impacts in water availability, and medium impacts on biodiversity. Here, we show that dropping demand is essential to avoid trade-offs and help consolidate bioPE as a sustainable alternative for future net-zero strategies.

The global production of plastics has been growing on average 8.4% per year (compound annual growth rate – CAGR) since 1950, and it is expected for it to grow between 3% and 4% until 2050[1,2]. This trend, however, does not come without consequences. Plastics production currently accounts for 5–7% of the global oil supply, and around 2% of the global greenhouse gases (GHG) emissions[3]. Although expressive, these shares do not represent the largest contributor in any of them. The issue resides, however, in the future. Following the trend, plastics could embody 20% of the global oil uptake and up to 15% of carbon emissions budget by 2050, considering the fossil energy sources phase-out required to limit global temperature increase to 1.5 °C[4].

This growing demand for plastics also raises more concern regarding pollution and its effects on ecosystems quality and human health. Microplastics and nanoplastics severely impact the food chain and water supplies, with their cumulative behavior having long-term implications in human tissue and cells[5]. This being a direct result of global plastic waste leakage to the environment, one of the consequences of the linearity of the current plastic value chain. In fact, around 80% of the plastic pollution in the oceans is derived from terrestrial littering[3], and this flow could triple by 2040, if urgent measures are not implemented, such as Advanced Recycling (AR) methods, substitution of packaging materials and products redesign[6].

Given the long-term impacts that plastic production will have in terms of pollution, contribution to GHG emissions, and fossil resources uptake, four main strategies are available to reduce plastic demand, promote value-chain circularity, and increase renewability[4,7,8]:

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i. Substitution: replacement of fossil-based plastics with renewable alternatives, such as biobased plastics (bioplastics), promoting the capture and use of atmospheric carbon dioxide, either reducing value chain emissions, or promoting carbon stocks, when long-term applications for plastics are concerned.
ii. Integration: plastic value chains are also over reliant on fossil energy sources and other inputs that carry substantial dependance on fossil resources, such as additives[7] and colorants, so this strategy promotes integration with renewable energy and substitution of the remaining inputs with renewable alternatives.
iii. Circularity: adoption of advanced recycling strategies, including mechanical, chemical, and biological methods, in order to transition from a linear value chain to a circular one, substantially reducing virgin plastic demand.
iv. Reduction: promote redesign of products, change public perception of single-use materials and substitution with renewable non-plastic materials, in order to reduce future plastic demand, and ease the environmental burden from virgin plastic production, reverse logistics, recycling, and final disposal.

The concept of circular economy is characterized by diminishing the demand for virgin materials and upgrading the perspective on residues to the status of feedstock[8]. In 2016, however, only 16% of the plastic waste was collected for recycling, and 25% of it was lost through process inefficiencies[9]. This is due to the nature of mechanical recycling processes, where material quality is gradually reduced through processing, affecting closed-loop efficiency, and being considered as downcycling[10,11]. Chemical and biological recycling methods can be seen as upcycling alternatives, since plastics can be converted back to their monomeric precursors, with no losses in quality, allowing for it to serve as raw material for new plastics, in a closed-loop value chain, or for new products and materials, contributing to the economy's circularity[3,10,12].

In addition to alternative materials, such as paper packaging[6], bioplastics are often considered as direct substitutes to fossil plastics. By embedding biogenic carbon in their structures, originated from biomass or organic residues, bioplastics can be regarded as low-carbon materials and potential carbon-sinks for long term applications such as building and construction[4,13]. Even though, currently, bioplastics correspond to only 0.5% of the global market for virgin material[3]. Important trade-offs, however, may emerge in other environmental impact categories with this transition, and a holistic approach must be applied, regarding not only changes in production processes, but also on end-of-life scenarios and additional inputs[14].

Moreover, the transition towards biobased materials still depends on consumption patterns, that rely on psychological traits from the consumers. Choosing a more sustainable alternative is not always straight-forward per se, it depends on how much effort must be put on the decision-making process, extra time and personal resources to be destined to comply with reverse logistics, and also personal convictions towards sustainability itself[15,16]. Alternatively, changes in product and value chain design are applicable to effectively reduce demand for plastics, from an upstream perspective, and consumers behavioral changes will then follow, driven by prosocial and environmental education initiatives, with progressive effect in the long term[17,18].

The implementation of circularity and substitution into polymers value chains also have large implications on energy and material consumptions, that will both stress the restrict carbon budgets and demand for renewable alternatives[7]. The adoption of low-carbon energy sources is fundamental to this aspect, also contributing to circularity if residue-based technologies are implied, such as for biomass and waste-to-energy pathways[19].

Sugarcane bioethanol has a legacy of over four decades in Brazil, benefitting from important technological advances in agricultural and industrial aspects, promoting energy and material efficiency[20]. One of sugarcane bioethanol main highlights is its little reliance on fossil resources from an industrial standpoint, with sugarcane mills being self-sufficient in energy, due to bagasse use in cogeneration facilities[21]. The bioethanol dehydration into ethylene, and its posterior conversion into biobased polyethyelene (bioPE) is already deployed in industrial scale and represents a potential alternative to fossil PE[22].

Another important aspect of bioplastics is their potential pressure over natural resources and land use, that may compete over cropland or even among other biobased products, such as biofuels[23]. While existing studies have addressed the prospective GHG emissions mitigation of fossil plastics substitution with biobased alternatives[7] and the potential environmental impact considering the Planetary Boundaries[24,25], it is essential to consider context-specific conditions and synergies and trade-offs regarding land-based alternatives[26]. However, there is lack of spatially explicit data over land availability to support plastics' growing demand, while preserving natural biomes, avoiding stress on water reserves and accounting for land use change emissions, especially considering Brazilian conditions, where biomass cultivation is often cogitated[3,14].

This work, thus, aims to evaluate the GHG emissions mitigation potential of the implementation of an integrated biobased value chain for bioPE production in Brazil, profiting from the Brazilian experience on sugarcane cultivation and bioethanol production, while also proposing alternatives for recycling and energy-integration. Finally, a spatially explicit assessment will point out the land availability for the necessary sugarcane expansion to supply the PE projected demand in 2050, considering the potential impact on water resources, biodiversity, and emissions constraints, proposing an environmentally safe zone for bioPE expansion in Brazil.

Results

Value chain integration

A total of six scenarios were evaluated, considering different combinations of base year, PE demand, end-of-life composition, bioPE substitution, sugarcane expansion rationale, and recycling technology, named Current, Trend, Future SR 1 G, Future SR 1G2G, Future AR 1 G, and Future AR 1G2G. Figure 1 illustrates the value chain emissions for each of the evaluated scenarios, under a life cycle perspective. Land use change (dLUC) emissions are addressed on "Spatial analysis". For the future scenarios with widespread bioPE adoption, End-of-Life (EoL) emissions reduce in 29.5% and the emissions for virgin bioPE manufacturing are notably lower than for fossil PE (at least in 52%). As a result, bioPE itself may function as a carbon sink, embodying more CO_{2e} than its life cycle emissions.

For the Advanced Recycling (AR) scenarios, a larger share of waste PE is processed through mechanical recycling, rather than through chemical recycling. Since the later presents a larger carbon footprint than the former, the overall life cycle emissions are lowered. Moreover, for the AR scenarios, a larger closed-loop efficiency for circularity is achievable, demanding less virgin material (bioPE) to be produced, contributing to lower GHG emissions for the whole value chain. The lower virgin material input, however, reflects in a lower carbon stock as well. By comparing the two technologies for ethanol production (1 G and 1G2G), only a small difference is seen in terms of emissions, with the recycling scenarios representing a larger impact in overall GHG balance.

Emissions from the EoL phase decrease their volume and impact when the future scenarios are considered. It is mainly related to the transition to municipal incineration arrangements with energy use, resulted from the transition for bioPE production associated to biogenic carbon as the value-chain virgin material. The transition from disposal options with a lower sanitary standard (namely, open dumps and unsanitary landfills) to sanitary landfills also contributes to lower emissions, although at a smaller degree.

By upscaling life cycle emissions towards the value chain level and correlating different GHG emissions with projected demand scenarios

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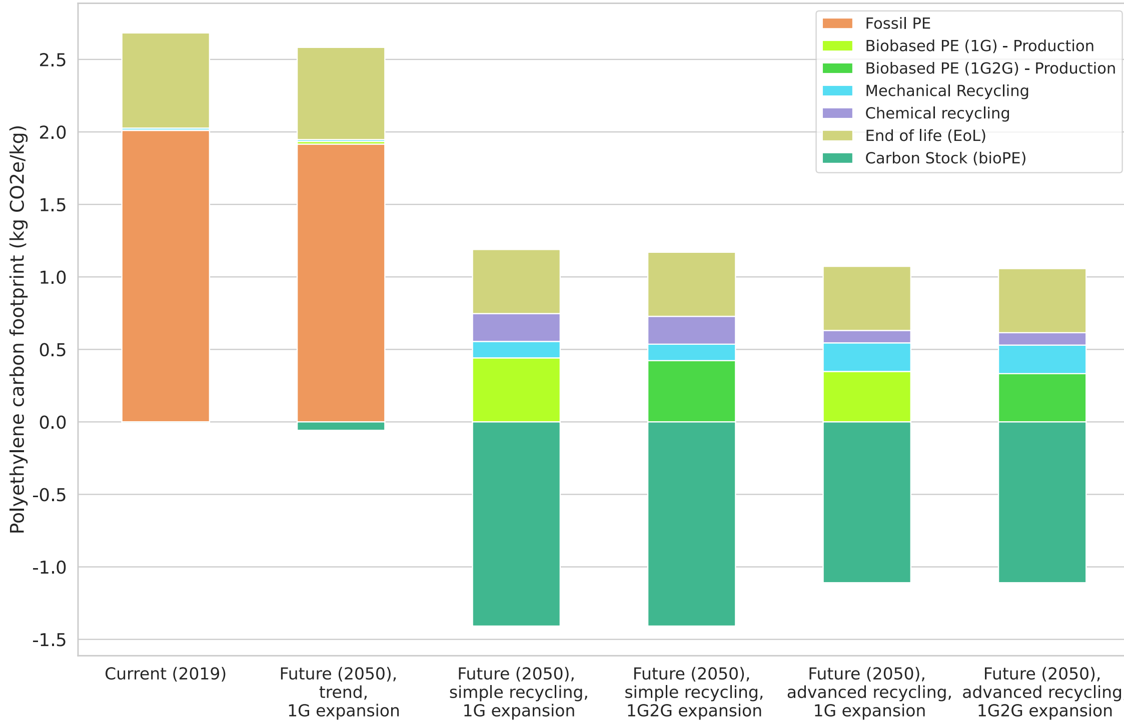

Fig. 1 | Life-cycle emissions composition for polyethylene (PE) value chain across different scenarios. PE carbon footprint includes production, recycling, end of life and carbon stock, considering scenarios of simple and advanced recycling and 1G and 1G2G technologies for ethanol production (functional unit = 1 kg of PE in use).

Table 1 | Value chain emissions for polyethylene (PE) across different trajectories

	PE carbon footprint ($kgCO_{2e}.kg^{-1}$)	PE value-chain emissions ($MtCO_{2e}.\ year^{-1}$)	Emissions increase[a]	Share of global emissions[b]
Current (2019)	2.67	293.6	-	0.50%
Future (2050), trend, 1 G	2.53	602.5	105%	6.03%
Future (2050), SR, 1 G	−0.219	−52.3	−118%	−0.52%
Future (2050), SR, 1 G2G	−0.238	−56.8	−119%	−0.57%
Future (2050), AR, 1 G	−0.036	−8.7	−103%	−0.09%
Future (2050), AR, 1 G2G	−0.052	−12.4	−104%	−0.12%

[a]compared to Current (2019).
[b]Current (2019) emissions consider 59 $GtCO_{2e}$[69], and Future (2050) consider the carbon budget projection of 10 $GtCO_{2e}$ from SSP1-1.9[69]

for PE in 2050 (Table 1), some aspects for the different trajectories become clearer. By shifting all PE production to biobased pathways, the sector could contribute with an offset of up to 0.6% (56.8 $MtCO_{2e}$) in the global emissions for 2050 considering the SR scenarios results. Regarding AR and Simple Recycling (SR) scenarios, they always present negative net GHG emissions due to incorporated biogenic carbon in bioPE.

The AR scenarios present net GHG emissions about 5-fold lower than the SR scenarios (Table 1), even though AR scenarios present lower positive emissions of about 16% when compared to SR scenarios (Fig. 1). The lower net GHG emissions associated to AR scenarios are due to gains of closed-loop efficiency, that destinates less bioPE to downcycling (12 Mt, Fig. 2c) when compared to SR scenarios (28 Mt, Fig. S1 - Supplementary Information), ending up in a lower input of virgin material (84 Mt, Fig. 2c) in the former. In this case, the lower need of virgin material in AR scenarios implies lower inputs of biogenic carbon in the production cycle to meet the same future demand of bioPE as in SR scenarios.

The impacts associated to the recycling-based scenarios (circularity) become more evident when the annual value chain mass flows for polyethylene demand and supply are showed (Fig. 2). While the Future trend scenario for 2050 retains the linear aspect of the Current scenario, it is worth noticing that both the Future trend scenario and Future advanced recycling scenario address the same projection for future PE demand, but with the latter approaching it in a circular way.

Future advanced recycling scenario destinates 4-fold the amount of material to recycling when compared to Future trend scenario, which results in a 63% lower demand for virgin feedstock. The rest of the demand for virgin material in Future advanced recycling scenario is supplied by closed-loop recycled material. In this case, the material quality of which is guaranteed by advanced mechanical recycling complemented by chemical recycling.

Spatial analysis

As shown in the previous section, the choice of AR over SR scenarios has a larger effect over GHG emissions than the technological pathway for ethanol production (1 G or 1G2G), in both the product and value-chain levels. However, there is a change is this trend when assessing the required area for sugarcane expansion. On Table 2, it is displayed the number of new facilities, within the expansion area, required to supply the projected demand for virgin bioPE in 2050, considering the four combinations of either simple or advanced recycling and 1 G and 1G2G expansions.

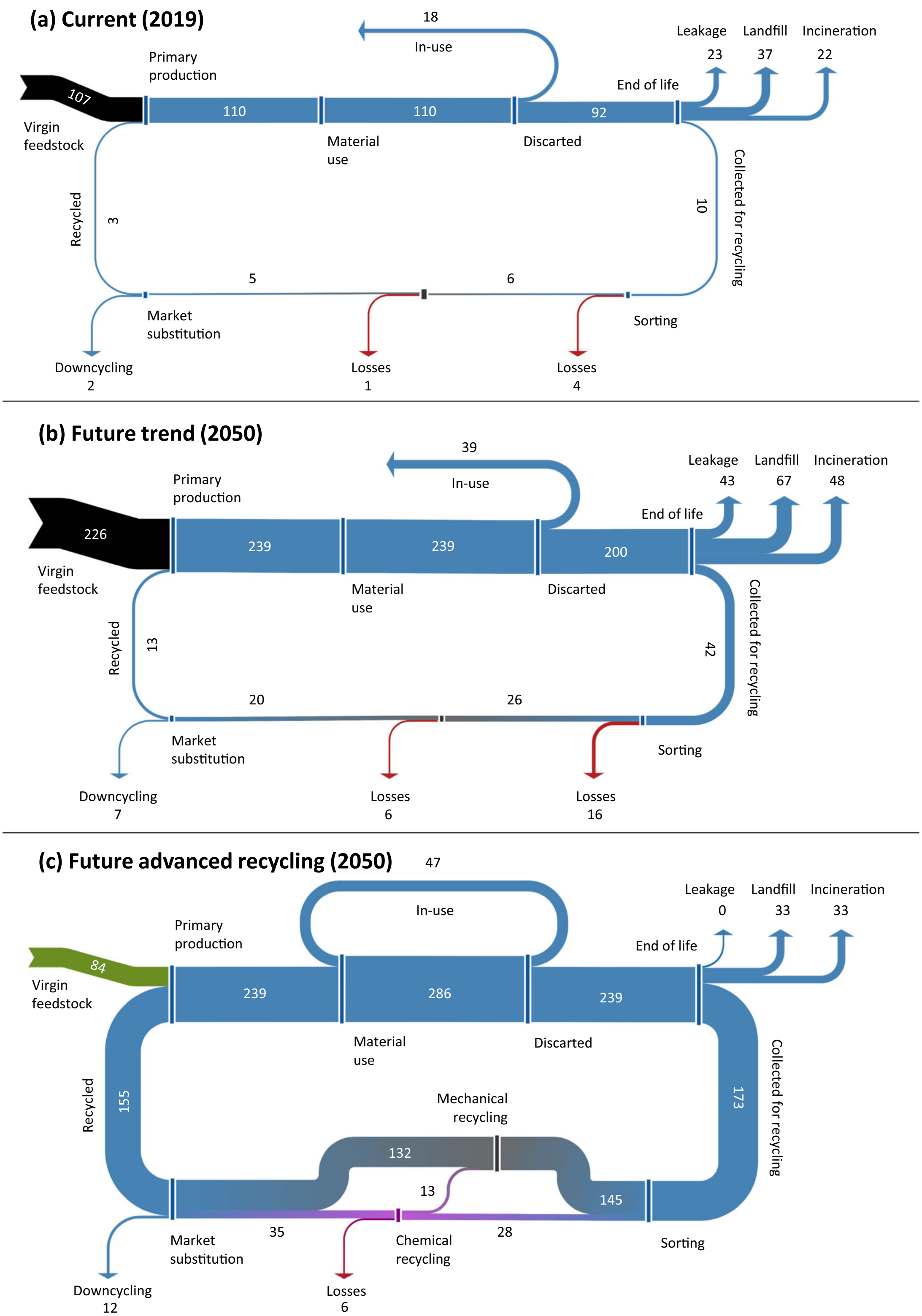

Fig. 2 | Annual value chain mass flows, in Mt, for polyethylene demand supply considering different scenarios. Virgin feedstock required, recycling and end of life composition vary for current (2019) (**a**), future trend (2050) (**b**) and future advanced recycling (2050) (**c**) scenarios.

The combination of SR and 1 G expansion would require 38.5 Mha of new sugarcane land, almost 5-fold the current sugarcane cultivation area in Brazil (8.4 Mha)[27]. This could be reduced in 17%, by either implementing AR or promoting a 1 G2G expansion. While the first promotes a reduced demand for bioPE due to increased circularity efficiencies, the latter promotes a more optimized land use. Individually, both options have a similar effect over the land requirement, but when combined, it can result in an area of 22.2 Mha, representing a 42% reduction. Nonetheless, it still represents 2.6 times the current sugarcane cultivated area in Brazil.

All the four expansion scenarios would, at least, triple the current sugarcane cultivation area, so there is a concern if this demand can be sustainably accommodated. On Fig. 3, it is presented three sustainability criteria for sugarcane expansions: (i) water scarcity vulnerability, (ii) carbon stock change, and (iii) biodiversity loss vulnerability, along with their overlay, pointing out synergy areas with less vulnerability for expansion (3.4 Mha), mostly located in Mato Grosso do Sul state (51.3%). While this area is sufficient to supply the future demand for ethanol, as expected by the RenovaBio biofuels policy[28], it would accommodate only 15% of the least land-demanding scenario (AR + 1 G2G). That is, for the remaining required area for expansion of sugarcane production, compromises are needed in the form of trade-offs. On Fig. 4, it is showed the different criteria combinations and the resulting available area and the associated potential carbon stock change.

Table 2 | Sugarcane processing facilities and land demand for each PE production expansion scenario

	Simple Recycling	Advanced Recycling	Unit
Virgin PE demand (2050)[a]	106.9	84.2	Mt
Integrated facilities	264	208	u
Supplier facilities (1 G)	417	328	u
Supplier facilities (1 G2G)	234	184	u
Area for 1 G Expansion	38.5	30.3	Mha
Area for 1 G2G Expansion	28.1	22.2	Mha

[a]considering bioPE total (virgin and recycled) projected demand of 238.6 Mt for 2050[46].

The SR combined to 1 G is the only scenario that would not fit in the considered expansion area. The remaining scenarios would fit outside the synergy area, occupying areas with trade-offs among the assessed sustainability criteria. Results show at least 33.5 Mha in the considered expansion area that would completely comply with water availability. There is 15.3 Mha where dLUC GHG emissions will be negative, which means that LUC in those areas could bring positive impacts on carbon stock. The most restrictive sustainability constraint is biodiversity loss since there is only 10.2 Mha classified as low in terms of biodiversity loss vulnerability. Although only 15.3 Mha out from the 35.6 Mha considered for sugarcane expansion are classified as areas with carbon stocks regarding dLUC, it worth to mention that the balance in the total area result in a final carbon stock of 14.1 $MtCO_{2e}$.

The most representative area regarding the criteria combination is representing by 9.4 Mha with low water scarcity vulnerability, 38.8

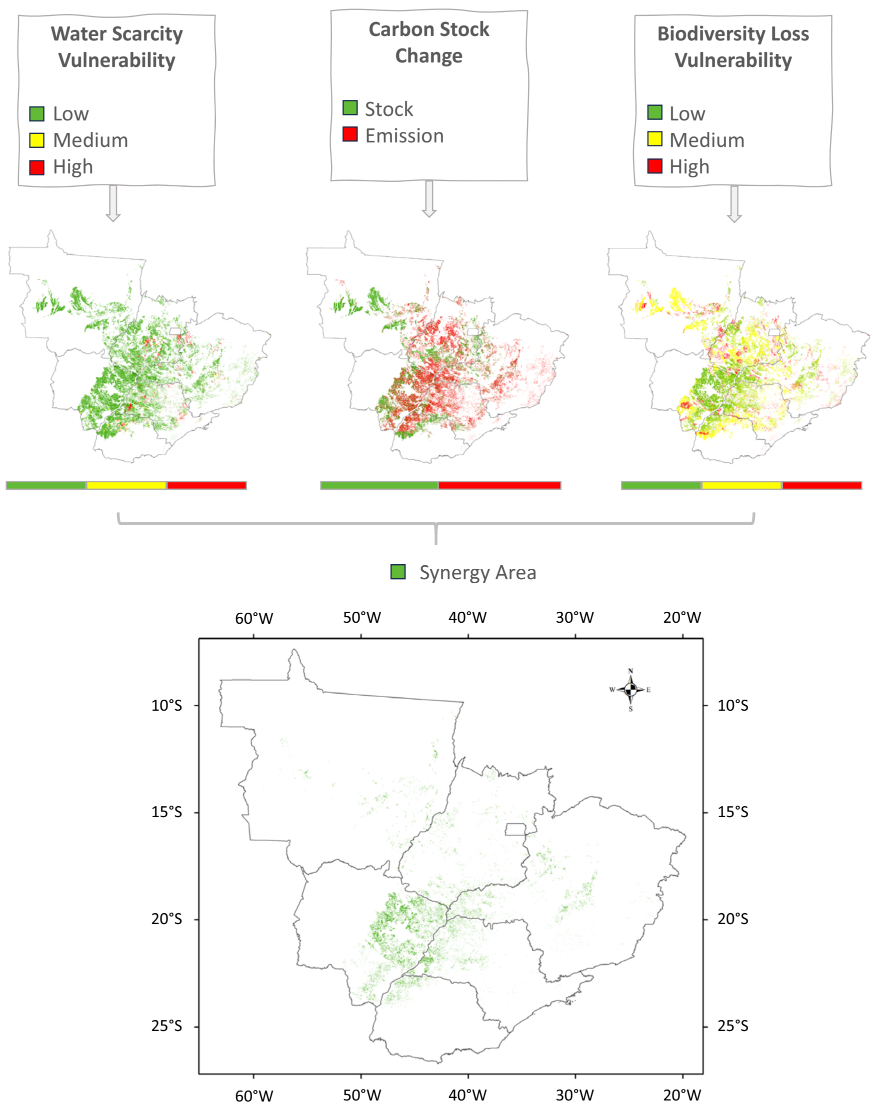

Fig. 3 | Spatially explicit assessment of sugarcane expansion. Within each 30 m-pixel across the expansion area, the classes for the three defined criteria (water scarcity vulnerability, carbon stock change and biodiversity loss vulnerability) were established and used to estimate synergy area through crossing the green classes.

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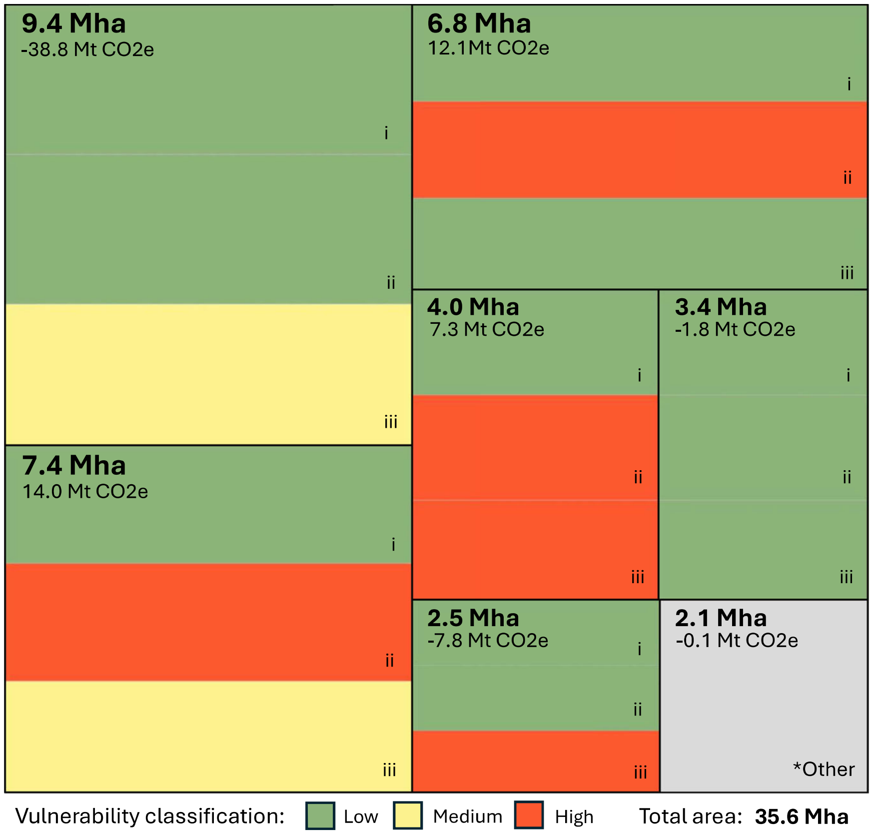

Fig. 4 | Area and GHG emissions from carbon stock change for the criteria-crossing-combinations in the sugarcane expansion area. Each box represents a combination and is divided into 3 parts, one for each criterion (water scarcity vulnerability (i), carbon stock change (ii), and biodiversity loss vulnerability (iii)) with the corresponding vulnerability classification (low, medium and high). Dimensions are proportional to the area and the remaining combinations were grouped into the last box (*Other).

$MtCO_{2e}$ of carbon stock related to dLUC, and medium biodiversity loss vulnerability. Combinations also show 6.8 Mha consistent with water availability and biodiversity conservation, however presenting emissions of 12.1 $MtCO_{2e}$ related to dLUC. In 7.4 Mha water availability is not an issue, however biodiversity loss is classified as medium and emissions of 14 $MtCO_{2e}$ are associated to dLUC. These three areas combined with the synergy area (3.4 Mha) account for nearly 27 Mha, capable to accommodate both the AR + 1G2G and the AR + 1 G scenarios, and with a final dLUC carbon stock of 14.5 $MtCO_{2e}$ and medium impacts on biodiversity loss.

Demand supply for 2050 and GHG emissions

Aside from its land use implications and trade-offs for water availability and biodiversity vulnerability, bioPE may still be presented as a carbon sequestration and stock alternative, either in the form of long-term applications, such as construction materials, or in stable EoL destinations, such as landfills[3,4]. On Fig. 5, it is displayed the GHG emission profile considering the four scenarios, across the whole assessed expansion area in Brazil. The facility candidates were sorted considering their area-specific dLUC emissions, from the largest carbon stock to the highest emission potentials. The vertical dotted lines show the total area required to meet the bioPE demand for each scenario, and the dotted curve shows the accumulated GHG balance until that point.

Both SR and AR scenarios considering 1 G ethanol production show similar profiles for total emissions, achieving negative values (stocks) when considering the occupation of the total area for expansion. However, in SR case, despite the larger carbon stock compared to AR, the total area is not capable to meet the 2050 bioPE demand. In SR 1 G case, the total emissions benefit from lower emissions in EoL and from the larger requirement of virgin material with biogenic carbon content when compared to AR 1 G. Conversely, the larger requirement of virgin material in SR 1 G is also responsible for the inability to supply the future BioPE demand within the available area.

SR and AR scenarios with 1G2G ethanol production show similar results than those considering 1 G, however, in this case both recycling technologies leading to meeting the future demand for bioPE within the available area considered. SR scenarios require about 6 Mha of additional area to accommodate the 2050 demand than the AR scenarios. All scenarios show a large portion of GHG emissions balance associated to the bioPE carbon incorporation (bioPE carbon stock), with values compatible to the aggregate of all other categories together.

AR considering 1G2G ethanol production requires 22.2 Mha and if produced in the first areas after sorted by carbon stock change, it would promote a carbon stock of 52.1 $MtCO_{2e}$ per year to reach the expected demand, as opposed to a carbon stock of 85.7 $MtCO_{2e}$ per year if SR with 1G2G ethanol is considered, requiring an area of 28.1 Mha. Scenario AR with 1 G ethanol would be reached at 30.3 Mha, with a stock of 33.6 $MtCO_{2e}$ per year, 36% and 61% less than AR with 1G2G and SR with 1G2G, respectively, and requiring more land than both.

Discussion

This work addressed Brazil's potential to sustainably accommodate future bioplastics production for global supply, considering projections for 2050. Current land availability for sugarcane cultivation, in an environmentally conservative zoning, would be sufficient for total substitution of fossil PE to bioPE, if state-of-the-art technology is

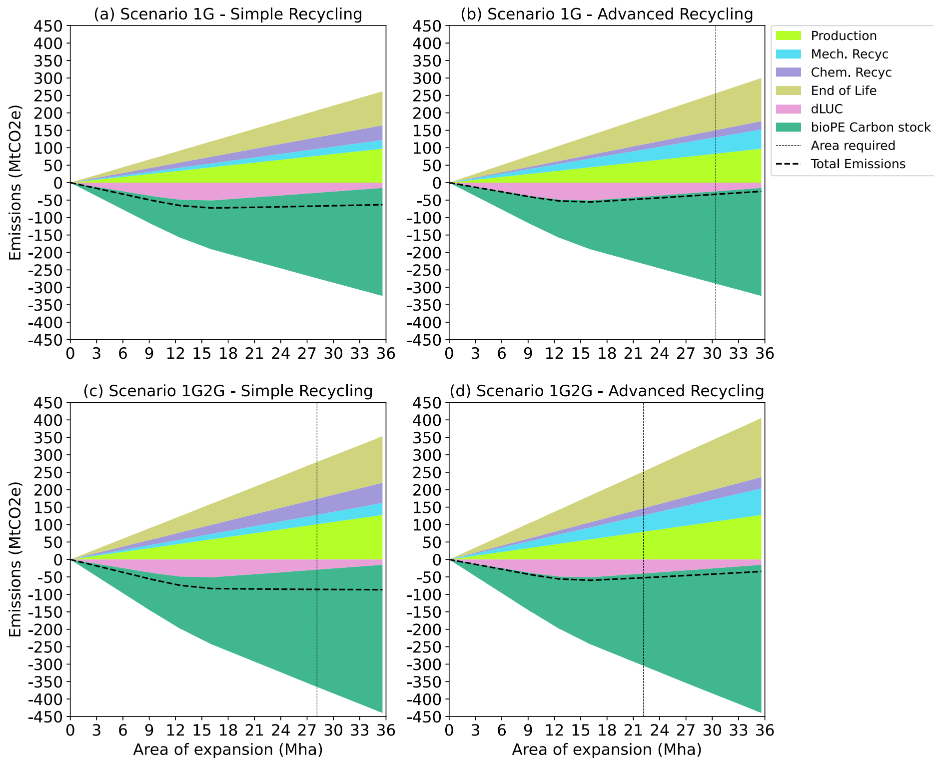

Fig. 5 | Life cycle emissions profile for bioPE value-chain over the sorted area of expansion across different scenarios. Scenarios include 1 G – Simple Recycling (**a**), 1 G – Advanced Recycling (**b**), 1 G2G – Simple Recycling (**c**) and 1 G2G – Advanced recycling (**d**), all for 2050. 1 G (first generation) and 1G2G (first and second generation) are different technologies for ethanol production. The GHG emissions balance includes production, mechanical recycling (Mech. Recyc), chemical recycling (Chem. Recyc), end of life, direct land use change (dLUC) and bioPE carbon stock. Area required to meet the bioPE demand for each scenario are shown in the vertical lines, and area required for Scenario 1G – Simple Recycling is not reached.

deployed for recycling and increased closed-loop efficiency for the PE value-chain, as well as leakage avoidance. These future recycling scenarios rely on the deployment of current technologies that are not yet economically competitive with virgin plastic production, such as advanced mechanical and chemical recycling, and specialists also point that high circularity levels, such as those suggested in the AR scenarios, depend on future technology not currently available[6]. So, even with such assumptions, Brazil would struggle to supply, sustainably, all the virgin PE future demand, which is still about one third of the plastics resins market[1].

Among the scenarios with recycling, SR considering 1 G ethanol production is the only one that cannot be fully accommodated in the assessed area. That is, either (or both) AR arrangements or 1G2G expansion would be necessary. If AR is to be considered, an important distortion emerges. AR results in a more efficient closed-loop circularity for PE, lowering demand for virgin material, stocking less carbon from the atmosphere. This effect can be seen by comparing the AR with SR curves, with SR presenting larger carbon stocks until the 12–15 Mha mark and maintaining this stock throughout the remaining expansion area and production (Fig. 5).

Carbon sink alternatives, such as long-term use bioplastics, are pivotal for net-zero targets, since hard-to-abate sectors, such as aviation transport and steel industry, need compensation by sequestration and stock technologies, and their development will dictate how flexible future carbon budgets will be, especially towards the middle of the century. However, an important distortion may emerge if carbon stocks are to be appreciated over efficient closed-loop circularity, exemplified by the comparison of the SR with AR scenarios. Efficient recycling reduces virgin material demand and EoL disposal. This might not be an issue when approaching fossil-based plastics, but with biobased plastics such as bioPE, this means less captured CO_2 in circulation and in storage.

While these stocks are to be profited from, EoL environmental issues from plastic residues leakage need to be accounted for, as well as their subsequent impact in terrestrial and aquatic ecosystems. Nonetheless, it is still to be determined how labile these materials can be, especially in conditions such as those in landfills; and trade-offs in other impact categories, such as the case of plastic leakage to the environment. Even so, when considering the severally reduced global carbon budget for 2050, the AR with 1G2G scenario could represent a stock of up to 52.1 $MtCO_{2e}$, that corresponds to 0.52% of the carbon budget of SSP1-1.9 scenario.

Beyond land availability, there are trade-offs in the assessed sugarcane expansion area to accommodate future bioplastics production. For non-degraded pastureland and areas of annual crop production on the considered expansion area, not only there is medium vulnerability on the region's biodiversity but also risks regarding food production, LUC and deforestation are higher. Those are not marginal lands, and the land use competition and prices might be higher than those in degraded lands.

Most of the combinations of trade-offs include emissions from carbon stock change, but those values are lower than those from the conversion of areas with high carbon stocks such as native vegetation, which were previously excluded from the considered expansion area. In this case, despite most of the area mapped show emissions instead of carbon stocks related to dLUC, the overall balance represents a stock of 14.1 $MtCO_{2e}$ per year if all the considered area were occupied with sugarcane. This approach evinces the impacts not only in considering land use constraints regarding areas with high carbon stocks, but also the impacts in considering the overall landscape instead of an isolated facility when pursuing to attend sectorial GHG emissions mitigation.

Water availability is the least concerning issue in the considered area since most of the areas do not include high or medium water scarcity vulnerability. Despite this criterion referring to current land use, and the possibility of emerging risks due to the expansion, irrigation was not considered for sugarcane and both land use change scenarios evaluated (pastureland or annual crops converted into sugarcane) are not expected to worsen the water availability[29,30].

Another aspect related to the expansion area and feedstock potential production is that it considers the current sugarcane agroecological zoning and historical climate data. However, climate change can affect the suitability of sugarcane production and, on the most pessimistic climate change projections, the level of congruence between different climate change projections in the agroecological zoning region are low, which could imply a reduction on the land availability for sugarcane expansion[31]. These effects are to be monitored as the climate change mitigation alternatives, such as the bioPE production, and their associated trade-offs can be strictly affected by climate change itself.

Recycling is important to maintain the required area to meet the projected demand within the considered area. Without recycling measures, an area of 63 Mha (1G2G) or of 86 Mha (1 G) would be necessary, with the assessed expansion being available to accommodate only 56.2% and 41.1% of these. In this case, the potential developments are either expansion on non-suitable land, on native vegetation or on annual crops outside considered area, that will represent a higher risk for sustainable development; or halt plastics growing demand, by changing product design for packaging, using alternative materials for plastics substitution, or even promoting larger reuse approaches for plastics.

Brazil is also expected to accommodate future demand for biofuels, renewable chemicals, and energy. Land is a finite resource, so each of the products should be approached as a land-based GHG mitigation solution and should be deployed considering both market needs and maximized mitigation[32–35]. Although only 9% of the assessed land for expansion (3.4 Mha) would be synergistic in relation to the evaluated criteria, this area is enough to double the current ethanol production in Brazil. These results indicate, for instance, that the future demand envisaged for RenovaBio program could be supplied by new areas with less risk of trade-offs considering the carbon stock change due to dLUC, biodiversity loss and water scarcity vulnerability criteria. That is, land occupation by dedicated feedstock for biorenewables, food crops and biomes restoration will, imperatively, follow public policy targets, carbon stock and ecosystem services maximization and market needs.

Despite the feedstock production potential of Brazil, land use, land use change and forestry (LULUCF) is the sector with the most GHG emissions in the national inventory[36]. However, the increase in the former does not necessarily have to compromise the latter, and context-specific conditions matter. The findings of this study are useful for searching for synergistic solutions when halting climate change, preserving biodiversity, and reducing pollution. Additionally, it enlightens the importance of identifying trade-offs and pointing out them for policymakers, either to attempt to reduce them or for completeness on sustainability assessments. Further investigation of feedstock potential for bio-based products on the considered expansion area including other sustainability criteria, such as those related to social aspects not addressed in this study, and implications on United Nations' Sustainable Development Goals are to be future studied.

Aside from the three main strategies available to reduce plastic demand, promote value-chain circularity and increase renewability (substitution, integration, and circularity), the need of the fourth, namely consumption reduction, becomes clear. Without reduction of plastic demand, there will be a certain natural resources stress, either in the form of land use or fossil resources availability, or plastics pollution, no matter how the resulting GHG balance is associated with it. And since there will be no major generational gap for behavioral change until 2050, to curb plastic demand from the consumer end[16,18], changes in product design and policy making are to be deployed in order to foster this reduction[15,17], such as the directives proposed by the European Union[37]. For instance, this could come by substantially reducing single-use plastics, that accounts for about half of the current demand[1].

Methods

Industrial production of biopolyethylene

The industrial modeling was performed using the commercial process simulator Aspen Plus® for all stages, except for poly-ethylene polymerization where spreadsheet calculations were used. A brief description of the industrial processes involved is made as follows. The first steps in the industrial modeling consider the production of ethanol, either from sugarcane juice (1 G ethanol) or from the sugars obtained from the breaking of lignocellulosic material (2 G), in this case, bagasse and straw. 1 G ethanol production involves the extraction of juice from sugarcane stalks in mills, the chemical and physical treatment of the juice to remove impurities, and juice concentration followed by alcoholic fermentation using native *Saccharomyces cerevisiae*. The last step is ethanol purification in distillation columns to obtain hydrated ethanol (93% in mass of ethanol). Steam is generated on the plant on boilers through bagasse burning and electricity is generated from steam, making these units self-sufficient. For 2 G ethanol, the first stages of the process are the pre-treatment of the lignocellulosic material through steam-explosion followed by enzymatic hydrolysis. The objective of these initial operations is to obtain monomeric sugars from cellulose and hemicellulose. The following steps of the process are similar to 1 G ethanol production, except for the microorganism used in xylose fermentation (genetically modified *Saccharomyces cerevisiae*).

Ethanol is then sent to the ethylene production sector of the plant. Vaporized ethanol is heated in a furnace and sent to the multi-tubular reactor containing the catalyst. The exit stream containing ethylene and other sub-products (n-butene, propene, etc.) is cooled and enters a quench tower for water removal. The ethylene is then compressed on a series of compressors and sent to a caustic scrubber for removal of impurities (mainly CO_2). The resulting stream is then sent to molecular sieves for further removal of water and lastly to a cryogenic distillation/stripping system, where polymer-grade ethylene is obtained[38].

The typical arrangement for sugarcane mills in Brazil is based on energy self-sufficiency, using internally generated lignocellulosic biomass (bagasse) as fuel in the Cogeneration of Heat and Power (CHP) unit boilers, that can be complemented with harvest residues (straw)[21]. This integration allows for sugarcane ethanol to be produced independently from fossil energy sources, at least within the industrial level, and with an energy surplus and a lower carbon footprint. To profit from this surplus, the ethanol dehydration and ethylene polymerization units were integrated to a sugarcane ethanol distillery (either 1 G or 1G2G), designed to provide enough steam for these processes, and to generate surpluses of electricity and biogas, with the last being generated from the anaerobic digestion of stillage (vinasse). Also, additional sugarcane mills were considered as ethanol suppliers to meet the dehydration capacity of the integrated facility (400 kt.year^{-1}). Surplus electricity and biogas from these facilities were also available for use in the integrated mill. For the 1 G expansion scenario, each integrated facility demands other 1.58 ethanol supplier mills, and for the 1 G2G expansion, 0.89 (Fig. 6). Each sugarcane mill is modeled after a stalk processing capacity of 4 Mt.year^{-1}, a typical size in Brazil due to its economic feasibility and equipment dimensions[39].

Each inventory combines different industrial pathways applied for the polymerization of ethylene, such as gas-phase, suspension, and

https://doi.org/10.1038/s41467-024-53201-9

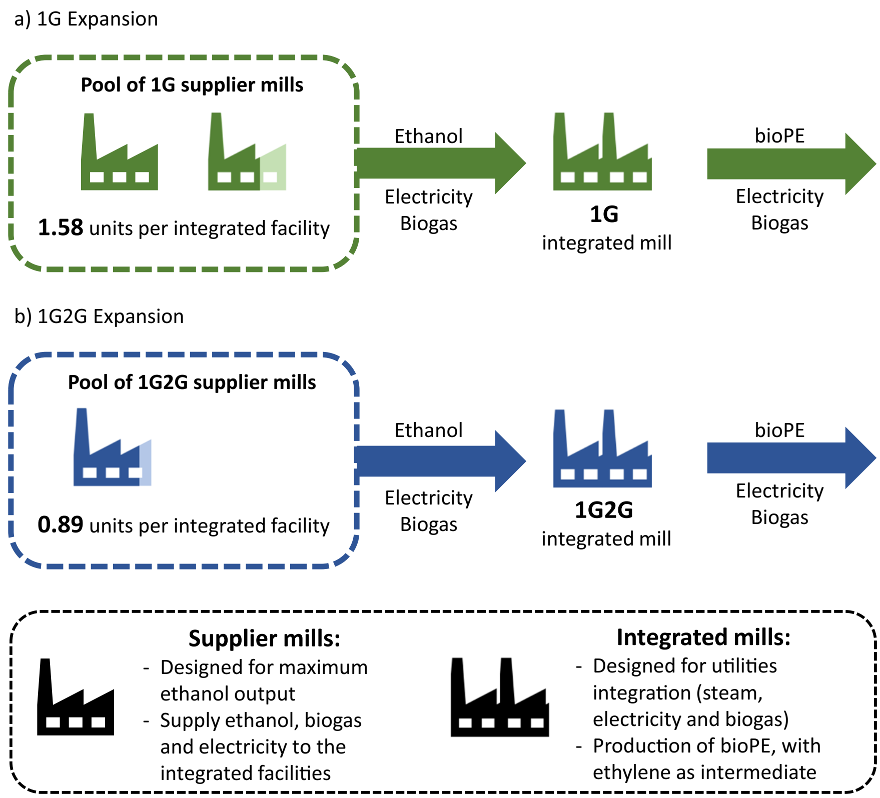

Fig. 6 | Supply and integration arrangements for bioPE production using different ethanol technologies for expansion. Expansions considered using first generation (1G) ethanol mills (**a**) or first and second generation (1G2G) ethanol mills (**b**).

solution polymerization processes[40], according to their market share. Ecoinvent presents separate inventories for each PE grade, namely High-Density Polyethylene (HDPE), Low-Density Polyethylene (LDPE) and Linear Low-Density Polyethylene (LLDPE)[41–43]. These inventories were used to describe fossil-based PE and adapted for bioPE production, by introducing biopolyethylene and performing energy integration with sugarcane mills (Fig. 6).

Polyethylene recycling and end-of-life

For the modeling of PE post-consumption, it was considered (i) mechanical recycling, with two technological options, assuming simple (SR) and advanced (AR) levels; (ii) chemical recycling, with PE depolymerization and subsequent monomer processing into PE; (iii) End-of-Life (EoL), considering current and future compositions of final disposal, encompassing open dumps, landfills, leakage, and incineration. Modeling of waste polyethylene final disposal (EoL) considered a selection of inventories from ecoinvent, built specifically for PE, namely open burning, open dump, landfill (unsanitary and sanitary), and municipal incineration. Plastic waste leakage, or littering, was used for accounting purposes only, since no Life Cycle Impact Assessment (LCIA) methods available today are able to classify and characterize this flow into potential environmental impact[14]. Such specific LCIA characterization factors are being developed by the Marine Impacts in LCA (MarILCA) project, for areas of protection such as human health and ecosystem quality[44].

Mechanical recycling inventories (simple and advanced) consider three main circularity efficiencies: sorting, based on how much of the collected plastic residue is processed in recycling units; processing, based on the technical yield of the recycling process; market substitution, associated with actual circularity of the recycled material, in terms of material quality and application. Advanced mechanical recycling aims for a more thorough separation of different polymers among the plastic waste stream and removal of impurities, such as ferrous and non-ferrous metallic material[11]. Chemical recycling assumes a combination of a depolymerization inventory and an adaptation of the polymerization inventories for the three PE grades. Depolymerization is carried out by catalyzed thermolysis, and the resulting monomers are assumed to be direct substitutes to their virgin counterparts[12]. The inventories used are presented in Tables S2, S3 and Table S4 (Supplementary Information).

Scenarios definition

Carbon footprint calculations were carried out with a cradle-to-grave approach using the Global Warming Potential (GWP) impact category from ReCiPe 2016 (H) 1.09 impact assessment method. It was chosen as the functional unit 1 kg of PE in use. It was assumed that only the inlet of virgin bioPE in the value chain would account for biogenic carbon stocks, even though uncertainties are in place regarding circularity, long-term applications and disposal in landfills. Also, aspects regarding the long-term stability of these carbon stocks and the temporal dynamics of material accumulation within the circular economy of plastics, due to its expected growing demand for the following decades, are still to be determined[3,4]. Still, the use of biobased plastics (and other materials) as carbon sinks can be of great importance for net-zero emission strategies and should be further explored in the future.

Two scenarios were designed, the first one considering current practices and the second one projecting 2050's PE demand and increased renewability and recyclability in the value chain. For the current scenario, based on 2019 data, 83.6% of all the produced PE (virgin and recycled) was assumed to be discarded[45] and, from this amount, 10.2% is collected for recycling and 24% incinerated[1]. The remaining 38.8% is accounted as leakage, and the rest is destined to dumps and landfills[45]. For the future scenarios (2050), two technological options were considered for recycling (Simple and Advanced). On the Simple option, it was assumed that the production volume of virgin

Table 3 | Scenario definition for current and future projections

Scenario	Base year	Total demand for PE (virgin and recycled)	End of life composition*	bioPE substitution	Sugarcane ethanol technology	Recycling technology
Current	2019	109.8 Mt	a	0.28%	-	Simple
Trend	2050	238.6 Mt	b	2.4%	1 G	Simple
Future SR 1 G	2050	238.6 Mt	c	100%	1G	Simple
Future SR 1G2G	2050	238.6 Mt	c	100%	1G2G	Simple
Future AR 1G	2050	238.6 Mt	c	100%	1G	Advanced
Future AR 1G2G	2050	238.6 Mt	c	100%	1G2G	Advanced

*End-of-life composition:

[a]Literature-based statistics (refer to text for details);

[b]OECD projections;

[c]Use of recycling options to achieve circularity targets (specific for each scenario) and prioritization of sanitary landfills and incineration to avoid leakage.

Table 4 | Criteria choice for the assessment of synergies and trade-offs in the sugarcane expansion area

Criteria	Reference	Classes	Definition
Water scarcity vulnerability	Basin water balance status	Low	No problem
		Medium	Qualitative problem
		High	Quantitative and quali-quantitative problem
Carbon stock change	Organic carbon stock change from soil and biomass (dLUC emission)	Stock	dLUC < 0
		Emission	dLUC > 0
Biodiversity loss vulnerability	Biological importance of areas and reported biodiversity impacts (direct and indirect) considering sugarcane expansion on current land use	Low	Degraded pastureland
		Medium	Annual crop and non-degraded pastureland
		High	High biological importance areas

PE from 2019 would be maintained in 2050, and all the additional PE demand would be supplied by recycled plastic. For the Advanced option, the gains in efficiency and circularity are reflected in a reduced demand for virgin plastic, assuming the same waste PE collection volume for recycling as the Simple option. For both the future scenarios, 50% of the discarded PE that is not recycled is sent to municipal incineration and 50% to sanitary landfills, with no plastic leakage.

PE global demands for 2019 and 2050 were based on the projections from OECD[46], segmented into HDPE and LDPE/LLDPE. It was assumed that all virgin fossil PE production would be substituted by bioPE by 2050, as an effort to limit GHG emissions from this value-chain, even though this substitution is expected to reach only 2.4%, if the current trend for bioplastics demand growth is followed (CAGR 8.3%)[47]. An additional scenario for 2050 was also considered, using OECD future projections, that was called “trend”, and assumes that all future bioPE production will rely on 1 G ethanol expansion. The proposed future scenarios consider an increased reuse of PE, that ultimately would result in more material available for recycling, as opposed to the “trend” scenario. This is a generalization to represent a more environmentally idealistic scenario for future bioplastics. Table 3 summarizes the differences among the scenarios.

Biomass production modeling and criteria for selection of areas

Sugarcane expansion areas were first delimited by the original Sugarcane Agroecological Zoning (SAEZ), a zoning for sugarcane expansion in Brazil developed by the Brazilian Agricultural Research Corporation (EMBRAPA)[48]. Further updates on this zoning were suggested in previous studies[49], excluding areas that are currently occupied by sugarcane, unsuitable for mechanical harvesting due to slope, and environmentally relevant, as well as remaining native vegetation. The focus was directed to the states within the Brazilian Center-South region that mostly contribute to the current sugarcane production[27]. Building upon these updates, a new update has been made considering only current pastureland and annual crops classified by the Annual Mapping Project of Land Use and Cover in Brazil (MapBiomas)[50] for sugarcane expansion. In the case of pastureland, the level of degradation classified by vegetative vigor was also extracted from MapBiomas.

Sugarcane yield was estimated using the Crop Assessment Tool (CAT), an agrometeorological model based on the Agroclimatic Zoning methodology[51] with adaptations for the Brazilian Center-South characteristics regarding climate and sugarcane cultivation[52], using historical climate data in a resolution of 27 km as input[53]. Sugarcane agricultural operations were modeled with CanaSoft, developed by the Brazilian Biorenewables National Laboratory (LNBR/CNPEM)[54]. Input data for CanaSoft on crop yield and sugarcane straw recovery were assumed to be the average for the expansion area within the revised SAEZ.

Three criteria associated with ecosystem functions and services were chosen to assess trade-offs and synergies in the considered expansion area, addressing the possible impacts related to land use change from current land use to sugarcane: water scarcity vulnerability; carbon stock change; and biodiversity loss vulnerability (Table 4). The maps from the three established criteria were crossed and the resulting areas and emission or stock associated to land use change from each overlay combination were calculated and presented.

Qualitative and quantitative water balance status was extracted from Brazilian water and sanitation agency (ANA)[55] and the 30 m-pixels in the expansion area were divided in three classes for water scarcity vulnerability: low, medium and high. Pixels with qualitative problems were classified as medium vulnerable, while quantitative and quali-quantitative problematic ones were classified as high. As quantitative balance refers to the relationship between withdrawal flows and water availability, this is critical for the development of agriculture and a compromised balance represents higher risks to water availability in the basins. The qualitative balance classification was made by ANA considering basin’s ability to assimilate domestic organic loads, being more assertive for residential than for agricultural expansion outside urban centers.

Carbon stock change for the sugarcane expansion was calculated considering soil and biomass carbon stock in the expansion area using spatially explicit sugarcane yield, current land use classification, guidelines from IPCC[56] including equations S1 and S2 (Supplementary Information) and the emission factors presented in the Table S1 (Supplementary Information). The area was divided in two classes for the criterion: carbon emissions and carbon stocks.

For the biodiversity loss vulnerability, the same area was divided in three classes: low, medium, and high. The areas currently occupied by pasturelands or annual crops but classified as areas of high biological importance by the Brazilian Ministry of Environment (MMA)[57] were classified as a high biodiversity loss vulnerability, presenting higher risks. Degraded pastureland pixels were classified as a low vulnerability, as they are expected to fail to regain previous biodiversity levels on their own if abandoned[58] and have low deforestation risks associated when occupied, being pointed as less vulnerable for energy crops expansion[59]. It is worth mentioning that sugarcane expansion has historically occurred over pastureland in Brazil[60, 61].

Despite the efforts by studies to determine relationships between agricultural production and biodiversity[62,63], it is difficult to evaluate the direct impacts of the sugarcane expansion on biodiversity for anthropized areas. Studies have suggested a decrease in macrofaunal abundance and diversity when sugarcane replaces pastureland[64], however, the activity represents a lower indirect land use change (iLUC) risk over native vegetation if compared to annual crops, that have also a higher impact on food production[65,66].

It's worth noting that in Brazil a large part of annual crops corresponds to soybean with maize as a second crop, in addition to the use of conservative agricultural practices, such as crop rotation, minimum soil disturbance, and soil cover maintenance[67], which might attenuate the impacts on reduction of biodiversity communities[68]. Nevertheless, native vegetation and original biodiversity have already been suppressed. Therefore, considering the involved uncertainties regarding those land use changes to sugarcane, and its direct and indirect possible impacts, both annual crops and non-degraded pastureland were classified as a medium biodiversity loss vulnerability.

Data availability

The raw and calculated data of figures and tables generated in this study have been provided in the figshare database available at https://figshare.com/s/a7abc068cec9db42d996?file=47847163. Additional information and inventories are presented in the Supplementary Information.

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Acknowledgements
This research used facilities of the Brazilian Biorenewables National Laboratory (LNBR), which is part of the Brazilian Centre for Research in Energy and Materials, a private nonprofit organization under the supervision of the Brazilian Ministry for Science, Technology, and Innovations.

Author contributions
G.P.N. contributed to Conceptualization, Methods, Formal analysis, Writing - Original Draft and Writing - Review & Editing. G.P.P. contributed to Conceptualization, Methods, Software, Formal analysis, Writing - Original Draft, Visualization and Writing - Review & Editing. M.F.C. contributed to Methods and Formal Analysis. I.L.M.S. contributed to Methods and Writing - Original Draft. L.Z.O.M. contributed to Methods. T.L.J. contributed to Methods and Writing – Original Draft. E.R.M. contributed to Conceptualization, Methods and Writing – Original Draft. T.A.D.H. supervised the work and contributed to Conceptualization, Methods, Formal analysis, Writing – Original Draft and Writing - Review & Editing.

Competing interests
The authors declare no competing interests.

Additional information
Supplementary information The online version contains supplementary material available at https://doi.org/10.1038/s41467-024-53201-9.

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Peer review information *Nature Communications* thanks Sameh Samir Ali, Gabriel Granco and the other, anonymous, reviewer(s) for their contribution to the peer review of this work. A peer review file is available.