

### Climate tipping indicators for improved environmental sustainability assessment of bio-based materials

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Climate tipping indicators for improved environmental sustainability assessment of bio-based materials

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PhD Thesis February 2021

DTU Management Technical University of Denmark



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### PREFACE

This PhD thesis titled "Climate tipping indicators for improved environmental sustainability assessment of bio-based materials" was conducted at the Quantitative Sustainability Assessment Section of the Department of Management at the Technical University of Denmark (DTU), between September 2017 and February 2021. The main supervisor was Senior Researcher Mikołaj Owsianiak and the co-supervisor was Professor Michael Z. Hauschild. The PhD was funded by the EU Horizon 2020 project BioBarr (project no. H2020-745586) and co-financed by DTU. During the project period, a research external stay was carried out at the Centre for Biodiversity and Environment Research, University College London (UCL) under the supervision of Dr. Tim Newbold, and four journal articles were prepared. The articles are included as appendices and, throughout the text, they are referred to using roman numerals as indicated below:

- Article I Fabbri S., Hauschild M. Z., Lenton, T. M. Owsianiak, M. (2021).
  Multiple climate tipping points metrics for improved sustainability assessment of products and services. *Environmental Science and Technology*. DOI: 10.1021/acs.est.0c02928
- Article II Fabbri S., Owsianiak M., Newbold T., Hauschild M. Z. Development of metrics for climate tipping in life cycle assessment based on damage to ecosystems. *Manuscript in* preparation intended for submission to Ecological Indicators.
- Article III Fabbri S., Hauschild M. Z., Owsianiak M. Implications of accounting for multiple climate tipping impacts in life cycle assessment: examination of two case studies. *Manuscript in preparation intended for submission to Sustainability*.

Article IV Vea E. B., Fabbri S., Spierling S., Owsianiak M. Environmental performance of polyhydroxyalkanoate (PHA)-based plastics with improved barrier properties. *Submitted to ACS Sustainable Chemistry and Engineering*.

In addition, contribution to the following article was carried out during this PhD project.

Rodríguez L. J., Fabbri S., Orrego C. E., Owsianiak M. (2020). Comparative life cycle assessment of coffee jar lids made from biocomposites containing poly(lactic acid) and banana fiber, *Journal of Environmental Management*, 266. DOI: 10.1016/j.jenvman.2020.110493.

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### SUMMARY

Introduction of bio-based materials represents one of the key strategies in the transition to a bio-based economy, as these materials are thought to contribute to climate change mitigation through reduction of fossil-related GHG emissions. However, currently recommended metrics used in life cycle impact assessment (LCIA), i.e. the global warming potential (GWP) and the global temperature change potential (GTP), do not account for the potential of GHG emissions to trigger dramatic and potentially irreversible changes in the climate system (so called, climate tipping points). Climate tipping points are crossed when the global temperature reaches specific thresholds. Earlier efforts to include climate tipping in LCIA are limited to the climate tipping potential (CTP) metric, which considers only the loss of Arctic sea ice as tipping point. Yet, several other tipping points are foreseen to be crossed within this century. Examples include the collapse of the ocean circulation in the Atlantic or the irreversible melting of the Greenland ice sheet. This makes climate tipping particularly relevant to consider for bio-based materials, as they are often designed for biodegradability and may contribute to crossing multiple climate tipping points.

The objectives of this PhD work were (1) to develop a methodology to account for multiple climate tipping points for assessing the climate performance of products in life cycle assessment (LCA), and (2) to apply this methodology to selected case studies on bio-based materials. This resulted in the development of new characterization factors, the multiple climate tipping points potentials (MCTP), at both midpoint and endpoint level. Substance-specific MCTP, expressing the impact per unit of emitted substance, were calculated for the three major anthropogenic GHGs: carbon dioxide (CO<sub>2</sub>), methane (CH<sub>4</sub>) and nitrous oxide (N<sub>2</sub>O).

The MCTP at midpoint level was built taking the earlier climate tipping potential (CTP) of Jørgensen et al. (2014) as starting point. The CTP depends on the proximity of an emission to the tipping point (Arctic summer sea ice loss) and on the share of carrying capacity up to this tipping point that is taken up by emissions. Their framework was expanded and adapted to include 12 additional projected climate tipping points, which were selected based on a set of criteria defined to ensure feasibility of modelling. Each tipping point was then modelled considering the potential effects that crossing a tipping point has on speeding up the next tipping points, while accounting for uncertainties in the temperature thresholds triggering tipping. The resulting midpoint MCTP gives a measure of the potential contribution of a product's life cycle GHG emissions to crossing multiple climate tipping points. The MCTP depends on the emission year and it assigns larger impacts to those emissions occurring right before when a tipping point is expected. Given this dynamic character, MCTPs are provided as sets of year-specific factors. The method, however, is not without limitations. Particularly, the calculation of year-specific MCTP factors depends on knowledge about future expected tipping points and development of the background atmospheric GHGs concentration, which are uncertain.

Building on the midpoint MCTP methodology, the framework was further developed by translating the contribution to tipping (midpoint level impacts) into potential temperature increase and then into potential loss of species following the temperature increase. The resulting MCTP at endpoint level therefore expresses the damage to ecosystems quality in terms of potential loss of terrestrial species resulting from the contribution of GHG emissions to cross climatic tipping points. To improve comparability with other indicators for species loss used in LCA, the endpoint MCTP factors were expressed as either local loss of species, i.e. loss from delimited areas that can be reverted through recolonization from other areas, or global loss of species, i.e. irreversible extinction across the world. Being generally proportional to the MCTP at midpoint, the resulting endpoint MCTP attributes a larger potential species loss to emissions with higher contribution to crossing tipping points, given that crossing could intensify warming and exacerbate species loss. It follows that the main advantage of the endpoint MCTP is to express impacts in terms of damage to terrestrial species. This, however, warrants further harmonization efforts to make them fully comparable with endpoint indicators representing other impact categories.

To demonstrate the potential added value of MCTPs in environmental sustainability assessment of bio-based materials, the developed MCTPs at midpoint level were applied to three 'cradle-to grave' case studies on: (i) engineered biochar obtained from biomass residues, (ii) engineered hydrochar obtained from green waste and (iii) polyhydroxyalkanoate (PHA) bio-plastic produced from molasses. The cases on hydrochar and PHA showed that MCTPs can bring additional insights compared to GWP and GTP metrics. While with GWP the climate performance improved with increasing stability of the bio-based material, due to larger benefits from carbon storage, MCTP showed the opposite trend because when degradation is slow a substantial share of emissions occurs in proximity to tipping points, where climate tipping impacts are the largest. In the case of biochar, MCTP did not lead to additional insights, showing that the performance of very stable materials like biochar depends more on total amount of emissions released over a certain timeframe rather than on emission timing and proximity to tipping points. Thus, the use of MCTP is more relevant for assessing bio-based materials that slowly degrade over time but achieve at least 95% degradation in about 70 years. This is also expected to be the case for the endpoint MCTPs.

In conclusion, this PhD work contributed to the development of a more robust LCIA methodology accounting for climate tipping impacts of products' life cycle GHG emissions. Climate tipping represents a new impact category in the context of climate change impacts and thus the developed MCTP factors should be considered

complementary, and not a substitute, to the recommended GWP and GTP. Their use for assessment of the climate tipping impacts of selected bio-based materials can add new insights on their environmental sustainability performance depending on the stability of the bio-based material. A practical implication of the new MCTP factors is the requirement for emission inventories to be provided in time-differentiated format, where relevant and where necessary.

### RESUMÉ (DANISH)

Introduktion af biobaserede materialer er en af nøglestrategierne i overgangen til en biobaseret økonomi, da disse materialer menes at bidrage til at begrænse klimaændringer ved at reducere udledning af fossile drivhusgasser. De anbefalede indikatorer anvendt i livscyklus konsekvensvurdering (LCIA) er hhv. det globale opvarmningspotentiale (GWP) og det globale temperaturændringspotentiale (GTP). Disse tager dog ikke højde for potentialet for drivhusgasemissioner for at udløse dramatiske og potentielt irreversible ændringer i klimasystemet (såkaldte klimatippepunkter). Et klimatippepunkt krydses, når den globale temperatur specifik grænse. Tidligere bestræbelser på at inkludere overstiger en 'klimatippepunkter' i LCIA er begrænset til klimatippepotentialet (CTP), som kun betragter tabet af arktisk havis som et tippepunkt. Alligevel forventes adskillige andre tippepunkter at blive overskredet inden for dette århundrede, så som kollaps af havcirkulationen i Atlanterhavet eller den irreversible smeltning af det grønlandske indlandsis. Dette gør det særlig relevant at overveje klimatippepunkter for biobaserede materialer, da de ofte er designet til at være bionedbrydelige og kan bidrage til at krydse flere klimatippepunkter.

Formålet med dette ph.d.-projekt var (1) at udvikle en metode som tager højde for flere klimatippepunkter når produkters klimapåvirkning vurderes i livscyklusvurdering (LCA) og (2) at anvende denne metode til udvalgte casestudier omkring bio-baserede materialer. Dette resulterede i udviklingen af nye karakteriseringsfaktorer, adskillige klimatippepotentialer (MCTP), på både midtpunkt og slutpunkt niveau. Substansspecifikke MCTP'er, der udtrykker påvirkningen per enhed af udledt substans, blev beregnet for de tre vigtigste menneskeskabte drivhusgasser: kuldioxid (CO<sub>2</sub>), metan (CH<sub>4</sub>) og lattergas (N<sub>2</sub>O). MCTP på midtpunkt niveau blev udarbejdet ved at anvende CTP fra Jørgensen et al. (2014) som udgangspunkt. CTP afhænger af hvor tæt en emission er på tippepunktet (tab af arktisk sommer havis) og hvor stor en andel af bæreevnen til tippepunktet er nået, der er optaget af emissioner. Denne metode blev udvidet og tilpasset til at omfatte 12 yderligere forventede klimatippepunkter, der blev valgt på baggrund af et sæt kriterier, der var defineret for at sikre at modelleringen var gennemførlig. Hvert tippepunkt blev derefter modelleret i betragtning af de potentielle påvirkninger, som overstigningen af et tippepunkt har på at fremskynde de næste tippepunkter, samtidig med at der tages højde for usikkerhed i temperaturgrænserne, der udløser at punktet tippes. Den resulterende midtpunkt MCTP er altså et mål for det potentielle bidrag som et produkts drivhusgasudledninger i dets livcyklus har på overstigningen af flere klima tippepunkter. MCTP afhænger af emissionsåret, og det tildeler større påvirkninger til de emissioner, der opstår lige før et forventet tippepunkt. I betragtning af denne dynamiske karakter, er MCTP faktorer til rådighed som sæt af årsspecifikke faktorer. Metoden er dog ikke uden begrænsninger. Især afhænger beregningen af årsspecifikke MCTP-faktorer af viden om fremtidige forventede tippepunkter og udvikling af baggrundsatmosfæriske drivhusgas koncentrationer, som er usikre.

Baseret på midtpunkt MCTP, blev metoden videre udviklet ved at oversætte bidraget til (påvirkninger klimatippepunkter på midtpunktsniveau) til potentiel temperaturstigning og derefter til potentielt tab af arter på bagrund af temperaturstigningen. Det resulterende MCTP på slutpunktsniveau, udtrykker derfor skade på økosystemers kvalitet med hensyn til potentielt tab af terrestriske arter, som følge af drivhusgasemissioners bidrag til at krydse klimatippepunkter. For at forbedre sammenligneligheden med andre indikatorer for artstab, der bliver brugt i LCA, udtrykkes slutpunkt MCTP'er enten som lokalt tab af arter (dvs. tab fra afgrænsede områder, der kan tilbageføres gennem rekolonisering fra andre områder) eller som globalt tab af arter (dvs. irreversibel udryddelse verden over). Da

endepunkt MCTP'er generelt er proportional med midtpunkt MCTP'er, tilskriver den et større potentielt artstab til emissioner med højere bidrag til krydsning af tippepunkter, da krydsning kan intensivere opvarmningen og forværre artstabet. Det følger heraf, at den største fordel ved slutpunkt MCTP-faktorer er at udtrykke påvirkninger med hensyn til skader på terrestriske arter. Yderligere arbejde i harmonisering bør prioriteres, for at gøre dem fuldt sammenlignelige med slutpunktsindikatorer, der repræsenterer andre påvirkningskategorier.

at demonstrere den potentielle værdi af MCTP'er i miljømæssig For bæredygtighedsvurdering af biobaserede materialer, blev de udviklede midtpunkt MCTP'er anvendt til tre 'cradle-to-grave' casestudier på: (i) biokul fremstillet fra biomasserester, (ii) hydrokul fremstillet af grønt affald og (iii) polyhydroxyalkanoat (PHA) bioplast fremstillet af melasse. Studierne på hydrokul og PHA viste, at MCTP'er kan give yderligere indsigt sammenlignet med GWP- og GTP-indikatorer. Hvor GWP viser en forbedret klimaprofil med øgende stabilitet af det biobaserede materiale, på grund af større fordele ved kulstofopbevaring, viser MCTP den modsatte tendens. Dette skyldes, at ved en langsom nedbrydningen udledes en betydelig andel af emissionerne tæt på de tippepunkter, hvor påvirkning fra klimatipning er størst. I tilfælde af biokul førte MCTP ikke til yderligere indsigt, hvilket viser, at ydeevnen for meget stabile materialer som biokul afhænger mere af den samlede mængde emissioner, der frigives over en bestemt tidsramme end af emissionstidspunktet og hvor tæt på tippepunkter de udledes. Således er brugen af MCTP mere relevant til vurdering af biobaserede materialer, der langsomt nedbrydes over tid, men opnår mindst 95% nedbrydning på cirka 70 år. Dette forventes også at være tilfældet for slutpunkts-MCTP'erne.

Afslutningsvis bidrog dette ph.d.-projekt til udviklingen af en mere robust LCIAmetode, der tager højde for hvordan klimatippepunkter påvirker drivhusgasemissionerne fra produkters livscyklus. Klimatippepunkter repræsenterer

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en ny påvirkningskategori i forbindelse med klimapåvirkninger, og derfor bør de udviklede MCTP-faktorer betragtes som supplerende og ikke en erstatning for den anbefalede GWP og GTP. Ved at anvende dem til at vurdere klimapåvirkninger fra udvalgte biobaserede materialer, kan ny indsigt i deres miljømæssige bæredygtighedsprofiler tilføjes, afhængigt af stabiliteten af det biobaserede materiale. En praktisk konsekvens af de nye MCTP-faktorer er kravet om, at emissionsopgørelser skal leveres i et tidsdifferentieret format, hvor det er relevant og hvor det er nødvendigt.

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### **ABBREVIATIONS**

ACTP	Absolute climate tipping potential
CF	Characterization factor
GHG	Green hose gas
GIS	Greenland ice sheet
GTP	Global temperature change potential
GWP	Global warming potential
HTC	Hydrothermal carbonization
IPCC	Intergovernmental Panel on Climate Change
LCA	Life cycle assessment
LCIA	Life cycle impact assessment
MCTP	Multiple climate tipping points potential
NPK	Fertilizer (Nitrogen Phosphorus Potassium)
NTCF	Near-term climate forcer
PDF	Potentially disappeared fraction of species
PHA	Polyhydroxyalkanoate
RCP	Representative Concentration Pathway
RE	Radiative efficiency
RF	Radiative forcing
SSPs	Shared Socioeconomic Pathways
THC	Thermohaline ocean circulation

### **1. INTRODUCTION**

After thousands of years where humans survived and prospered with the sole physical and animal strength, we have learned how to harness the immense power of fossil fuels, leading to an unprecedent exponential technological growth and expansion on the globe. In less than 300 years from the industrial revolution, the consequences of the uncontrolled use of fossil fuels have been wiping out entire ecosystems and causing serious threats for the future of humanity. Biomass application and the development of bio-based materials that are fully of partly derived from biomass are re-gaining more and more attention to replace fossil fuels. Examples are bio-based polymers (bioplastics), chemicals, fibre composites or engineered chars. Today the production of these materials represents a pillar in the transition to a bio-based economy and their growth is expected to continue in the future with further technological advances and novel applications (European Commission, 2018).

Biobased materials are promoted as greener alternatives compared to their petroleum-based counterparts mainly because of their potential to reduce the need for non-renewable resources and greenhouse gas (GHG) emissions. However, their sustainability is being scrutinized closely as their climate mitigation potential is not assured (e.g. due to GHG emissions from land use changes) and may come at the expenses of other impacts that are not properly addressed in current environmental impact assessment methods (Piemonte and Gironi, 2010). To reduce the risk of burden-shifting and guide strategic decision making, it is necessary to carry out thorough analyses of all environmental impacts of bio-based materials and, for this, it is important that appropriate methods exist for assessing advantages and disadvantages.

The standardized Life Cycle Assessment (LCA) methodology (ISO, 2006a, 2006b) is the most comprehensive and utilized method to assess the environmental impacts of products, including bio-based materials. LCA analyses the full life cycle of products, starting from the extraction of raw materials, to production, use and final disposal. During the life cycle impact assessment (LCIA) phase of an LCA, flows of emissions and resources exchanged between the product system and the environment are first classified based on the environmental impacts they cause and then translated into potential contribution to those impact categories. This is done by multiplying each flow with a corresponding characterization factor (CF), representing the potential impact per unit of emission or resource consumption (Hauschild and Huijbregts, 2015). Each impact category may be expressed through different indicators, which represent quantifiable aspects of the impact and to which are associated different sets of substance-specific characterization factors (CFs). LCA covers a broad range of environmental impacts, with climate change being the focus of most LCA studies on bio-based materials and on products in general (Martin et al., 2018).

Currently, the default metric for climate change impacts used in LCA is the global warming potential (GWP) proposed by the Intergovernmental Panel on Climate Change (IPCC) (IPCC, 2013). The UNEP-SETAC Life Cycle Initiative recommended use of the GWP in LCA to assess shorter-term climate change impacts, i.e., addressing the "rate of climate change" over the next decades (Jolliet et al., 2018). For addressing "long-term effects from climate change" over the next centuries, the global temperature change potential (GTP) proposed by (Shine et al., 2005) and considered by the IPCC (IPCC, 2013), was instead recommended (Jolliet et al., 2018). These two metrics were chosen as there is no single one that can appropriately assess both shorter-term and long-term impacts, highlighting that more than one metric is needed "to represent the complexity of climate change impacts" (Jolliet et al., 2018; Levasseur et al., 2016b).

One effect of GHG emissions that neither GWP nor GTP consider is the potential to push the level of GHG emissions reaching the point where dramatic and potentially irreversible changes in the climate system take place, crossing so-called climate tipping points. Several climate tipping points could be passed within this century as a consequence of human-induced climate change and increasing global atmospheric temperature (Lenton et al., 2008). The most imminent example is the seasonal, or even year-round, loss of sea ice in the Arctic which is expected to become an irreversible and self-enforcing process at around 1-3°C degrees warming above preindustrial levels (Steffen et al., 2018). (Lindsay and Zhang, 2005) suggested that a tipping point in the Arctic might have already been crossed. Passing critical tipping points will induce further and intensified changes, which will eventually cause damages to ecosystems and humans, such as loss of biodiversity and increased human health hazards (Meredith et al., 2019). Currently recommended LCA metrics for climate change do not consider climate tipping points. An attempt to consider the Arctic summer sea ice loss in LCIA methods has been made, however no robust methodology exists to account for multiple tipping points.

This PhD work aimed to address this deficiency to improve the assessment of climate change impacts of bio-based materials, which are often designed for biodegradability and may contribute to crossing multiple climate tipping points. Before describing in more detail the objectives of this PhD thesis and the relevance of considering bio-based materials (Chapter 3), an overview of climate tipping points, their expected occurrence and possible consequences from crossing them will be provided in Chapter 2. Current practice and recent advances in LCIA methods for assessing climate change and climate tipping impacts will also be presented in the same chapter.

## 2. CLIMATE TIPPING POINTS AND THEIR CONSIDERATION IN LCIA

#### 2.1 MULTIPLE CLIMATE TIPPING POINTS

In colloquial terms, the expression 'tipping point' is associated with the notion that "little things can make a big difference" (Gladwell, 2000). The climate science has adopted this concept for describing phenomena in which a small initial change in some control parameters can have large consequences on a system and cause profound transitions. In this context, the term 'climate tipping point' indicates "a critical threshold at which the future state of a system can be qualitatively altered by a small change in forcing" (Lenton et al., 2008; O'Riordan and Lenton, 2014). A 'tipping element' is a component of the earth system (identifiable as a region or a group of regions of the globe) that can be pushed toward a tipping point. Climate-altering human activities, increasing atmospheric GHG concentrations and the associated increase in global atmospheric temperature levels are the dominant drivers forcing the tipping elements to cross their tipping point.

There are several tipping elements that could cross a tipping point (Figure 1). They could be categorized in three general groups based on the type of changes involved: (i) melting of large masses of ice, (ii) changes in atmospheric and ocean circulation, and (iii) loss of biomes (Lenton, 2012). To name a few, loss of Arctic sea ice, permafrost (i.e. frozen soil in Siberia and North America) or melting of the Greenland ice sheet (GIS) fall within the first group. Circulation changes include disruption of the West African monsoon patterns or collapse of the Atlantic thermohaline ocean circulation (THC), while biome losses occur in the case of the Amazon forest dieback and the deterioration of coral reefs. Each tipping element

depends on specific variables (e.g. ice thickness, local temperature gradient, precipitation flux) which control the state of the system and can lead to a shift if pushed to cross a threshold level. These control variables are all influenced by global temperature patterns to some extent, however many uncertainties arise when trying to link these controls with global warming (Lenton, 2011). Despite this, thresholds for tipping are mostly given in terms of global mean surface temperature change (compared to a reference period) at which the tipping is triggered (Lenton, 2011). Estimates of temperature thresholds indicate that tipping points are expected to be triggered at different temperature levels ranging across 1 to >8°C of global warming above pre-industrial levels (Lenton, 2012; Schellnhuber et al., 2016; Steffen et al., 2018). The current level of warming is estimated between 0.8 and 1.2°C above preindustrial levels (IPCC, 2018), suggesting that some of the earliest predicted tipping elements, like coral reefs or Arctic summer sea ice, are very close to cross their tipping point. Others are expected at higher warming levels, such as thawing of permafrost, for which a tipping point is unlikely to be passed before 5°C warming (Drijfhout et al., 2015; Schellnhuber et al., 2016). The timing when tipping points are expected to be crossed will depend on the future development of global warming.



**Figure 1**: Map of potential climate tipping elements in the earth's system (non-exhaustive overview) Figure adapted from (O'Riordan and Lenton, 2014).

A key feature of tipping dynamics is the presence of self-enforcing (or positive) feedback mechanisms. These dominate the system dynamics after the tipping point is crossed and have the potential to trigger irreversible processes (Lenton et al., 2008; Levermann et al., 2012). The ice-albedo feedback is a typical example of self-enforcing mechanism. A loss of snow and ice area leaves larger portions of darker surface exposed to solar radiation, absorbing more heat and reducing surface albedo. In turn, this intensified warming further decreases the snow and ice area, amplifying the initial perturbation. The existence of positive feedbacks implies that the change in the state of the system, e.g. from perennial to seasonal or even ice-free cover, could potentially be irreversible, meaning that even if the forcing level is returned below the tipping point, the system will not recover to its original state (O'Riordan and Lenton, 2014). However, a tipping point may, in principle, also be reversible

(Lenton et al., 2008). For an overview of climate tipping elements and their feedback mechanisms see Table S1 in Supporting Information-1 of **Article I**.

The timescale of the transition into a new state is also a relevant factor for understanding the danger of climate tipping points. According to the formal definition of climate tipping points, which were initially referred to as 'large-scale discontinuities' (Smith et al., 2009) or 'abrupt climate change' (Alley et al., 2003), the transition can be either abrupt or gradual. Abrupt is when the "changes observed are faster than the time scale of the external forcing" (Drijfhout et al., 2015), meaning that even a slow but stable increase in global temperature can cause rapid changes such as the complete loss of Arctic sea ice cover in less than 10 years (IPCC, 2007). By contrast, a gradual transition takes place over timescales of centuries, as found for the shutdown of the ocean circulation in the Atlantic (Drijfhout et al., 2015) or millennia, as the case of the GIS meltdown (Robinson et al., 2012).

Regardless of whether abrupt or gradual, the transitions that follow the crossing of tipping points would certainly lead to dangerous climate changes with severe impacts at both regional and global levels (Schellnhuber et al., 2006). In many cases, tipping is expected to cause a further increase in warming via different mechanisms. For example, thawing of permafrost activates the microbial decomposition of the organic material that is stored in the soil, estimated to contain between 1460 – 1600 Gt of carbon (almost two times the carbon currently in the atmosphere) (Schuur et al., 2018). This could release large amounts of carbon dioxide and methane, which amplify warming. Other mechanisms are the reduction of the albedo effect from the loss of ice and snow cover, and the decline in the strength the earth's most important climate sinks derived from dieback of the Amazon rainforest or a shutdown of the Atlantic Ocean circulation (Wang and Hausfather, 2020). Impacts from tipping include also sea level rise, with a projected 7 meters rise from an ice-free Greenland (Gregory and Huybrechts, 2006), changes in global climate and weather patterns,

including intensified droughts and storms (Duque-Villegas et al., 2019), and massive losses of biodiversity, especially from biome-related tipping points (Howard, 2013; Veron et al., 2009). Moreover, the different tipping elements could interact with one another creating tipping cascades, where tipping of one element increases or reduces the likelihood of tipping the others (Cai et al., 2016; Kriegler et al., 2009; Levermann et al., 2012). For instance, freshening of the North Atlantic Ocean caused by melting of Greenland ice sheet could trigger the collapse of the Atlantic thermohaline ocean circulation. This, in turn, leads to warming of the Southern Ocean increasing the probability of ice loss from the West Antarctic ice sheet.

With increasing understanding of the imminent threats of crossing dangerous climate tipping points and the consideration that rising production and consumption patterns of products (including bio-based materials) could contribute to cross them, it is deemed particularly relevant to develop metrics that account for climate tipping impacts of products.

### 2.2 CLIMATE CHANGE IMPACT ASSESSMENT IN LCA: CURRENT PRACTICE

In LCA, climate change impacts are currently assessed considering emissions of well mixed GHGs stemming from the life cycle of products (other causes of climate change such as aerosols emissions are currently not accounted for). The overall impact pathway linking emissions to impacts considers sequentially (i) the increase in atmospheric concentration of the released gas, (ii) the change in radiative forcing (defined as the change in the net energy flux (in W·m<sup>-2</sup>) at the tropopause caused by an external driver of climate change, such as GHG emissions (IPCC, 2013)) resulting from the increased concentration, (iii) the change in atmospheric temperature due to

the change in radiative forcing and (iv) the final damage caused to ecosystems and humans through the induced warming (Figure 2).



**Figure 2**: Simplified impact pathway for climate change impacts considered by currently used metrics.

All existing LCIA methods proposing characterization factors (CF) for assessing climate change impacts use the global warming potential (GWP) as metric at midpoint level, i.e. located at some intermediary point in the impact pathway up to final damage, which is the endpoint level. The GWP expresses the potential change in radiative forcing due to a pulse GHG emission aggregated over a chosen time horizon (typically 100 years) and relates it to that of carbon dioxide (CO<sub>2</sub>), chosen as reference gas. The other complementary metric at midpoint level is the global temperature change potential (GTP), which goes one step further in the impact pathway. It expresses impacts as the change in global mean surface temperature at a chosen point in time (after 100 years) due to a pulse GHG emission, relative to that of CO<sub>2</sub>. The two metrics have been recommended by the UNEP-SETAC Life Cycle Initiative as they cover shorter-term and long-term impacts of climate change (Jolliet et al., 2018).

Considerably more challenging is the quantification of damage to ecosystems or humans from the climate change induced by GHG emissions (endpoint level). This is due to the complexity of the mechanisms involved and their dependency on highly uncertain dynamics, such as the ability of systems to adapt to the changes (Rosenbaum et al., 2018). In LCIA, damage to ecosystems is traditionally expressed as loss of species biodiversity (Curran et al., 2011; Woods et al., 2018). No specific recommendations for endpoint metrics have been developed yet. However, most LCIA methods derive endpoint CFs starting from the midpoint GWP-based factors. Midpoint to endpoint factors are then used to estimate the potential temperature change and the resulting potential loss of species caused by emissions, obtaining damage-oriented GWP CFs. Damage to human health was not addressed in this PhD thesis, therefore it will not be discussed hereafter.

The current metrics are relevant for evaluating the different types of impacts derived from either short- and long-term temperature changes, such as consequences due to lack of ecosystems adaptation in the short term or consequences from future sea level rise (Jolliet et al., 2018; Levasseur et al., 2016b). However, they do not specifically evaluate how much the changes induced by GHG emissions can potentially contribute to crossing of specific tipping points. For instance, the GTP of 1 kg of methane released today tells us the additional temperature increase that will be caused in 100 years, but without providing any information on whether that increase could contribute to triggering an irreversible loss of sea ice. Therefore, there is a need for complementary metrics that can address climate tipping.

### 2.3 RECENT ADVANCES IN CONSIDERATION OF CLIMATE TIPPING IN LCIA

Among the several alternative metrics for climate change that have emerged in recent years (see for instance the review of Levasseur et al., 2016a), the climate tipping potential (CTP) developed by Jørgensen et al. (2014) is the only example that considers climate tipping. The CTP expresses the impact of unit GHG emissions (for either CO<sub>2</sub>, CH<sub>4</sub> or N<sub>2</sub>O) based on their potential contribution to pass the tipping point for the Arctic summer sea ice. This potential contribution is quantified by considering how much the time-integrated radiative forcing change due to a pulse emission, expressed as CO<sub>2</sub>-equivalents concentration increase, contributes to deplete the remaining capacity of the atmosphere to absorb this change without crossing the Arctic tipping point. The remaining capacity up to the tipping point is defined as the time integrated atmospheric CO<sub>2</sub>-equivalents concentration increase that can still take place before reaching the tipping point. Thus, contribution to tipping is measured by contribution to deplete the remaining capacity and the final impact represents the fraction of remaining capacity taken up by a unit emission, expressed in parts per trillion of remaining capacity, ppt<sub>rc</sub>.

The CTP approach laid the foundations for including climate tipping in LCIA climate metrics, however there are some limitations to overcome in order to obtain a more robust metric. First, as it was specifically developed to capture urgent impacts and the need to stay below a critical level of warming, the CTP considers only Arctic summer sea ice as tipping point and takes a very short-term perspective by accounting only for impacts up to that point. This neglects longer term impacts given by the potential contribution of emissions to cross other expected tipping points. Second, considering only one tipping point disregards the possible consequences from passing the tipping point, which can influence occurrence of the next tipping points and thus the remaining capacity up to those points. Third, the method strongly depends on the time when the tipping point is expected and precise temperature thresholds triggering tipping are found to be rather uncertain (Kriegler et al., 2009), however no uncertainties were considered. Finally, the CTP was developed only at the midpoint level, therefore a further development step consists in providing CFs also at the endpoint level, expressing the potential species loss from contribution to climate tipping.

Recently, there has been an increasing interest in developing 'absolute' LCIA methods able to account for the carrying capacity of the environment to withstand anthropogenic pressures "without experiencing negative changes in structure or functioning that are difficult or impossible to revert" (Bjørn and Hauschild, 2015; Ryberg et al., 2018; Tuomisto et al., 2012). Considering the carrying capacity in the characterization factors as done in the CTP is one possible approach. In this context, the remaining capacity of the atmosphere up to tipping points could be seen as a limited 'resource' and tipping points would represent the 'boundaries' delimiting a 'safe operating space' to act without triggering dangerous climate changes.

### 3. OBJECTIVES AND THESIS OUTLINE

Biomaterials have very different degradability properties, which may vary from fast (within one year) to very slow (>100 years) (Emadian et al., 2017; Zimmerman and Gao, 2013). These timeframes make these materials relevant when considering climate tipping impacts as they could be potential contributors to crossing multiple tipping points. Indeed, the emissions resulting from degradation could occur right before the time when climatic tipping points are expected, potentially contributing to cross the tipping and, thus, causing more impact than mitigation. Thus, development of a robust metric for assessing climate tipping impacts could support environmental sustainability assessments of bio-based materials.

The objectives of this PhD project were (1) to develop a methodology accounting for multiple climate tipping points in LCIA that addresses the limitations of existing methods and (2) to apply this methodology to selected case studies on bio-based materials. Taking the earlier climate tipping point potential (CTP) as a starting point, this PhD work resulted in the development of new characterization factors, the multiple climate tipping points potentials (MCTP), at both midpoint and endpoint levels. Substance-specific MCTP, expressing the impact per unit of emitted substance, were calculated for the three major anthropogenic GHGs: carbon dioxide (CO<sub>2</sub>), methane (CH<sub>4</sub>) and nitrous oxide (N<sub>2</sub>O).

The remaining structure of the thesis is as follows: Chapter 4 presents the methodology for calculating MCTP factors at midpoint level and is supported by **Article I**; Chapter 5 presents the methodology at endpoint level and is supported by **Article II**; Chapter 6 illustrates the application of MCTP factors to selected case studies on bio-based materials using results from Articles **III-IV**. Finally, Chapter 7

concludes by summarizing the contributions of this PhD work and highlighting priorities for further improvements.

# 4. THE MULTIPLE CLIMATE TIPPING POINTS POTENTIAL (MCTP) AT MIDPOINT LEVEL

This chapter describes the methodology accounting for multiple climate tipping points developed to assess climate tipping impacts at the midpoint level in LCIA. The first methodological improvement consisted in considering multiple climate tipping elements beyond Arctic summer sea ice, therefore, the selected tipping elements and their potential occurrence are first presented. Next, the overall approach and conceptual framework are illustrated followed by a more detailed presentation of the mathematical framework used for computing the new characterization factors at midpoint. This is done considering other two method improvements, i.e. the possible consequences from crossing of tipping points and the uncertainties surrounding tipping points occurrence. Lastly, trends of the obtained characterization factors are highlighted.

All contents of this chapter are based on **Article I**. The parts that are taken directly from the article are marked with "…".

### 4.1 SELECTED TIPPING ELEMENTS AND THEIR POTENTIAL OCCURRENCE

From a review of the potential earth systems that could pass a tipping point with increasing warming, a list of 23 potential climate tipping elements was found (see Table S1 in Supporting Information-1 of **Article I**). To ensure that the tipping elements are relevant and can be modelled, 13 out of 23 were selected based on three

criteria which were defined as follows (all three definitions are taken from Article I):

- 1. "There is an evidence of a critical threshold beyond which a small change in one variable controlling the system (control variable) causes a large qualitative change in the system (that is, the system exhibits threshold behaviour)."
- "There is an evidence that the system's critical control variable that may pass a threshold is influenced by changes in atmospheric CO<sub>2</sub>-equivalent GHGs concentration."
- 3. "Tipping threshold estimates and their relative uncertainties can be expressed as global mean temperature change above pre-industrial levels."

Only tipping elements meeting all three criteria were considered. This excluded tipping elements that (i) were not supported by a minimum scientific evidence published in at least two peer-reviewed journals, (ii) show only a gradual change in state without a specific threshold that triggers the change, (iii) are not affected by changes in  $CO_2$ -equivalent GHGs concentration (but are affected by i.e. aerosol pollution) and (iv) tipping elements for which the critical threshold is expressed only in terms of local physical parameters (e.g. sea ice thickness) and cannot be related to either global mean temperature change above pre-industrial levels or atmospheric  $CO_2$ -equivalents concentration.

The selected tipping elements include Arctic summer sea ice loss and other 12 tipping elements listed in Table 1. According to data found in the literature, a range of temperature thresholds was assigned to each tipping element. This range indicates the interval of global mean atmospheric temperature change (above pre-industrial levels) at which tipping is likely to occur. The occurrence of tipping points depends on whether their temperature thresholds are reached and this, in turn, depends on the future evolution of the atmospheric GHG concentrations which determine the global

temperature level. Therefore, temperature projections under different Representative Concentration Pathways (RCP) of the IPCC obtained in (Meinshausen et al., 2011) were used to determine their possible occurrence (including their specific timing). As shown in Table 1, under the highest emission pathway RCP8.5 (reaching a total radiative forcing of 8.5 Wm<sup>-2</sup> in 2100) all 13 tipping points could be crossed, whereas under the lower emission pathways RCP4.5 (stabilization at 4.5 Wm<sup>-2</sup> after 2100) and RCP6 (stabilized at 6 Wm<sup>-2</sup> after 2100) some cannot occur, as expected at higher temperatures than those projected.

**Table 1**: Selected tipping elements, their temperature thresholds and potential occurrence under three RCP pathways. A tipping element is marked as 'potential' when tipping could happen also at higher temperature levels than those projected in the RCP pathway. Further details on temperature thresholds and tipping elements in general are found in **Article I**. Table taken from Supporting Information-1 in **Article I**.

Selected tipping element	Temperature threshold range (global mean temperature above pre-industrial level in °C)	Occurrence		
cicinent		RCP4.5	RCP6	RCP8.5
Arctic summer sea ice loss (AS)	1.5 – 2.6	Expected	Expected	Expected
Greenland ice sheet melt (GI)	1.6 – 3.5	Potential	Expected	Expected
West Antarctic ice sheet collapse (AI)	1.9 – 4.8	Potential	Potential	Expected
Amazon rainforest dieback (AF)	2.8 - 5.0	Potential	Potential	Expected
Boreal forest dieback (BF)	3.4 - 5.4	Not expected	Potential	Expected
El Niño-Southern Oscillation change in amplitude (EN)	3.4 - 5.9	Not expected	Potential	Expected
Permafrost loss (P)	5 - 8.5	Not expected	Not expected	Expected
Arctic winter sea ice loss (AW)	4.8 - 8.2	Not expected	Not expected	Expected
Atlantic thermohaline circulation shutoff (TC)	3.1 – 4.6	Not expected	Potential	Expected
North Atlantic subpolar gyre convection collapse (SG)	1.2 – 3.8	Potential	Expected	Expected
Sahara/Sahel and West African monsoon shift (AM)	2.9 - 4.4	Potential	Potential	Expected

Alpine glaciers loss (AG)	1.2 – 3.0	Expected	Expected	Expected
Coral reefs	1.2 - 2.5	Expected	Expected	Expected
deterioration (CR)				

#### 4.2 OVERALL APPROACH

The method for calculating the climate tipping potential (CTP) of Jorgensen et al. (2014) was further developed in this PhD work to include all 13 selected tipping elements. The resulting characterization factors (CFs) were referred to as multiple climate tipping points potentials (MCTP). When considering one tipping point the approach is as follows (in practice, the CTP approach): first the time-integrated radiative forcing due to 1 kg emission of greenhouse gas *i* is calculated, second this impact is expressed as atmospheric CO<sub>2</sub>-equivalent concentration and finally related to the remaining capacity of the atmosphere to absorb this increase in  $CO_2$ -equivalent concentration without reaching the level that could trigger the tipping point. The resulting CF represents the share of remaining CO<sub>2</sub>-equivalent concentration up to the tipping point (i.e., the remaining capacity) that is taken up by the unit emission. The concept is illustrated in Figure 3a. Here the background increase in anthropogenic GHG emissions leads to crossing the first tipping point in year  $T_{\text{tipping,1}}$  = 2030. The radiative forcing change caused by an emission that is part of that background increase and occurring in year  $T_{\text{emission}} = 2025$  (represented with a red triangle) will take up a certain share of the remaining capacity up to the tipping point (represented with a red border shape). This share represents the contribution of the emission to cross the tipping point and thus its climate tipping impact.

This approach is extended to the other selected tipping elements, by considering that now the emission at  $T_{\text{emission}}$ = 2025 will also contribute to consuming part of the remaining capacity up to the next tipping points after the first. Figure 3b, in which only two tipping points are considered for simplicity, shows that the emission
contributes to crossing both the tipping point in 2030 and the second tipping point expected in 2043. Therefore, the total climate tipping impact of an emission released in a specific year  $T_{\rm emission}$  will be the sum of the contribution to crossing all tipping points expected after  $T_{\rm emission}$ .

Similarly, an emission occurring after the first tipping point, but before the second, e.g. at  $T_{emission}$  = 2035, contributes to crossing the second tipping point. However, in this case passing the first tipping point causes an extra impact on the climate. This can be translated into an increase in CO<sub>2</sub>-equivalent concentration, which is added to the background impact (dark shaded shape in Figure 3c). Therefore, the crossing of the first tipping point causes a reduction of the remaining capacity up to the second tipping point and, thus an acceleration of the tipping year (from 2043 to 2040 in Figure 3c). This effect from tipping is accounted for in the calculation of impacts of all those emissions occurring after a tipping point has already been crossed.



**Figure 3**: Conceptual illustration of the approach underlying the calculation of MCTP factors for a unit emission occurring in different years considering one (**a**) and two (**b** and **c**) tipping points. The horizontal time axis is divided in discrete time intervals of 1-year, as indicated with capital letters, and vertical bars represent annual CO<sub>2</sub>-equivalents concentration

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increases.  $T_{emission}$  indicates the emission year;  $T_{tipping,1}$  and  $T_{tipping,2}$  indicate the year of tipping of the first and second tipping point, respectively.  $C(T_{tipping,1})$  and  $C(T_{tipping,2})$  represent the level of CO<sub>2</sub>-equivalent concentration that stabilizes the climate at the temperature threshold triggering the first and the second tipping point, respectively. Figure taken from **Article I**.

Overall, the main features of the new approach are:

- The total contribution of an emission to cross multiple climate tipping points is determined by considering the contribution to deplete the remaining capacity up to each expected climate tipping point.
- The climate tipping impact of a unit emission is based on the remaining capacities: what is relevant is not much the radiative forcing induced by the emission *per se*, but how much this radiative forcing, expressed as CO<sub>2</sub>-equivalent concentration, depletes the remaining capacity up to a specific tipping point.
- The impact of an emission depends on the time when the emission is released. This is because timing determines which tipping points could be influenced by the emission and how much remaining capacity is left up to these tipping points. Therefore, MCTP CFs for a given GHG are provided as a set of year-specific values, providing the impact per unit of emission released in different years.
- MCTP factors are influenced by the background level of anthropogenic GHG emissions. This because background emissions determine the timing of the tipping points, which in turn, affect the remaining capacity that is used to calculate the MCTP. Therefore, MCTP CFs were calculated for different Representative Concentration Pathways (RCP).
- Generally, the approach used to develop MCTP characterization factors can be considered as in line with an *average* modelling approach. In this approach, the impact attributed to the assessed product represents the

contribution of the product to the total background impact rather than the small additional impact on top of this background (Huijbregts et al., 2011). Therefore, the GHG emissions associated to a product's life cycle are assumed to be part of the anthropogenic background GHG emissions. This is different from the *marginal* modelling approach adopted by most other metrics like GWP, which aims to quantify the very small (marginal) impacts induced by emissions on top of a background situation (Huijbregts et al., 2011).

#### 4.3 MODELLING FRAMEWORK FOR CALCULATION OF MIDPOINT MCTP FACTORS

Specific definitions in this section are taken from Article I.

The multiple climate tipping points potential, MCTP<sub>*i*</sub>, in  $[ppt_{rc} \cdot kg_i^{-1}]$  (parts per trillion of remaining capacity taken up by a unit emission) of gas *i* emitted at year  $T_{emission}$  was defined as the sum of the ratios between the *impact of the emission* (that is part of anthropogenic background emissions) and the corresponding remaining capacity for each of the *m* tipping points occurring after the emission year:

$$MCTP_{i}(T_{\text{emission}}) = \sum_{j=1}^{m} \frac{I_{\text{emission},i,j}(T_{\text{emission}})}{CAP_{j}(T_{\text{emission}})}$$
(1)

where *j* indicates the *j*th tipping point occurring after the emission year (in order of occurrence) and can take any value from 1 to *m*, which is the total number of exceeded tipping points;  $I_{\text{emission},i,j}$  is the *impact of the emission* of gas *i* with respect to the *j*th tipping point,  $CAP_j$  is the remaining capacity up to the *j*th tipping

point, and the emission year  $T_{\text{emission}}$  is any year in which life cycle emissions take place.

The  $I_{\text{emission},i,j}$  [ppm CO<sub>2</sub>e · yr · kg<sub>i</sub><sup>-1</sup>] (where CO<sub>2</sub>e is the CO<sub>2</sub>-equivalent concentration) of gas *i* with respect to the *j*th tipping point was defined as the absolute climate tipping potential (ACTP) of gas *i* in [W · m<sup>-2</sup> · yr · kg<sub>i</sub><sup>-1</sup>] divided by the radiative efficiency (RE) of 1 ppm CO<sub>2</sub> [W · m<sup>-2</sup> · ppm CO<sub>2</sub><sup>-1</sup>](Jørgensen et al., 2014):

$$I_{\text{emission},i,j}(T_{\text{emission}}) = \frac{ACTP_{i,j}(T_{\text{emission}})}{RE_{\text{CO}_2}} = \frac{\sum_{k=1}^{n} RF_i(T_{k-1}) \cdot \Delta T}{RE_{\text{CO}_2}}$$
(2)

where the ACTP is equal to the radiative forcing of gas  $i (RF_i)$  integrated over time between the emission and the tipping. This integral is written using Riemann sum notation, in which n is the number of time steps (dimensionless). n is equal to the difference between the year of tipping  $T_{\text{tipping},j}$  (i.e. the year when the *j*th tipping point is exceeded) and the year of emission,  $T_{\text{emission}}$ , divided by the length of the time step,  $\Delta T$ . The  $\Delta T$  is always equal to 1 year. Division by  $RE_{\text{CO}_2}$  is necessary to make the unit of the *impact of the emission* consistent with that of the remaining capacity, in ppm CO<sub>2</sub>e · yr.

The  $CAP_j$  [ppm CO<sub>2</sub>e · yr] is defined as the increase in atmospheric CO<sub>2</sub>-equivalent concentration that can still take place before reaching the concentration level (in ppm CO<sub>2</sub>e) that stabilizes the climate to the temperature level that could trigger the tipping. It is calculated considering the effect of crossing any preceding tipping points in terms of CO<sub>2</sub>-equivalent concentration increase caused by tipping,  $C_{tip}$ , which reduces the remaining capacity and expressed using Riemann sum notation calculated for 1-year time steps:

 $CAP_j(T_{\text{emission}})$ 

$$= C(T_{\text{tipping},j}) \cdot (T_{\text{tipping},j} - T_{\text{emission}})$$
$$- \sum_{k=1}^{n} [C(T_{k-1}) + C_{\text{tip}}(T_{k-1})] \cdot \Delta T$$
(3)

where,  $C(T_{\text{tipping},j})$  is the atmospheric CO<sub>2</sub>-equivalent concentration at the year of tipping  $T_{\text{tipping},j}$ , C(T) is the CO<sub>2</sub>-equivalent concentration from background emissions at time T and  $C_{\text{tip}}(T)$  is the change in CO<sub>2</sub>-equivalent concentration at time T caused by all tipping points occurred before  $T_{\text{emission}}$  (all terms expressed in ppm CO<sub>2</sub>e). The calculation of  $C_{\text{tip}}(T)$  is further detailed in Section 4.3.1.

The framework was used to compute year-specific MCTP factors for CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub>O under the three RCP pathways RCP4.5, RCP6 and RCP8.5 to account for the influence of the background GHG concentration development path. To account for the uncertainties in the occurrence of tipping points, a triangular probability distribution was assigned to the range of possible temperature thresholds found for each considered climate tipping element (shown in Table 1) and included in the computation of MCTP factors in 10000 Monte Carlo simulations. Each simulation represents a possible scenario with different timing and sequence of tipping points. Final MCTP factors were calculated as the average (geometric mean) from the 10000 simulations.

#### 4.3.1 CALCULATING EFFECTS FROM CROSSING TIPPING POINTS

 $C_{\rm tip}(T)$ , here indicated with  $C_{\rm tip}(T_{\rm effect})$  to indicate dependency on the year in which effects caused by tipping points unfold ( $T_{\rm effect}$ ), was obtained from estimates of radiative forcing (RF) changes caused by passing each specific tipping point. This

radiative forcing was then converted to the  $CO_2$ -equivalents concentration increase (in ppm  $CO_2e$ ) that would lead to the same RF change, to allow accounting for this effect in the calculation of the remaining capacity (which is expressed in ppm  $CO_2e$ ). At any year  $T_{effect}$ , the total effect from tipping is given as the sum of the effects from tipping resulting from each tipping element:

$$C_{\rm tip}(T_{\rm effect}) = \sum_{a} C_{\rm tip,a}(T_{\rm effect})$$
(4)

where *a* indicates a tipping element that passed its tipping point before  $T_{\text{emission}}$ , and  $C_{\text{tip},a}$  is the CO<sub>2</sub>-equivalent concentration increase caused by crossing the tipping point of the tipping element *a*.

For Arctic summer and winter sea ice loss, changes in RF are due to reduced sea ice albedo derived from ice loss (Hudson, 2011). This results in a constant annual increase of 22.2 and 52.0 ppm CO<sub>2</sub>e for the two tipping elements, respectively. For six of the selected tipping elements (i.e. Greenland ice sheet melt, West Antarctic ice sheet collapse, El Niño-Southern Oscillation change in amplitude, permafrost loss, Amazon rainforest and Boreal forest dieback) estimated changes in RF are due to carbon emissions that could be released after tipping (either in the form of CO<sub>2</sub> or methane). Such emissions originate from mechanisms like anomalous fire events or flooding of low-lying permafrost (Cai et al., 2016; Steffen et al., 2018). For these tipping elements, calculation of  $C_{tip,a}$  was done by adapting the dynamic GWP approach of Levasseur et al. (2010) to obtain time-dependent (dynamic) yearly equivalents of GHGs concentration increase resulting from the carbon emissions. The first step was to compute the instantaneous dynamic characterization factor of the pulse emission of gas *i* (derived from tipping) at any year *T*,  $DCF_{inst,i}(T)$ , and express it as time-integrated CO<sub>2</sub>-equivalent concentration as follows:

$$DCF_{\text{inst},i}(T) = \int_{t_{\text{ini}}-1}^{t_{\text{ini}}} \Delta C_i \cdot IRF_i(t) \cdot \frac{RE_i}{RE_{\text{CO}_2}} dt \qquad \text{for } T = 1,2,3,\dots$$
(5)

Where the  $DCF_{inst,i}(T)$  [ppm CO<sub>2</sub>e · yr · kg<sub>i</sub><sup>-1</sup>] is calculated for relative time *intervals* of 1-year length (i.e. T = year 1, year 2, etc.) defined within an initial and a final point in time,  $T = [t_{ini}, t_{end}]$ , and where time t is relative and continuous. The  $\Delta C_i$  [ppm<sub>i</sub> · kg<sub>i</sub><sup>-1</sup>] is the change in atmospheric GHG concentration due to a unit emission of gas i;  $IRF_i(t)$  is the impulse response function of gas i representing the decay of the gas after a pulse emission;  $RE_i$  is the radiative efficiency per ppm of gas i and  $RE_{CO_2}$  is the radiative efficiency per ppm CO<sub>2</sub>. By combining the  $DCF_{inst,i}$ , relative to one pulse emission, with the evolution of these pulse emissions from tipping over the years (as emissions are not released all at once after the tipping but are distributed over time), the effect from tipping element a was obtained:

$$C_{\text{tip},a}(T_{\text{effect}}) = \sum_{i} \sum_{T=T_a+1}^{T_{\text{effect}}} e_i(T) \cdot DCF_{\text{inst},i}(T_{\text{effect}} - T)$$
(6)

Where  $T_a$  is the year of tipping of the element a,  $e_i(T)$  [kg<sub>i</sub> · yr<sup>-1</sup>] is the annual release of gas *i* (either CO<sub>2</sub> or methane depending on the tipping point) at year *T*, i.e. at any year before the year of calculation of the dynamic effect ( $T_{effect}$ ) since the year following the tipping ( $T_a + 1$ ). The total carbon emissions from tipping were equally distributed over the transition period of the tipping event, so that the annual released amount ( $e_i(T)$ ) is constant during the transition. Carbon emissions were assumed to cease at the end of the transition period, unless their release is considered permanent, as for tipping of the El Niño-Southern Oscillation (Cai et al., 2016). The resulting effect from tipping from each tipping element as a function of time,  $C_{tip,a}$ , is shown in Figure 4. Note that for five of the selected tipping elements (Atlantic thermohaline circulation shutoff, North Atlantic subpolar gyre convection collapse, Sahara/Sahel and West African monsoon shift, Alpine glaciers, and coral reefs), the effect from tipping could not be modelled, due to lack of data or lack of direct effects on the climate after crossing the tipping point.



**Figure 4**: Temporal evolution of the effects from tipping (expressed as  $CO_2$ -equivalent concentration increase) for eight of the selected tipping elements. AS = Arctic summer sea ice loss, GI = Greenland ice sheet melt, BF = Boreal forest dieback, EN = El Niño-Southern Oscillation change in amplitude, AW = Arctic winter sea ice loss, P = Permafrost loss, AI = West Antarctic ice sheet collapse, AF = Amazon rainforest dieback. Figure taken from Supporting Information-1 of **Article I**.

#### 4.4 DERIVED MIDPOINT MCTP CHARACTERIZATION FACTORS

The MCTP of a unit emission varies over time depending on the emission proximity of to the tipping time. As the emission approaches the tipping year, the remaining capacity becomes smaller, thus the fraction of remaining capacity taken up by the emission increases, resulting in larger MCTP values (more details are presented in **Article I**). Therefore, the closer an emission occurs to a tipping point the larger is its climate tipping impact. Inclusion of uncertainties in tipping occurrence shows that these uncertainties are currently so large that timing of single tipping events is not clearly identifiable. Despite this, average MCTP factors from ~10000 Monte Carlo simulations are still larger for emissions occurring in periods with higher probability that several tipping points will occur. They vary by up to one order magnitude depending on the emission time and the considered RCP pathway (Figure 5).



**Figure 5**: Average (geometric mean) year-specific multiple climate tipping points potentials (MCTP) for 1 kg CO<sub>2</sub> (solid line) and corresponding 5<sup>th</sup> and 95<sup>th</sup> percentiles of yearly results (red dotted lines) computed assuming RCP4.5 (**a**), RCP6 (**b**) and RCP8.5 (**c**). Grey dots indicate MCTP results for 10000 model simulations. Note the different scales of the x-axes. Figure rearranged from **Article I**.

# The choice of RCP pathway influences both the magnitude and the trends of MCTP factors, which depend on (i) differences in number type and sequence of occurring tipping points in each RCP, (ii) different rates of GHG concentrations increase projected across the RCPs and (iii) variations in how climate responds to the concentration increase in the three RCPs. The latter explains why MCTP factors are larger under RCP4.5 compared to the other two pathways. In RCP4.5 tipping points are passed at lower levels of CO<sub>2</sub>-equivalent concentration, resulting in lower remaining capacities and thus larger MCTP values. This somewhat counterintuitive finding reflects the inability of midpoint CFs to capture the larger damages that would normally be expected under higher emission scenarios.

As a development of the CTP method of Jørgensen et al. (2014), the metric is designed to penalize emissions occurring in periods when there is higher chance to cross tipping points. Assuming that background emissions follow the RCP6 pathway, this would correspond to the period between 2040 and 2060. Thus, use of the MCTP aims to discourage emissions (attributed to product life cycles) that will occur when it is most likely that these will lead to passing tipping points and result in largest damage. This could contribute to postponing the tipping and allow the implementation of climate change mitigation and/or adaptation solutions (Jørgensen et al., 2014; Jørgensen and Hauschild, 2013).

### 5. THE MCTP AT ENDPOINT LEVEL

This chapter illustrates the methodology used to obtain MCTP CFs at endpoint level focusing on damage to ecosystems. An overview of the adopted approach is first given, followed by a detailed presentation of the modelling framework and a brief description of the obtained characterization factors.

All contents of this chapter are based on Article II.

#### 5.1 OVERALL APPROACH

Like most of the LCIA methods assessing damage to ecosystems, the developed MCTP CFs at endpoint level (MCTP<sub>endpoint</sub>) focus on biodiversity loss. The framework used to calculate MCTP factors at midpoint was further developed to translate the contribution of emissions to crossing tipping points into potential temperature increase and then into potential loss of species resulting from that temperature increase. Similarly to the midpoint methodology, here emissions attributed to a product are assumed to be part of background anthropogenic GHG emissions. Therefore, rather than considering the marginal impact on top of the background, the potential temperature increase from emissions represents a share of the total projected background temperature increase. This means that the loss of species due to this share depends also on the background temperature increase itself and on how this increase is affected by crossing tipping points. For this, the additional warming caused by crossing tipping points was included in the quantification of potential species loss.

The damage quantified by the  $MCTP_{endpoint}$  CFs addresses the potential loss of terrestrial species. The loss could be either at local level, when species disappear

from delimited areas but are still present in other areas, or at global level, when species become extinct across the whole planet. CFs were thus developed at both local and global levels, given that the two measures complement each other and are important to ensure ecosystem functionality and prevent irreversible extinction of species (Jolliet et al., 2018; Verones et al., 2020). Consistently with midpoint CFs, MCTP<sub>endpoint</sub> were calculated for the three major gases CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub>O, and for the three GHG concentration pathways RCP4.5, RCP6 and RCP8.5, to account for the dependency on background concentration levels.

#### 5.2 MODELLING FRAMEWORK FOR CALCULATION OF ENDPOINT MCTP FACTORS

Specific definitions in this section are taken from Article II.

The endpoint MCTP (MCTP<sub>endpoint</sub>, in potentially disappeared fraction of species, PDF  $\cdot$  kg<sup>-1</sup>) of given GHG *i* emitted at year  $T_{\text{emission}}$  is derived from the midpoint MCTP by using a 'midpoint-to-endpoint' factor:

$$MCTP_{\text{endpoint},i} (T_{\text{emission}}) = MCTP_i (T_{\text{emission}}) \cdot MEF(T_{\text{emission}})$$
(7)

where  $MCTP_i$  [ppt<sub>rc</sub> · kg<sub>i</sub><sup>-1</sup>] is the multiple climate tipping points potential at midpoint of gas *i* emitted at year  $T_{\text{emission}}$ , and MEF [PDF · ppt<sub>rc</sub><sup>-1</sup>] is the midpointto-endpoint factor at year  $T_{\text{emission}}$ . The *MEF* translates the impact from the contribution of the emission to cross tipping points, to potentially disappeared fraction of species [PDF] at either local or global level. The MCTP<sub>endpoint</sub> factors are given as average (geometric mean) over 10000 Monte Carlo simulations taking into account uncertainties in tipping occurrence, as done in **Article I**. The *MEF* is obtained through eq.8:

$$MEF(T_{\text{emission}}) = \frac{\Delta TEMP(T_{\text{emission}})}{1 \cdot 10^{12}} \cdot \frac{\Delta PDF(T_{\text{emission}})}{\Delta TEMP(T_{\text{emission}})}$$
(8)

where  $\frac{\Delta TEMP(T_{emission})}{1\cdot 10^{12}}$  [°C · ppt<sub>rc</sub><sup>-1</sup>] is the global temperature change ( $\Delta TEMP$ ) resulting from one part per trillion reduction of the remaining capacity [ppt<sub>rc</sub>] (i.e., per unit of the midpoint MCTP) and  $\frac{\Delta PDF(T_{emission})}{\Delta TEMP(T_{emission})}$  [PDF · °C<sup>-1</sup>] is the rate of potentially disappeared fraction of species, at either global or local level (PDF<sub>global</sub> and PDF<sub>local</sub> respectively), per unit change in global average atmospheric temperature. The factor  $1 \cdot 10^{12}$  [ppt<sub>rc</sub><sup>-1</sup>] is used to convert the midpoint *MCTP<sub>i</sub>* into unitless fraction of remaining capacity.

The factor  $\frac{\Delta TEMP(T_{emission})}{1\cdot 10^{12}}$  links the fraction of remaining capacity depleted by the emission (midpoint impact) to the temperature increase that is associated to depleting that fraction of remaining capacity. The two variables were related by considering the overall remaining capacity from the emission year to the year when the last expected tipping point is crossed (expressed in the denominator) and the average background temperature increase expected to occur over the same period ( $\Delta TEMP$ ). This background temperature increase was calculated starting from the temperature projections of the chosen RCP pathway and by adding the additional temperature rise due to crossing tipping points. To obtain this, the increment in CO<sub>2</sub>-equivalent concentration from crossing tipping events (estimated in **Article I** for 8 of the 13 considered tipping points) was first added to the projected RCP concentration, obtaining a new concentration profile. Then, the new temperature profile was obtained by associating the new concentration level with the corresponding temperature level derived from the RCP pathway.

The factor  $\frac{\Delta PDF(T_{emission})}{\Delta TEMP(T_{emission})}$  was calculated considering the difference between the foreseen fraction of species lost ( $F_{lost}$ ) at the highest considered temperature increase (that triggering the last tipping point) and the foreseen fraction of species lost at the temperature level in the emission year. This  $\Delta PDF$  was then related to the expected temperature change over the same period ( $\Delta TEMP$ ).

## 5.2.1 FRACTIONS OF LOCAL AND GLOBAL SPECIES LOST WITH RISING TEMPERATURE

The fraction of species lost at local and global levels ( $F_{lost}$ ) were derived from two different studies estimating species loss under climate change. Local species losses were obtained from Newbold (2018), who used species distribution models for estimating a global average of local losses of four major terrestrial vertebrate groups in response to future climate change projected in four RCP scenarios. The study was chosen as it focuses on local biodiversity loss due to climate change and allows deriving a curve for local species loss as a function of global mean temperature. Global species losses, instead, were taken from Urban (2015), who gathered data from 131 studies predicting extinction risk for seven taxonomic groups and using different modelling techniques to derive the global mean extinction risk per unit of temperature increase. The study of Urban (2015) was used also in other LCIA methods, such as ReCiPe 2016 and LC-IMPACT, to obtain endpoint-level GWP CFs expressing impacts as global species loss (Huijbregts et al., 2017; Verones et al., 2020). More details about the treatment of the data from Newbold (2018) and Urban (2015) are found in Article II. The resulting fractions of local and global species lost plotted as functions of global mean temperature show that the rate of species loss per unit of temperature change is not constant but accelerates with global temperature increase (Figure 6). This indicates that more species are expected to be lost at higher temperature levels.



**Figure 6**: Fraction of local and global species lost as a function of global temperature change above pre-industrial levels. Single data points indicate the original data taken from the models of Newbold (2018) and Urban (2015). Solid lines indicate the curves obtained from linear regression of the logit-transformation of the original data points. Figure taken from **Article II**.

#### 5.3 DERIVED ENDPOINT MCTP CHARACTERIZATION FACTORS

The obtained MCTP<sub>endpoint</sub> factors are generally proportional to their corresponding MCTP factors at midpoint and, overall, follow a similar trend (Figure 7). Under RCP6, for instance, larger MCTP<sub>endpoint</sub> factors are observed for emissions occurring between 2040 and 2060, as found also for midpoint MCTPs (Figure 5). This means that impacts at both midpoint and endpoint levels are higher for emissions occurring in periods when the contribution to deplete the remaining capacity and cross tipping points is larger. Given that tipping could amplify warming and further affect species loss, emissions with larger contribution to tipping have a higher potential to cause damage to species.

Despite this proportionality to midpoint impacts, overall  $MCTP_{endpoint}$  values decrease over time. Indeed, emissions occurring later in the century are attributed a lower potential species loss (of up to almost 2 orders magnitude) compared to the initial increase observed under the considered RCP pathway. This might seem unexpected given that the model accounts for the acceleration of species loss with increasing temperature levels (Figure 6), which suggests that the impact should be higher for later emissions occurring at higher levels of warming. However, this decline, due to decreasing contribution of emissions to temperature rise over time, is in line with the average approach to model characterization factors and should not be interpreted as, e.g., lower sensitivity of the climate to future emissions.



**Figure 7**: Average MCTP<sub>endpoint</sub> CFs of 1 kg CO<sub>2</sub> based on local (**a**) and global (**b**) species loss (solid lines) calculated under three RCP pathways and plotted as function of emission year. Shaded areas indicate uncertainty ranges enclosed between the  $5^{\text{th}}$  and  $95^{\text{th}}$  percentiles. Figure taken from **Article II**.

Compared to midpoint factors, the  $MCTP_{endpoint}$  allow for a more straightforward interpretation of impacts of GHG emissions because their values are larger under RCP8.5 and lower under RCP 4.5, in line with expectations that more species could be lost at higher temperature projections. In addition, expressing impacts as potentially disappeared fraction of species should ideally allow for comparison with

the damage caused through other environmental impacts (e.g., ecotoxicity) or other climate-related impact categories (such as damage GWP). However, further harmonization efforts between the category units are needed for direct comparisons. In particular, the MCTP<sub>endpoint</sub> does not include in the units the time dimension that, in other damage-oriented metrics, is associated to the duration (in years) of the exposure to the environmental pressure (such as damage GWP expressed in PDF·yr, Verones et al., 2019). This time indeed cancels out when relating the *impact of the emission* to the remaining capacity at midpoint (eq. 1). An idea to harmonize units consists in multiplying the MCTP<sub>endpoint</sub> factors by the total number of years from the first emission up to the last expected tipping point in each RCP pathway. For an emission occurring in 2021, this period corresponds to 70, 97 and 85 years for RCP4.5, RCP6 and RCP8.5, respectively. This would represent the relevant exposure period for climate tipping impacts.

# 6. APPLICATION TO CLIMATE IMPACT ASSESSMENT OF BIO-BASED MATERIALS

This chapter describes the findings from application of the developed MCTP factors at midpoint level in selected case studies on bio-based materials. Three full LCA case studies were examined. The first two focus on two types of engineered char obtained from biomass, namely biochar and hydrochar. They were analysed together in **Article III**, where two earlier LCA studies were considered for calculation of climate tipping impacts with the MCTP. The third case, examined in **Article IV**, is a new LCA case on bio-based plastics made from the polymer polyhydroxyalkanoate (PHA), where calculation of MCTP impacts was included in the LCIA phase of the study. These materials were chosen as representatives of bio-based materials that are currently gaining attention as potential solutions to mitigate climate change.

The structure of the chapter is as follows. First, the case studies and the considered scenarios are presented. Next, application of MCTP factors and calculation of impact scores are provided. Finally, results on the climate tipping impacts of the considered bio-based materials are illustrated, highlighting the potential of the developed MCTPs to bring additional insights compared to other complementary climate metrics.

The chapter draws on findings from the cases presented in Article III and Article IV.

#### 6.1 CASE STUDIES

#### 6.1.1 BIOCHAR

Biochar is a carbonaceous "solid material obtained from the thermochemical conversion of biomass in an oxygen-limited environment", typically resulting from a dry carbonization process like pyrolysis (IBI, 2015). It is mostly used as soil conditioner to increase crop productivity, but biochar can have several other applications, including utilization as energy source or for carbon sequestration and storage (Kambo and Dutta, 2015). The stability of biochar in soil can vary widely, but in general biochar is a very stable material that is believed to completely degrade to CO<sub>2</sub> (mineralization) over hundreds to thousands of years (Lehmann et al., 2009). The biochar case examined in Article III is based on the study of Owsianiak et al. (2018b), who considered the production of biochar from biomass residues and its application as soil conditioner for maize cultivation in Indonesia. The 'cradle to grave' LCA model and the GHG emissions inventories from this study were used as direct input for application of the developed MCTP factors and quantification of climate tipping impacts of the biochar system. The influence of biochar stability on potential contribution to climate tipping was investigated considering three scenarios representing slow, average, and fast kinetics for mineralization of biochar during its application to soil (Table 2).

#### 6.1.2 Hydrochar

Hydrochar is another carbonaceous material obtained from treatment of biomass residues that can be applied in agriculture as soil conditioner (Reza et al., 2014). It is produced through hydrothermal carbonization (HTC), in which biomass undergoes carbonization in the presence of water (Berge et al., 2011). Hydrochar is

also relatively stable in soil, but it degrades faster than biochar, typically within 100 years (Busch and Glaser, 2015; Gronwald et al., 2016). The hydrochar case study in **Article III** builds on the 'cradle to grave' LCA model and the GHG emissions inventories reported in Owsianiak et al. (2018a), which were used for calculation of climate tipping impacts of the hydrochar system using the MCTP. Owsianiak et al. (2018a) examined the full plant scale production of hydrochar from green waste for soil conditioning application in barley cultivation. Similarly to the biochar case, three scenarios were considered based on the different mineralization rates found for hydrochar in soil, representing slow, average and fast kinetics (Table 2).

**Table 2**: Overview of scenarios considered for the biochar and the hydrochar case studies.

 Scenario B4, which assumes application of biochar as energy source for household cooking,

 was considered in Article III but will not be discussed in this thesis. Table taken from Article III.

Details of the case	Biochar				Hydrochar		
study					•		
Goal of the underlying study	"to assess and compare life cycle impacts of biochar systems in Indonesia in order to support decision making related to the implementation of biochar as a waste management strategy in four Indonesian island communities"				"to evaluate the application of hydrochar to agricultural soils as a potential technology for carbon sequestration and temporary storage"		
Functional unit (f.u.)	"Treatment of 1 kg of biogenic carbon from biomass residues in rural areas in Indonesia"				"Average application and storage of 1 kg of biogenic HTC carbon to a temperate ag- ricultural soil"		
Scenario a,b	B1	B2	B3	B4	H1	H2	H3
Char application	Soil conditioner Energy source			Energy source	Soil conditioner		
Geographic location	Indonesia			Spain			
Biowaste type	Biomass residues			Green waste			
Production technique	low-cost pyrolysis technology based on "Kon Tiki" flame curtain kiln			Hydrothermal carbonization installation operating at full commercial scale			
Production capacity	~30 kg/day (dry weight)			~30,000 kg/day (dry weight)			
Replaced waste manage- ment system	None (not required by the functional unit)			Composting			
Avoided crop produc- tion	Maize			Not rele- vant	Barley		
Avoided fertilizer	NPK and urea			Not rele- vant	NPK		
Avoided heat generation process	Not relevant		Cooking using wood	Not relevant			
Negative priming effect	Considered		Not rele- vant	Not considered			

Mineralization rate con- stant of labile carbon pool (day <sup>-1</sup> )	Slow (1.67E- 03)	Average (7.18E- 03)	Fast (1.75E- 02)	Not rele- vant (im- mediate release)	Slow (1.20E-02)	Average (8.10E-02)	Fast (1.40E-01)
Mineralization rate con- stant of recalcitrant car- bon pool (day-1)	Slow (2.52E- 08)	Average (2.35E- 06)	Fast (1.67E- 05)	Not rele- vant (im- mediate release)	Slow (1.40E-04)	Average (3.00E-04)	Fast (1.40E-03)
Time differentiated life cycle process	Mineralization in soil		None	Mineralization in soil			

#### 6.1.3 POLYHYDROXYALKANOATE (PHA)-BASED PLASTICS

Polyhydroxyalkanoate (PHA) is a bio-based and biodegradable polyester polymer that can be produced by microbial fermentation starting from various feedstock, such as organic waste and by-product streams (Koller, 2017; Saratale et al., 2021). The case study in Article IV analysed the entire value chain, from production to disposal, of a PHA-based film used as food packaging material produced from the fermentation of molasses (a by-product of sugar beet processing). Potential addition of extra layers (lamination) of (poly)lactic acid (PLA) or metallization with aluminium (Al) or aluminium oxides (AlOx) to improve barrier properties of the PHA-based film were considered. PHA is generally considered as readily biodegradable depending on product characteristics and degradation conditions (Fernandes et al., 2020). However, the addition of other chemicals or blending with PLA were found to reduce degradability compared to the pure bio-based polymer (Meereboer et al., 2020) and it is not known how lamination and metallization could influence degradability. This was investigated by considering four different mineralization rate scenarios representing fast, medium, slow, and very slow kinetics during landfilling. Additionally, two scenarios considering a 20-years and 40-years lag phase, indicating delayed degradation that may occur due to differences in availability of water and oxygen during landfilling, were also explored. More details on the considered scenarios and the LCA model can be found in Article IV.

#### 6.2 CALCULATION OF MCTP IMPACT SCORES

The MCTP factors for a given GHG are time dependent and emission-year specific. Thus, their application requires availability of time differentiated GHG emission inventories, specifying amounts of emissions released in each year. This is the same as needed for dynamic LCIA methods such as the dynamic GWP (Levasseur et al., 2010). In the considered scenarios, mineralization of biochar and hydrochar in soil and degradation of PHA-based plastic during landfilling are the only relevant processes in which emissions are distributed over time. Thus, starting from the examined mineralization rates of the bio-based materials, annual amounts of mineralized  $CO_2$  were calculated for these processes.

The total midpoint MCTP impact score  $(IS_{MCTP})$  for a specific scenario was obtained by summing the score calculated for the time-differentiated processes in the life cycle and that for all remaining processes that are not temporally distributed.

The former score was calculated by multiplying masses of  $CO_2$  emitted in given years with the corresponding year-specific MCTP characterization factor and then summed over time, starting from the first year in which emissions take place (assumed in 2021) until the year of the last tipping point (eq. 9). The score for all remaining processes was calculated as the product between the total mass of  $CO_2$ aggregated over time and the MCTP factor corresponding to the year when that emission is expected to occur all at once (assumed in 2021).

$$IS_{\text{MCTP}} = \sum_{i} \sum_{T_{\text{emission}}=2021}^{T_{\text{tipping},j_{\text{last}}}} m_i(T_{\text{emission}}) \cdot \text{MCTP}_i(T_{\text{emission}})$$
(9)

Eq. 9 is a general equation valid for more GHGs (not only CO<sub>2</sub>), in which  $m_i(T_{\text{emission}})$  is the mass of GHG *i* emitted in a given year  $T_{\text{emission}}$ , and  $MCTP_i(T_{\text{emission}})$  is the midpoint MCTP of GHG *i* for year  $T_{\text{emission}}$ .

# 6.3 RELEVANCE OF CLIMATE TIPPING IMPACTS FOR THE ASSESSED BIO-BASED MATERIALS

The results from the three examined case studies show that the stability of the biobased materials is an important factor that influences the climate tipping impacts of the products. In the case of hydrochar, climate tipping impacts generally increase with increasing stability of hydrochar in the soil, with some differences depending on the assumed RCP pathway for MCTP factors (Figure 8). This is because, for the most stable (slow-degrading) hydrochar, CO<sub>2</sub> emissions from hydrochar mineralization are distributed over a longer period compared to fast-degrading chars. In such case, a larger portion of  $CO_2$  is emitted when there is higher risk that tipping points will be crossed and when MCTP factors are the largest. Similar results are obtained in the PHA-based plastic case, where climate tipping impacts increase with increasing stability of the bioplastic and are the largest when considering a 20-years delayed degradation during landfilling (Table 3). In this case the largest share of emissions is released around year 2050, when MCTPs (assuming RCP6), and thus potential contribution to tipping, are the largest. This shows that the different stability of the compared materials determines differences in timing of emissions, which are captured by the MCTP and result in different climate tipping impacts.



**Figure 8**: Characterized MCTP (a) and GWP100 (b) impact scores per functional unit (f.u.) for the slow (H1), average (H2) and fast (H3) mineralization rate scenarios of hydrochar applied to soil. MCTP scores are based on CFs calculated for three RCP pathways. Figure taken from **Article III**.

A comparison with the ranking between mineralization scenarios obtained with the global warming potential for 100-years' time horizon (GWP100) shows opposite trends. In both the hydrochar and the PHA-based plastic cases, GWP100 scores decrease with increasing stability because the slow-degrading bio-based material is assigned more credits for temporary storage of carbon compared to the other scenarios. This shows that the choice of metric influences the ranking of compared scenarios and the identification of the best performing case. While from the GWP100 perspective faster-degrading materials perform worse, because of lower benefits from carbon storage, they perform generally better from the climate tipping perspective, as less likely to contribute to crossing tipping points. One exception is for the very slow degrading PHA scenario which performs best according to MCTP, GWP100 and GTP100 (global temperature change potential for 100-years' time horizon) metrics due to incomplete degradation of the bioplastic over the considered time frames (100 years for GWP and GTP and 94 years for MCTP under RCP6) (Table 3).

	GWP100	MCTP <sub>RCP6</sub>	GTP100
Mineralization scenario	(kg CO <sub>2</sub> eq/f.u.)	(ppt <sub>rc</sub> /f.u.)	(kg CO <sub>2</sub> eq/f.u.)
Fast	5.25E-02	1.22E-03	1.04E-01
Medium	4.53E-02	1.40E-03	1.04E-01
Slow	3.57E-02	1.45E-03	1.03E-01
Very slow	2.81E-02	9.40E-04	9.31E-02
Fast with 20-yr lag phase	4.17E-02	4.95E-03	1.04E-01
Fast with 40-yr lag phase	3.08E-02	4.93E-03	1.04E-01

**Table 3**: Characterized impact scores per functional unit (f.u.) for the PHA-based plastic case, depending on the considered mineralization scenarios and climate metrics. Increasing red shading indicates increasing impact (per climate metric). Table adapted from **Article IV**.

For the biochar case, the climate tipping impacts of the considered mineralization scenarios follow a different trend compared to the cases of hydrochar and PHA, as they increase with decreasing stability in soil (Figure 9). This result, which is the same as that obtained with GWP100, is not due to the differences in emission timing and proximity to tipping points but is determined only by differences in the total amount of CO<sub>2</sub> released in the three scenarios, over the time frame covered by the MCTPs. Thus, according to both MCTP and GWP100, the fast-degrading biochar performs worse because the amount of CO<sub>2</sub> released from mineralization in this scenario is larger (and consequently lower carbon storage credits for GWP100). This is different from the hydrochar and the PHA cases, in which the total CO<sub>2</sub> emissions released in the compared scenarios (over the time frame considered by MCTP factors) are similar, making timing of emissions important for determining climate tipping impacts.



**Figure 9**: Characterized MCTP (a) and GWP100 (b) impact scores per functional unit (f.u.) for the slow (B1), average (B2) and fast (B3) mineralization rate scenarios of biochar applied to soil. MCTP scores are based on CFs calculated for three RCP pathways. The figure is taken from **Article III**. Results for scenario B4 (biochar used as energy source) are discussed in the article.

The case of biochar highlighted that in comparative LCA the MCTP does not always bring new insights compared to other metrics. The stability of the bio-based materials and total amount of carbon re-emitted as  $CO_2$  over the relevant time frame (for MCTPs) are important for determining whether MCTP can capture differences in emission timing between compared scenarios. The high stability of biochar means that only a part of the  $CO_2$  emissions occurs within the time frame considered by MCTP factors and this amount of re-emitted  $CO_2$  will differ depending on the mineralization kinetics. These differences will then dominate the MCTP scores. By contrast, for materials with lower stability, as the case of hydrochar and the PHAbased plastic, mineralization will be nearly completed within the time frame of MCTP factors and there will be no difference in total emissions between scenarios. Thus, timing of emissions becomes important in this case and determines magnitude of MCTP scores. Overall, MCTP is expected to be particularly relevant for comparing materials that degrade gradually over time but reaching at least 95% degradation in around 70 years.

## 7. CONCLUSIONS AND OUTLOOK

#### 7.1 OVERALL CONTRIBUTIONS AND IMPLICATIONS

This PhD work contributed to the development of a more robust LCIA methodology accounting for climate tipping impacts of products' life cycle GHG emissions. The main added value of the methodology is to provide a measure of the potential contribution of product-related emissions to cross multiple climate tipping points. This was achieved by developing a framework that (i) includes other 12 tipping elements besides Arctic summer sea ice, (ii) considers uncertainties in tipping occurrence, (iii) accounts for potential effects from crossing tipping points and (iv) enables expressing impacts also at the endpoint level. The above developments represent a significant progress toward making climate tipping operational as a new climate-related impact category in LCA. Therefore, the obtained MCTP metric at both midpoint and endpoint levels should be considered complementary, and not a substitute, to the recommended GWP, GTP and climate-related damage metrics in LCA.

Application of the midpoint MCTP factors to selected bio-based materials showed that the metric could offer new insights about the climate performance of the biobased materials. The metric was found to be mostly relevant in comparative assessments of materials that degrade almost completely within the next two centuries, which is the time frame relevant for climate tipping impacts. In such cases, materials with lower stability were generally found to perform better from the climate tipping perspective, as less emissions are released in close proximity to tipping points. This offers a different perspective compared to GWP (accounting for benefits from carbon storage), which considers lower stability a disadvantage because of limited carbon storage. The MCTP is expected to add less value in comparative LCA for (i) very fast-degrading bio-based materials, e.g. mineralization within one year, (ii) scenarios where there are no relevant time-differentiated processes and emissions occur all at once, e.g. incineration of the bio-material, and (iii) for highly stable materials that reach almost complete mineralization in more than two centuries.

As found also for dynamic LCIA methods (e.g. Levasseur et al., 2010), availability of temporarily disaggregated emission inventories, specifying emissions at the year resolution, is necessary for a meaningful use of the MCTP factors. The main implication for LCA practitioners is that currently calculation of MCTP impact scores must be done offline. In fact, dynamic assessments are not yet supported in current LCI (life cycle inventory) databases and LCA software programs. Further developments would require calculation and reporting of time-differentiated emission inventories and adaptation of LCA software programs for calculating impact scores using time-differentiated inventories and time-dependent characterization factors. To apply MCTP factors, it is thus recommended to (i) identify foreground life cycle processes for which temporal evolution of emissions is expected to be relevant (such as end-of-life processes, biomass growth, or deforestation), (ii) obtain a time-differentiated inventory for these processes and (iii) calculate MCTP impact scores as the sum of the time-differentiated and the aggregated emission inventories.

Application of the endpoint MCTP is expected to provide additional insights in line with those found at the midpoint level. Being overall proportional to the midpoint, the MCTP at endpoint attributes a larger potential species loss to emissions with higher contribution to crossing tipping points, given that crossing could intensify warming and exacerbate species loss. The added value of the endpoint characterization factors is that interpretation of impacts becomes more environmentally relevant, as expressed in terms of damage to terrestrial species. Moreover, the increasing damage estimated when considering higher RCP pathways is consistent with expectations, from ecology, that more species could be lost at higher temperature levels.

Dependency of MCTP factors on background GHGs development pathway might complicate interpretation of the LCA study results. However, assumptions regarding the future emission pathway are necessary for determination of the tipping points and, thus, for a meaningful estimation of climate tipping impacts. The analysed case studies on bio-based materials showed that the choice of RCP pathway had some influence on the relative performance of the compared hydrochar scenarios, but it did not affect the choice of the best performing one. This should therefore be assessed case by case, as the result depends on timing of emissions attributed to products' life cycles. Thus, it is recommended to use MCTP factors for all three RCP pathways to examine if and how this choice could influence the goal of the study.

In conclusion, this PhD project has resulted in a more robust LCIA metric that addresses the need to account for multiple climate tipping points and can provide new insights in environmental sustainability assessments of bio-based materials. Although it has been tested mainly with bio-based materials, the method could be applicable also to other products for which temporal evolution of GHG emissions is relevant. It is emphasized however that the method is not applicable to assessing large scale systems, such as economic sectors or countries, which could lead to a substantial modification of the background emission path that is not accounted for in the current method.

#### 7.2 PRIORITIES FOR FURTHER RESEARCH

Although the research conducted in this PhD has contributed to advance the assessment of climate tipping impacts in LCIA, further developments are recommended. First, to increase accuracy of the quantified climate tipping impacts, MCTP characterization factors should be calculated for other relevant GHGs in addition to CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub>O. This would be feasible for all GHGs for which the radiative efficiency and the atmospheric lifetime are known (as reported by the IPCC in (Myhre et al., 2013). Calculation of MCTP factors is deemed particularly relevant for near-term climate forcers (NTCF), such as sulphur dioxide (SO<sub>2</sub>) or carbon monoxide (CO). These have shorter lifetimes compared to  $CO_2$  or other well-mixed GHGs and are responsible for determining short-term climate impacts (Myhre et al., 2013), which makes them relevant contributors to the first expected tipping points within the next two decades. Moreover, in the MCTP approach short-lived gases are assigned a higher relative importance compared to longer-lived ones because of the shorter time horizons over which the radiative forcing is integrated (eq. 2). This was observed for the NTCF and well-mixed CH<sub>4</sub>, whose MCTP factors (under RCP6) are on average 51 to 107 times larger than that of  $CO_2$ . Thus, accounting for other NTCFs is expected to improve the quantification of climate tipping impacts.

Further, given the dependency on background GHG emissions development, consideration of updated emission pathways, such as the Shared Socioeconomic Pathways (SSPs) (IPCC, 2018; Riahi et al., 2017) would be relevant. This is feasible if detailed projections about future GHGs concentrations and global temperature are available. Similarly, the method could be improved as new knowledge unveils about future expected climate tipping points. This could be through inclusion of other potential tipping points in addition to the 13 selected in this PhD work, or consideration of the possible interactions between tipping elements that could lead to cascading tipping events. Inclusion of such interactions, in which crossing of one

tipping point influences the timing of the following tipping points, could result in an increase in MCTP values in the case more tipping points are triggered in close proximity to each other.

To increase the relevance of the developed MCTPs in the context of bio-based materials, the method should provide guidance on how to handle carbon sequestration through  $CO_2$  fixation in the biomass feedstock and temporary carbon storage in the material. Accounting for these mechanisms could indeed highlight potential benefits from bio-based materials that are currently disregarded. Particularly challenging seems to be the assignment of credits for temporary storage of carbon. The CTP of Jørgensen et al. (2014) addressed this by giving credits only to carbon that is stored beyond the considered climate tipping point for Arctic summer sea ice loss. However, using a similar approach within the MCTP framework is not straightforward, as the framework considers multiple tipping points besides Arctic sea ice and, for this, a carbon emission will always contribute to cross some tipping point regardless of when it is re-emitted.

Finally, further developments of the endpoint methodology are recommended. To allow comparison with other impact categories, harmonization of the MCTP units with those of other damage metrics, especially for incorporation of the time dimension, is required. Estimation of potential species loss associated to climate tipping could be improved by accounting for direct impacts from crossing tipping points on species diversity, rather than considering only the indirect effects through temperature increase after tipping. For instance, inclusion of species loss due to depletion of natural habitats from Amazon rainforest dieback or caused by intensified weather patterns such as droughts could be considered. Lastly, more research should explore the possibility of assigning a weight to the species loss. This could be for instance through the incorporation of a severity factor that considers how severe is the loss of given species at given times for maintain ecosystem functioning. This would contribute to provide a more realistic measure of the potential damage to ecosystems.

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# PAPERS

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# Article I

# Multiple Climate Tipping Points Metrics for Improved Sustainability Assessment of Products and Services

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# Multiple Climate Tipping Points Metrics for Improved Sustainability Assessment of Products and Services

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ABSTRACT: Mounting evidence indicates that climate tipping points can have large, potentially irreversible, impacts on the earth system and human societies. Yet, climate change metrics applied in current sustainability assessment methods generally do not consider these tipping points, with the use of arbitrarily determined time horizons and assumptions that the climate impact of a product or service is independent of emission timing. Here, we propose a new method for calculating climate tipping characterization factors for greenhouse gases (carbon dioxide, methane, and nitrous oxide) at midpoint. It covers 13 projected tipping points,



Supporting Information

incorporates the effect that the crossing of a given tipping point has on accelerating the crossing of other tipping points, and addresses uncertainties in the temperature thresholds that trigger the tipping points. To demonstrate the added value of the new metric, we apply it to emissions stemming from end-of-life of plastic polymers and compare them with commonly used metrics. This highlights the need to consider climate tipping in sustainability assessment of products and services.

#### INTRODUCTION

There are several elements of the earth system that could pass a tipping point within this century and trigger large abrupt, potentially irreversible changes.<sup>1</sup> Examples of tipping elements include Arctic summer sea ice, the Atlantic thermohaline circulation, and the El Niño-southern oscilation.<sup>2</sup> The crossing of these elements may be one of the most dangerous consequences of human-induced climate change.<sup>3</sup> From the economic perspective only, Cai et al. showed an eight time increase in monetary costs per 1 tonne of carbon dioxide emitted, when compared to the costs without considering the tipping.<sup>4</sup> These findings stress the need for consideration of climate tipping elements when developing metrics of climate impact for improved environmental sustainability assessment of products and services.

Life cycle assessment (LCA) is a tool that is often used to address the environmental sustainability of products and systems.<sup>5</sup> In LCA, the climate change impacts of a product or service are traditionally quantified using global warming potentials (GWP)<sup>6</sup> as characterization factors (CF), representing the impact per unit of emission. Amounts of individual greenhouse gases (GHG) that can be attributed to a specific product or service are first summed up and then multiplied by a GHG-specific GWP; the resulting indicator scores added. The sum represents the climate change impact score (also referred to as carbon footprint)<sup>7</sup> and expresses the potential contribution of a product or service to change radiative forcing (not the actual warming) over a defined time horizon, typically over 100 years. The procedure for calculating impact scores is the same for all other midpoint indicators of climate change

(where midpoint refers to the location of the indicator in the cause-effect chain linking emission inventories with final damage caused to environment or human health). For another midpoint indicator, global temperature change, the global temperature change potential (GTP)<sup>8</sup> is used and the resulting impact scores indicate the potential contribution of a product or service to global average temperature increase of the atmosphere at a future point in time, typically at 100 years.

Both GWP and GTP are recommended emission metrics by the IPCC<sup>6</sup> and have been suggested as complementary CFs for quantification of climate change impacts of products and services by the LCA community.<sup>9</sup> However, none of them considers climate tipping mechanisms in the earth system.<sup>9,10</sup> It is challenging to capture the dependence of the impact of emissions on the emission timing in relation to the time of the tipping points. As tipping points represent critical levels of warming that should not be crossed, tipping-orientated GHG emission metrics cannot simply measure radiative forcing (or temperature) change over a fixed time horizon for a pulse emission emitted at an arbitrary time. Instead, they should quantify how much that change can contribute to crossing the tipping points and should assess that for multiple pulse

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emissions, i.e., emitted at different times. To do this, an approach based on quantification of the carrying capacity of the atmosphere to absorb the emission without crossing the tipping point is necessary.<sup>11</sup> In this perspective, the effects of an emission will depend on how much carrying capacity is depleted by the emission and, thus, on the proximity to tipping points. This is at odds with current impact assessment practice where carrying capacities and dependency of impacts on emission timing are not embedded in the CF.<sup>11,12</sup>

The metric developed by Jørgensen et al.,<sup>13</sup> the climate tipping potential (CTP), introduced both aspects while accounting for the Arctic summer sea-ice loss as tipping element. Here, the impact of 1 kg GHG emitted at a given year was expressed as the fraction of carrying (or remaining) capacity, i.e., the time-integrated increase in atmospheric CO2equivalent concentration that can still occur before Arctic summer sea-ice loss, depleted by the time-integrated change in CO2-equivalent concentration caused by the emission. However, their metric only considers this one tipping point and thereby neglects several aspects that are required for a robust metric of climate tipping. First, it must consider emissions occurring after the tipping of a given element of the earth system as contributors to crossing other, subsequent tipping points.<sup>13</sup> Second, potential consequences of crossing a given tipping point on the acceleration tipping of other elements must be accounted for.<sup>14</sup> For instance, the reduction of sea ice albedo in the Arctic amplifies warming making the subsequent tipping point (e.g., Greenland ice sheet melting) occur faster than it would without tipping of the Arctic sea ice. Third, when taking multiple tipping points into account, sequence and timing of occurrence of individual climate tipping points depend on uncertain factors, like temperature thresholds triggering the tipping points,<sup>2,15</sup> and these uncertainties must be accounted for.

In this paper, we develop new climate tipping characterization factors (CF) for three major anthropogenic GHGs (carbon dioxide  $(CO_2)$ , methane  $(CH_4)$ , and nitrous oxide (N2O)), which meet these requirements. We first select relevant tipping elements, present the conceptual framework, and develop a method for computing multiple climate tipping points potentials (MCTPs) at midpoint. We apply the new MCTPs to end-of-life GHG emission inventories for plastic polymers made from different feedstock and spanning a wide range of temporal evolutions of GHG emissions in their endof-life. We also present practical implications of using the new CFs in LCA, where information about temporal evolution of GHG emissions might not be available or relevant. We argue that the new CFs are a useful supplement to (but not a substitute for) the currently used GWP and GTP CFs recommended by the IPCC.

#### METHODS

**Selection of Climate Tipping Elements.** We carried out a literature review to identify a broad list of potential tipping elements without considering potential differences in the formal definition of tipping point given by different authors (Table S1 in Supporting Information). From this broad list, 13 tipping points were selected for inclusion in the study based on a set of criteria that (1) define the tipping mechanism, (2) consider changes in atmospheric GHGs concentration as the potential triggers, and (3) consider modeling of the tipping points feasible when tipping thresholds can be expressed as global mean temperature. The selection criteria are presented in the Supporting Information. The selected tipping points are Arctic summer sea ice loss (AS), Greenland ice sheet melt (GI), West Antarctic ice sheet collapse (AI), Amazon rainforest dieback (AF), Boreal forest dieback (BF), El Niño-Southern Oscillation change in amplitude (EN), Permafrost loss (P), Arctic winter sea ice loss (AW), Atlantic thermohaline circulation shutoff (TC), North Atlantic subpolar gyre convection collapse (SG), Sahara/Sahel and West African monsoon shift (AM), Alpine glaciers loss (AG), and Coral reefs deterioration (CR) (Table S2).

**Conceptual Framework.** The method for calculating the climate tipping potential (CTP) for the Arctic summer sea-ice loss as tipping element proposed by Jørgensen et al.<sup>13</sup> was taken as a starting point. Their method is further developed to consider: (1) other selected tipping elements, (2) uncertainties of tipping points occurrence, and (3) the effect of crossing a tipping point on accelerating tipping of all subsequent tipping points. The new CFs are therefore referred to as multiple climate tipping points potentials (MCTP). Their main features are presented below.

First, the impact of a GHG emission represents timeintegrated radiative forcing of 1 kg emission of a greenhouse gas *i* and is expressed as atmospheric  $CO_2$ -equivalent concentration (in ppm of  $CO_2$ e·yr·kg<sup>-1</sup>). The integration is from the emission year to the year of tipping (rather than over a fixed time horizon like in the GWP).

Second, this impact is always given in relation to the remaining capacity of the atmosphere to absorb that impact without triggering the tipping point, also expressed in ppm of  $CO_2e\cdot yr\cdot kg_i^{-1}$  (rather than comparing impacts to that of a reference gas like  $CO_2$  as in GWP). The resulting MCTP CFs therefore represent the fraction of remaining capacity taken up by the unit emission (which is expressed in parts per trillion of remaining capacity,  $ppt_{rc}\cdot kg_i^{-1}$ ). MCTPs are dynamic because both the impact and the remaining capacity to absorb the impact without triggering the tipping point depend on emission time.

Third, remaining capacities depend on background anthropogenic GHG emissions, as they ultimately determine when the tipping point is triggered, and furthermore, the impact of a GHG emission attributed to a product or service can be considered as part of this background. Although GHG emissions from an individual product system will never be large enough to cause a tipping, a large number of products that are produced, used, and disposed of in our society and their attributed (often very small) quantities of GHG emissions have a real potential to cause the tipping. Thus, application of MCTP CFs to single product systems that are modeled in LCA gives a meaningful estimate of the product's contribution to passing critical tipping points. This is in line with the attributional approach to LCA, which aims to represent a product system in isolation to quantify the impact that the product is "responsible for".16 However, considering the effects from crossing a given tipping point on the reduction of the remaining carrying capacity for all subsequent tipping points could be seen as a marginal contribution that adds impact to the background pressure. This is more in line with the consequential approach to LCA, which aims to assess the environmental consequences of using a product or providing a service.

Finally, the aforementioned considerations imply that MCTP CFs are not applicable to assessments of large scale



**Figure 1.** Conceptual illustration of MCTP calculation for a unit (1 kg) emission of GHG *i* that is part of anthropogenic background GHG emissions, in different years with either one (a) or two (b and c) tipping points. The horizontal time axis is divided in discrete time intervals of 1-year, as indicated with capital letters, and vertical bars represent annual CO<sub>2</sub>-equivalents concentration increases.  $T_{emission}$  indicates the year of tipping of the first and second tipping point, respectively. Emissions occurring before the first tipping point (at  $T_{emission} < T_{upping,1}$  and  $T_{upping,2}$ ). Lemissions occurring after the first tipping point (at  $T_{emission} < T_{upping,1} < T_{emission} < T_{upping,1} < T_{emission} < T_{upping,1} < T_{emission} < T_{upping,2}$  for the second tipping point, in practice, reducing the carrying capacity of emissions at  $T_{upping,1} < T_{emission} < T_{upping,2}$  for the second tipping point. Note that the effect of crossing the first tipping is irrelevant for part a because this case considers only one tipping point (as presented in Jørgensen et al.<sup>13</sup>) and is not considered in calculation of remaining carrying capacity for an emission occurring before the first tipping point.

systems, e.g., at country level, which have the potential to substantially influence background emission levels.

Figure 1 provides a conceptual illustration of the framework: starting from one tipping element (in practice, CTP of

Jørgensen et al.<sup>13</sup>) (Figure 1a) through adding a second tipping point (Figure 1b) to considering effects from crossing the first tipping point on accelerating tipping of the second tipping point (Figure 1c). The figure is conceptual as (1) increase in atmospheric CO2-equivalent concentration due to background anthropogenic emissions is assumed linear, (2) the impact of the emission (part of anthropogenic background emissions) is simplified using triangles, (3) the remaining capacity is also simplified using triangle-like shapes, and (4) the effect of crossing the first tipping point is assumed to be equally distributed over the years which follow. Yet, the figure allows us to illustrate the framework. Background production and consumption activities increase atmospheric CO2-equivalent concentration so that the first tipping point is triggered in 2030. An emission before this tipping point, e.g., in 2025, contributes to the crossing of this tipping point as it consumes part of the carrying capacity that remains until the tipping point is triggered (Figure 1a). This is the principle of the original CTP-framework of Jørgensen et al.<sup>13</sup> Extension of their framework by considering another tipping element, here triggered in 2043, implies that an emission in 2025 now contributes to crossing of both tipping points as it also consumes part of the carrying capacity that remains until the second tipping point is triggered (Figure 1b). Finally, for an emission occurring after the first tipping point but before the second one, e.g., in 2035, one additional factor must be considered. Namely, crossing of the first tipping point in 2030 speeds up tipping of the second tipping point (from 2043 to 2040) because of the effect from the tipping of the first tipping point itself which adds to the background (Figure 1c). This accelerated tipping of the second tipping point reduces the remaining capacity for those emissions which occur after the first tipping point.

The same mechanisms apply if more tipping points are considered. Mathematical description of these mechanisms is detailed later.

Consideration of Time as a Variable. The MCTP framework requires that the time variable is used with different attributes. Specifically, we distinguish time interval (i.e., time step) where time is discrete as opposed to point in time where time is continuous. The interval is used when time indicates a portion (an interval) of time defined within two specific points in time. It is indicated with capital T. For instance, the emission year  $T_{\text{emission}}$  = 2021 indicates an emission occurred any time between first January, 00:00 and 31st December, 23:59 of the year 2021. Intervals of 1 year were considered the most realistic level of resolution for time-differentiated inventories of emissions and thus for the calculation of MCTPs. Points in time were used when integration over time was necessary. Time in those cases is a continuous variable and is indicated with lowercase t. We also distinguish between absolute time as opposed to relative time. Time is generally absolute in our framework because MCTPs depend on the specific years in which tipping points are triggered (e.g., 2021, 2022, etc.). By contrast, whenever the dependent variable does not depend on the proximity to tipping point, then relative time is used (e.g., year 1, year 2, etc.). A summary of the symbols used to refer to the time variable, their meaning, and where they are used in the paper is presented in Table S7 in Supporting Information.

**Calculation of Multiple Climate Tipping Points Potentials (MCTP).** With a consideration of *m* tipping points, the multiple climate tipping points potential,  $MCTP_i$ , in [ppt,-  $kg_i^{-1}$ ] (parts per trillion of remaining capacity taken up by a unit emission) of gas *i* emitted at year  $T_{emission}$  is defined as the sum of the ratios between the *impact of the emission* (that is part of anthropogenic background emissions) and the corresponding remaining capacity for each of the *m* tipping points occurring after the emission year

$$MCTP_{i}(T_{\text{emission}}) = \sum_{j=1}^{m} \frac{I_{\text{emission}, i, j}(T_{\text{emission}})}{CAP_{j}(T_{\text{emission}})}$$
(1)

where j indicates the jth tipping point occurring after the emission year (in order of occurrence) and can take any value from 1 to m, which is the total number of exceeded tipping points; I<sub>emission,i,j</sub> is the impact of the emission (part of anthropogenic background emissions) of gas *i* with respect to the *j*th tipping point,  $CAP_i$  is the remaining capacity up to the *j*th tipping point, and the emission year  $T_{\text{emission}}$  can be any year from 2021 (or the year when emissions are expected to start taking place) up to the year of the last tipping point. Defined in this way, the MCTP represents the total fraction of remaining capacity taken up by the unit emission and is expressed in parts per trillion of remaining capacity (ppt<sub>re</sub>  $kg_i^{-1}$ ). The  $I_{\text{emission},i,j}$  [ppm of  $CO_2 e \cdot yr \cdot kg_i^{-1}$ ] (where  $CO_2 e$  is the  $CO_2$ -equivalent concentration) of gas *i* with respect to the jth tipping point is here defined as the absolute climate tipping potential (ACTP) of gas *i* in  $[W \cdot m^{-2} \cdot yr \cdot kg_i^{-1}]$  divided by the radiative efficiency (RE) of 1 ppm of CO<sub>2</sub>  $[W \cdot m^{-2} \cdot ppm of$  $CO_2^{-1}]^{13}$ 

$$I_{\text{emission},i,j}(T_{\text{emission}}) = \frac{ACTP_{i,j}(T_{\text{emission}})}{RE_{\text{CO}_2}} = \frac{\sum_{k=1}^{\infty} RF_i(T_{k-1}) \cdot \Delta T}{RE_{\text{CO}_2}}$$
(2)

where the ACTP is equal to the radiative forcing of gas i ( $RF_i$ ) integrated over time between the emission and the tipping. This integral is written using Riemann sum notation. In this notation, n is the number of time steps (dimensionless). Given that  $\lim_{n\to\infty} (n \cdot \Delta T) = (T_{\text{tipping}_i} - T_{\text{emission}})$ , the n is equal to the difference between the year of tipping  $T_{\text{tipping}_i}$  (i.e., the year when the *j*th tipping point is exceeded) and the year of emission,  $T_{\text{emission}}$ , divided by the length of the time step,  $\Delta T$  (eq 3). The  $\Delta T$  is always equal to 1 year.

$$=\frac{T_{\text{tipping},j}-T_{\text{emission}}}{\Delta T}$$
(3)

Note that time is relative in the RF function because radiative forcing increase depends on the time that has elapsed from the emission, independently of the emission year. However, the ACTP and the resulting impact of the emission are emission-year specific because year of tipping is given. The  $RF_i$  is calculated as the product of the radiative efficiency of gas i ( $A_i$ ) (which represents radiative forcing per unit mass increase in atmospheric abundance of gas i) and the impulse response function (IRF), which for most non-CO<sub>2</sub> GHGs is represented with a single exponential decay and for CO2 with a sum of exponentials.8 However, unlike in the GWP approach, where radiative forcing of gas i is divided by the radiative forcing of the reference gas  $(CO_2)$ , the radiative forcing of gas *i* is divided here by the radiative efficiency of CO<sub>2</sub>, the RE<sub>CO2</sub>. This makes the unit of the impact of the emission consistent with the unit of remaining capacity (both given in ppm of

n

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CO<sub>2</sub>e·yr). Details of calculations of the impact are presented in Supporting Information.

The  $CAP_j$  [ppm of CO<sub>2</sub>e-yr] represents the increase in atmospheric CO<sub>2</sub>-equivalent concentration that can still take place before reaching the concentration level (in ppm of CO<sub>2</sub>e) that will trigger the tipping. It is emission-year specific as it depends on CO<sub>2</sub>-equivalent concentration from background anthropogenic emissions. The remaining capacity is reduced when the emission year approaches the year of tipping due to the effect of crossing any preceding tipping points,  $C_{\rm tip}$ (expressed in terms of CO<sub>2</sub>-equivalent concentration increase). This effect reduces the CO<sub>2</sub>-equivalent concentration increase that can still occur before reaching the year of tipping of subsequent tipping points thus accelerating their tipping. Equation 4 shows the calculation of the remaining capacity using Riemann sum notation for 1-year time steps

$$CAP_{j}(T_{\text{emission}}) = C(T_{\text{tipping},j}) \cdot (T_{\text{tipping},j} - T_{\text{emission}})$$
$$- \sum_{k=1}^{n} [C(T_{k-1}) + C_{\text{tip}}(T_{k-1})] \cdot \Delta T$$
(4)

where  $C(T_{\text{tipping},j})$  is the atmospheric CO<sub>2</sub>-equivalent concentration at the year of tipping  $T_{\text{tipping},j}$  C(T) is the CO<sub>2</sub>equivalent concentration from background emissions at time T, and  $C_{tip}(T)$  is the change in CO<sub>2</sub>-equivalent concentration at time T caused by all the tipping points that occurred before  $T_{\text{emission}}$  (all terms expressed in ppm of CO<sub>2</sub>e). The  $C_{\text{tip}}(T)$  is obtained from radiative forcing (RF) change induced by passing each specific tipping event (see Section S1.3.1 of Supporting Information). Time is absolute in eq 4 because both anthropogenic background emissions and effect of the tipping depend on the specific year. To avoid the capacity to become infinitely small and thus returning high peaks in MCTP, a cutoff of 6 [ppm of CO2e yr] was applied by taking the annual variability of atmospheric CO<sub>2</sub> concentration as a proxy for the uncertainties in measuring the atmospheric capacity (see Supporting Information).

Our representation of MCTP as a CF is somewhat different from the one that is typically used in LCIA. CFs typically represent either marginal or average "impact due to a unit emission".<sup>16-19</sup> The GWPs are derived in a marginal way,<sup>10</sup> and this is also the way the ACTP underlying  $I_{\mathrm{emission},i,j}$  in numerator of eq 1 is calculated (as in the GWPs, it is derived through radiative forcing per unit mass increase in atmospheric abundance of a given gas; see eq 2 and S1). Yet, the resulting impact I<sub>emission/i,j</sub> is related to the remaining carrying capacity, which depends on the background level, which in turn follows RCP pathway projections that are not influenced by the system being assessed in the LCA. This suggests that the resulting MCTP CFs are more in line with the average approach to calculating characterization factors (which could be supported for this type of impact owing to assumption of additivity of impacts of GHG emissions  $^{20}$ ). Consideration of carrying capacity in the CF is not usual but has been discussed and tested previously.  $^{21,22}$  Bjørn A. $^{23}$  showed how carrying capacity can be integrated into characterization factors for terrestrial acidification.

The framework presented above was used to compute the MCTP of the three main anthropogenic GHGs,  $CO_2$ ,  $CH_4$ , and  $N_2O$ , considering the selected tipping elements, in 10000 Monte Carlo simulations. Each simulation represents a possible sample scenario of triggered tipping points (i.e.,

different timing and order of occurrence) based on the propagation of current uncertainties in tipping occurrence. An average (geometric mean) MCTP was then calculated. We observe that iterations fail whenever tipping points are triggered in close proximity to each other (either in the same year or in consecutive years) as no remaining capacity can be calculated. This is taken into account by adjusting the number of total iteration runs so that failed iterations are excluded while the total number of runs is ~10000. Implications of this model limitation on the MCTP will be discussed.

Choice of Atmospheric GHG Concentration Development Pathway. Both the determination of the years of tipping and the evolution of the remaining capacity over time depend on the development of atmospheric GHG concentrations, expressed in CO2-equivalents. Here, the Representative Concentration Pathways (RCPs) and their extensions up to year 2500 are used.<sup>24,25</sup> The medium stabilization pathway RCP6 (total radiative forcing stabilized at 6 Wm<sup>-2</sup> after 2100) is chosen as baseline, assuming that even though current emission trajectories are closer to RCP8.5 projections,<sup>2</sup> ongoing mitigation efforts will prevent a continuous increase and will more likely lead to a peak-and-stabilization pathway as projected in RCP6. The MCTPs were also calculated for RCP8.5 (rising radiative forcing to 8.5 Wm·-2 after 2100) and RCP4.5 (stabilization at 4.5 Wm-2 after 2100), selected as potentially worst- and best-case (realistic) pathways, respectively. The low emission scenario RCP2.6 is excluded as the massive mitigation efforts required are considered mostly unfeasible.<sup>26,27</sup> The choice of RCP pathway influences which tipping points are triggered in each simulation as it depends on whether the threshold temperature of a specific tipping element is reached under the RCP pathway.

**Determination of Tipping Time.** Accurate predictions of the climate conditions triggering a tipping point and the time of occurrence are uncertain.<sup>3</sup> On the basis of available estimates of potential thresholds levels (Table S1), we assigned one possible range of temperature thresholds to each selected tipping element (Table S2). Uncertainties in the actual temperature threshold level were accounted for by assigning a triangular probability distribution function to the range of potential threshold levels; T(a,b,c), where *a* and *b* are the lower and upper limits of the range, respectively, and the most likely value *c* is assumed to be the central value of the assigned range. Triangular distribution was chosen because actual distributions were unknown and could not be generated with the limited data available.

The CO<sub>2</sub>-equivalent concentration that stabilizes the climate at a given temperature threshold and the year of tipping were obtained by the combination of data on temperature and GHG concentration equivalents development over time, according to the chosen RCP pathway. The data are retrieved with the climate model MAGICC6 (Model for the Assessment of Greenhouse Gas Induced Climate Change, v.6), which is a default model to harmonize projections of RCP and Extended Concentration Pathways (ECP).<sup>25,28</sup>

**Calculation of Effects from Crossing Climate Tipping Points** ( $C_{tip}$ ). Modeling of the possible consequences from passing a tipping point is constrained by the availability of quantitative estimates of the total magnitude of such effects, which are rather scarce in the scientific literature. We considered available estimates of the potential change in RF induced by tipping suggested in previous studies (Table S6),

and to allow for their quantification in relation to the remaining capacity, we converted these to the increase in equivalents of GHG concentrations (ppm of CO2e) that would lead to the same RF change. In some cases, the effect from tipping could not be modeled due to either lack of data (Atlantic thermohaline circulation shutoff, North Atlantic subpolar gyre convection collapse, Sahara/Sahel and West African monsoon shift, Alpine glaciers) or lack of consequences on the climate from the tipping point (coral reefs) (see Supporting Information). For Arctic summer and winter sea-ice loss, the RF change is due to reduced sea-ice albedo and conversion to annual concentration increase was done using the radiative efficiency of CO<sub>2</sub> per 1 ppm. This effect was assumed to unfold completely from the year after tipping and to remain constant over the years, as the evolution of radiative forcing changes after tipping was unknown. For the other six tipping points, i.e., Greenland ice sheet melt, West Antarctic ice sheet collapse, El Niño-Southern Oscillation change in amplitude, permafrost loss, Amazon rainforest and Boreal forest dieback, the RF change derives from emissions of carbon estimated to occur after tipping (Table S6). Here, C<sub>tip</sub> was calculated by adapting the dynamic approach of Levasseur et al.,29 originally developed for calculating time-dependent RF impacts of GHG emissions (that is, dynamic global warming potentials), to obtain time-dependent (dynamic) yearly equivalents of GHGs concentration increase due to the carbon emissions. The total carbon emissions, considered to be either CO<sub>2</sub> or methane emissions, depending on the tipping element, were assumed to be equally distributed over the transition period of the tipping event (see Table S6 in Supporting Information), obtaining a constant temporal profile of emissions. An exception is for El Niño-Southern Oscillation change in amplitude for which the release of carbon is considered basically permanent.<sup>4</sup> The effect of these emissions was then calculated considering the residence time of the two gases in the atmosphere. The result provides the equivalent increase in GHG concentrations at any time T after tipping, caused by the emissions released at  $\dot{T}$  and the nondecayed fraction of emissions that occurred before T since the tipping year. This approach does not account for the gradual changes that in reality occur before a critical point is reached (e.g., albedo changes from melting sea ice at current temperature levels) and may underestimate the actual effects from tipping. However, it was the most feasible modeling option considering model complexity constraints and lack of estimates on the gradual changes expected before reaching some of the considered tipping points. Details of these calculations are

**Illustrative Application.** The CFs proposed here depend on the year of emission, hence for each GHG, a set of yearspecific MCTPs is provided and this should be used in combination with a time-differentiated inventory specifying GHG emissions in each year. The resulting impact score is calculated by summing the product of the emitted amount of gas *i* at year  $T_{\text{emission}}$  with the corresponding MCTP factor at  $T_{\text{emission}}$  for each GHG *i* and each emission year  $T_{\text{emission}}$ 

presented in Section S1.3.1 of Supporting Information.

$$IS_{\rm MCTP} = \sum_{i} \sum_{T_{\rm emission}=2021}^{t_{\rm upping,last}} m_i(T_{\rm emission}) \cdot MCTP_i(T_{\rm emission})$$
(5)

where  $IS_{MCTP}$  is the MCTP impact score,  $T_{tipping,j_{last}}$  is the last possible year when a tipping point can be triggered across

10000 model runs,  $j_{\text{last}}$  is the last triggered tipping point across 10000 model runs,  $m_i(T_{\text{emission}})$  is the mass of GHG *i* emitted at year  $T_{\text{emission}}$  and  $MCTP_i(T_{\text{emission}})$  is the corresponding MCTP for gas *i* and emission year  $T_{\text{emission}}$ . The double summation indicates that the product  $(m_i(T_{\text{emission}}))$ .  $MCTP_i(T_{\text{emission}})$  is first summed over time, starting from the first emission of GHG *i* released by the assessed product (assumed to be year 2021 in eq 5) up to the year when MCTPs are relevant  $(T_{\text{tipping}, j_{\text{last}}})$ , and then summed over each GHG *i*.

We apply the MCTPs calculated for the RCP6 scenario to CO<sub>2</sub> and CH<sub>4</sub> emission profiles (over 100 years) from incineration and landfilling of 1 kg of fossil-based (polycaprolactone (PCL), polybutylene succinate (PBS), polystyrene (PS)) and biobased (poly)lactic acid (PLA)) biodegradable polymers. These materials are selected as they degrade over different timespans when landfilled. Six landfilling scenarios are considered with four representing a possible range of degradation rate constants (corresponding to fast, medium, slow, and very slow first order<sup>30</sup> degradation kinetics under anaerobic conditions) and two accounting for delays in GHG emissions for a material with fast kinetics (20 and 50 years delay) as found for different fossil- and biobased plastic types.<sup>30-33</sup> For each scenario, the assumed carbon content of the degrading material is 0.5 kg C/kg plastic (stoichiometric calculation from a hypothetical polymer with 3 carbon atoms) of which 100% is released as CO<sub>2</sub> in the incineration scenario, whereas 71% is emitted as CO2 and 29% as methane in the landfilling scenarios.33 Note that only emissions stemming from the carbon contained in the plastic are considered. By multiplying the yearly emitted amount with the corresponding average MCTPs per unit emission (under RCP6), we used eq 5 to calculate total tipping impacts corresponding to degradation of 1 kg of plastic. For comparison, we also compute impact scores using the complementary CFs GWP20,6 GWP100,6 GWP100<sub>ILCD</sub>, i.e., including credits for temporary carbon storage using the method in the ILCD Handbook,  $^{34}$  dynamic GWP100,  $^{29,35}$  and GTP100.  $^{8,10}$  While GWP100 treats emissions over 100 years as a pulse emission in the first year, dynamic GWP100 expresses the time-dependent contribution of emissions to radiative forcing change over 100 years, accounting for the actual emission timing.  $GWP100_{ILCD}$ includes credits for temporary carbon storage to account for the storage due to delayed or incomplete degradation of the plastic materials over 100 years. In consistency with recommended practice,  $^{12}\,$  all GWP CFs are inclusive of climate-carbon cycle feedbacks. Methods for calculating impact scores using all these CFs are summarized in Table S9 in Supporting Information.

#### RESULTS

Multiple Climate Tipping Potentials. Results of two successful Monte Carlo simulations show that the number and type of tipping points actually triggered depends on the probability that the threshold temperature picked in the simulation is within the temperature increase projected under the chosen pathway (Figure 2a,b). They also show that MCTPs are particularly sensitive to the proximity of an emission year to the year of tipping. The MCTP can increase by up to a factor of 6 compared to the MCTP for an emission in year 2021 when emission year approaches the year of tipping, and it drops consistently after the tipping point is



Figure 2. Emission-year specific multiple climate tipping point potentials (MCTP) per emission of 1 kg CO<sub>2</sub> under RCP6. (a, b) MCTPs from two illustrative model simulation runs (solid line). Vertical dotted lines indicate occurrence of tipping points (Table S8). Green dashed curves are the same simulations computed without considering the effect from the tipping (tipping occurrence not shown in this case). AS = Arctic summer sea ice loss, AM = West African monsoon shift, SG = North Atlantic subpolar gyre convection collapse, AI = West Antarctic ice sheet collapse, GI = Greenland ice sheet melt, AF = Amazon rainforest dieback, P = Permafrost loss, AW = Arctic winter sea ice loss, TC = Atlantic thermohaline circulation shutoff. (c) MCTP results for 10000 model simulations (gray dots), their geometric mean (solid line) and uncertainty ranges (5th and 95th percentiles of yearly results, red dotted lines).

crossed, causing discontinuities in the MCTP curve. The steep increases in the MCTP are caused by fast reduction in the remaining atmospheric capacity assigned to these tipping points when emission years approach respective years of tipping (see Figure S3 in Supporting Information). The drop in the MCTP after crossing a given tipping point is caused by capacities assigned to the subsequent tipping always being significantly larger when compared to the remaining capacity assigned to the preceding tipping event. Accounting for direct effects from crossing tipping points in these two simulations reduces the remaining capacity from 10 to 99% (depending on the emission year) when compared to model results without considering the effect from the tipping on remaining capacity pubs.acs.org/est

up to the next tipping point(s). This accelerates the occurrence of the subsequent tipping points by 3 to 31 years.

The tendency of MCTP to peak with the proximity to a tipping point is masked by the large uncertainties around the year of tipping, which influence the number and sequence of tipping points and make individual tipping points overlap. Average (geometric mean) MCTP derived from ~10000 Monte Carlo simulations varies from 0.0074 to 0.020 ppt<sub>rc</sub> per 1 kg of CO<sub>2</sub> emission (Figure 2c). In 90% of the iterations, MCTPs ranged from 0.0034 to 0.033 pptr per 1 kg of CO<sub>2</sub> emission across all emission years. Yet, there is a relatively high probability of several tipping points occurring between 2040 and 2060, resulting in a peak of average MCTPs around 2050 with almost a doubling of the MCTP magnitude (average 0.014 ppt<sub>rc</sub>) in comparison to emissions occurring in 2021 (average 0.0074 pptrc). Average MCTPs of CH4 and N2O follow the same trends as observed for CO<sub>2</sub> in Figure 2c but are on average 83 and 273 times higher, respectively, when compared to  $CO_2$  (Figure S4). The impact of a unit emission of CH4 is higher than that of CO2 in the MCTP approach when compared to GWP100, because the time integrations in ACTP are over shorter time periods compared to the 100 years' time horizon of GWP, and with shorter time horizons, the impacts of short-lived gases like CH4 become larger.

Consideration of direct effects from the tipping increases the average MCTPs by up to 37% when compared to the average MCTP computed without considering the effect from the tipping (with greater increases for emissions occurring later in time). This corresponds to the last tipping point occurring, on average, 17 years earlier (Figure S5).

The MCTPs calculated for different RCP pathways follow different trends (Figure 3). They are larger when assuming a low background concentration pathway (RCP4.5) and become progressively smaller for higher concentration paths RCP6 and 8.5. The MCTPs increase until 2035 in all pathways, but then they fluctuate over the middle in RCP6, increase in RCP4.5, and follow a downward trend in RCP8.5. The number of tipping points that can be triggered also varies between RCP scenarios, depending on whether threshold temperatures are reached (Table S2). In the high emissions pathway RCP8.5, all the 13 elements can have their tipping points crossed. In RCP6, the permafrost loss and Arctic winter sea ice loss are not triggered, while under RCP4.5, additionally Boreal forest dieback, El Niño-Southern Oscillation change in amplitude, and Atlantic thermohaline circulation shutoff are not triggered. These differences in the number of tipping points determine the time horizon for which MCTPs are relevant (until 2085, 2115, and 2210 in the RCP4.5, RCP6, and RCP8.5 scenarios, respectively).

**Example of Degradation of Plastic Polymers.** We find that using new MCTPs leads to additional insights when compared to those gained from using other metrics (Table 1). Impact scores in the MCTP approach increase with decreasing degradation rates (scenarios 2–4) because there is higher probability that a significant portion of emissions is released in close proximity to tipping points, where MCTPs are the largest (Figure S6). By contrast, impact scores generally decrease with decreasing degradation rate in the GWP-based and GTP100 approaches owing to (1) decreasing emissions released within the 20 (GWP20) and 100 years (GWP100, GTP100) time horizons, (2) increasing benefits from temporary carbon storage (GWP100<sub>ILCD</sub>), and (3) delayed emissions and smaller values of their matching dynamic GWP100. With MCTP, a 20-

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Figure 3. Emission-year specific multiple climate tipping points potentials (MCTP) of 1 kg of CO<sub>2</sub> under RCP4.5 (a) and RCP 8.5 (b) scenarios. MCTPs for 10000 model simulations (gray dots), their geometric mean (solid line), and uncertainty ranges (5th and 95th percentiles, red dotted lines). Notice the different scale of the x-axes.

Table 1. Total Impact Scores for Different End-of-Life Scenarios of Plastic Polymers Calculated Using GWP20, GWP100, GWP100, GWP100, GTP100, and New MCTPs<sup>1</sup>

End-of-life degradation scenario	GWP20 (kg CO <sub>2</sub> eq/kg plastic)	GWP100 (kg CO2eq/kg plastic)	GWP100 <sub>ILCD</sub> (kg CO <sub>2</sub> eq/kg plastic)	Dynamic GWP100 (kg CO <sub>2</sub> eq/kg plastic)	GTP100 (kg CO2eq/kg plastic)	MCTP, under RCP6 (ppt <sub>rc</sub> /kg plastic)
1. Incineration <sup>a</sup>	1.8	1.8	1.8	1.8	1.8	0.014
Plastic degradation rate <sup>b</sup>						
2. Fast <sup>c</sup>	18	8.3	8.2	4.7	3.8	0.089
3. Medium <sup>d</sup>	14	8.3	7.4	4.6	3.8	0.14
4. Slow <sup>e</sup>	6.4	7.3	5.5	3.8	3.4	0.16
5. Very slow <sup>f</sup>	0.036	0.078	0.048	0.052	0.034	0.0020
Delayed degradation <sup>g</sup>						
6. After 20 years (fast rate)	0	8.3	6.9	4.5	3.8	0.21
7. After 50 years (fast rate)	0	8.3	5.1	4.1	3.8	0.16

<sup>*a*</sup>Incineration of fossil-based plastic where all carbon is emitted as CO<sub>2</sub> in the first year. <sup>*b*</sup>Degradation under anaerobic conditions, resulting in release of methane. <sup>c</sup>90% degradation of polycaprolactone (PCL) in 2 years.<sup>31</sup> <sup>*d*</sup>90% degradation of polybutylene succinate (PBS) in 31 years.<sup>32</sup> <sup>*c*</sup>90% degradation of polybutylene succinate (PBS) in 105 years.<sup>30</sup> <sup>*f*</sup>1% degradation of biobased PLA in 100 years.<sup>33</sup> <sup>*s*</sup>Potential short (20 years) and long (50 years) lag phase in degradation of PCL based on ref 33. <sup>*h*</sup>Ranking between scenarios 1–7 is illustrated within each column with different colors. Red shading indicates the highest impact scores and green the lowest impact scores. The GWP100<sub>ILCD</sub> includes credits for the temporary carbon storage of delayed or incomplete degradation of the material over 100 years calculated using the ILCD approach.<sup>34</sup>

and 50-year lag phase of degradation of the polymers are seen as worse and second worse scenarios, respectively, because of proximity of emissions to tipping points, whereas with GWP100 and GTP100, which are not able to capture differences in emission timing, impact scores are the same as without a lag phase (scenario 2). The MCTP results for these two scenarios are also different from GWP20, which does not assign any burden to emissions occurring after the 20 year time horizon. For very slow degradation kinetics, impact scores are almost independent of the type of metric chosen. This is because the vast majority of emissions in this slow degradation scenario occurs beyond the time frames for which MCTP and their complementary GWPs are considered relevant. Incineration is seen as the second best option with all other metrics, because no methane emissions occur and, for MCTP, also because of small CF values for emissions of CO<sub>2</sub> in year 2021.

Ranking of these different end-of-life scenarios was not very sensitive to the RCP pathway for which MCTPs were computed (Table S10); however, slight variations reflect the different contribution to tipping that emissions have in the three RCPs. In particular, under RCP4.5, the largest contribution is observed after 2060; therefore, a polymer with 50 years lag phase, emitting mostly around 2070, performs worse. In terms of magnitude, impact scores with RCP4.5 are larger for each end-of-life scenario, as the corresponding MCTP factors are larger.

#### DISCUSSION

**Importance of GHGs Development Pathway.** We find that the magnitude of the MCTPs is larger under RCP4.5 and lower under RCP8.5. This somewhat counterintuitive finding can be explained by two factors. First, the MCTP is a metric expressing midpoint impacts and, as such, it does not consider the severity of the damage on ecosystems or humans caused by crossing tipping points. These damages are expected to be larger for the RCP8.5 path when compared to those of the two other pathways. Thus, the impact expressed by our midpoint CFs should only be interpreted as the contribution of an emission that is part of the background to crossing tipping points and not as the overall damage caused by the emission

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the damage caused by the tipping itself. Second, climate responds differently to the same increase in GHG concentrations in the three RCPs: for example, to reach a tipping threshold of 2  $\,^{\circ}\text{C}$  under RCP8.5, the GHG concentrations should rise to about 574 ppm of CO2e, whereas 541 ppm of CO2e are already sufficient according to RCP4.5 projections (Figure S1). This is because the slow heat uptake of the oceans creates a delay in the response of the atmospheric temperature to an increase in CO<sub>2</sub> concentration,<sup>36</sup> and this delay depends on the different rate of CO<sub>2</sub> increase projected in each RCP pathway. In RCP8.5, CO2 concentrations increase rapidly, generating a larger lag in the climate response compared to RCP4.5. Therefore, RCP8.5 reaches 2 °C at higher concentrations, whereas in RCP4.5, the same temperature corresponds to lower concentration levels. This means that the contribution of an emission to crossing tipping points is proportionally larger under RCP4.5 because tipping points are triggered at lower concentrations when compared to RCP8.5 or RCP6. Consequently, for the same emission year, MCTPs are larger for RCP4.5 than for the two other pathways.

Differences in the temporal evolution of MCTPs observed between the RCP pathways are the result of a combination of several additional factors and it is not possible to determine one dominant driver. One factor is the different rate of projected GHGs concentration increase across the RCPs. In RCP8.5, GHGs concentration increases fast and, due to this, differences in concentration between consecutive years became larger over time (remaining capacity depends on the magnitude of the difference). In addition, tipping points are triggered at higher concentration levels, as explained above. This results in numerically larger remaining capacities for emissions in, e.g., 2080 than emissions in 2040 and explains why MCTP decreases over time. For RCP4.5, the opposite is true: MCTP increases over time because of relatively small differences in GHGs concentration between consecutive years (especially when the concentration starts to level off) and because tipping points are triggered at lower concentrations. Other factors to consider are the simultaneous dependency on evolution of impacts of the emission (as MCTPs are based on ratios between impacts of the emission and remaining capacities), the different number of tipping points that can be triggered in each RCP pathway, and the possibility, in RCP8.5, that tipping points occur at very high concentrations and very late in time (as opposed to no more tipping points beyond 2100 in RCP4.5).

Uncertainties. The major source of uncertainty in the MCTP CFs is that they do not consider interactions between the tipping elements.<sup>4</sup> Similarly, the MCTPs do not consider situations where tipping points are predicted to occur so close to each other that the remaining capacity is fully consumed by the preceding tipping points. Our results show that the probability that crossing a tipping point causes tipping of another (for at least one pair of tipping elements), even without considering other interactions,<sup>37</sup> is equal to 92% for the RCP6 scenario but is somewhat smaller for RCP4.5 and RCP8.5 (79 and 53%, respectively). This is consistent with earlier studies suggesting that the passing of some tipping points increases the likelihood of other tipping points due to positive feedbacks from the tipping.<sup>38,4</sup> The implication of this model limitation is that the time horizon for which MCTPs are relevant can be shorter. Another implication is that our MCTPs can be underestimated, particularly those occurring later where uncertainties about temperatures triggering the

tipping are larger. The combined effect of more tipping points triggered at once would indeed reduce the remaining capacity to the next tipping even further, resulting in higher MCTPs. This is particularly the case for the RCP6 pathway, where the chances of one or more tipping points triggered at the same time is the highest. However, *impacts of the emission* will simultaneously decrease, as tipping points approach, and whether this results in an increase in MCTP will thus depend on the magnitude of reduction of the *impact of the emission* in relation to the reduction in remaining capacity.

Implications for Life Cycle Assessment. We offer a new method that considers multiple climate tipping points in the quantification of the potential contribution of products to climate change impacts. As no other metric considers the contribution of emissions to deplete the remaining capacity up to multiple tipping points and the variability of this contribution based on emission timing, the new method represents a new life cycle impact category. This new impact category should be seen as being complementary to, but not a substitute for, global warming and global temperature change categories. A ranking of the three well-mixed GHGs (CO2, CH<sub>4</sub>, and N<sub>2</sub>O), in terms of their average MCTP, is comparable to the ranking of their GWP20s and ranges from 1:51:238 to 1:107:299 (RCP6), depending on emission year, in comparison to the constant ranking of 1:86:26810 for the GWP20. This stresses the need to consider short-term climate impacts, as in both CFs, the radiative forcing is integrated over shorter time horizons (through the ACTP and AGWP), resulting in larger impacts assigned to short-lived gases like methane. Despite this similarity, the added value of the MCTP is that it captures those emissions and short-term impacts occurring beyond the 20-year time.

We showed that the use of MCTPs offers new insights when applied to temporarily differentiated GHG emission inventories. The best performance, from the climate tipping perspective, is achieved when emissions from the product occur when their contribution to crossing tipping points is the lowest rather than when these emissions are just delayed. Indeed, there is a high probability of several tipping points occurring from ca. 2040 to 2060, where MCTPs are the largest. An accounting for the uncertainties in the triggering of tipping points eventually results in a more robust, but perhaps less straightforward, assessment of climate tipping impacts from products. These uncertainties are currently so large that individual tipping points are not clearly discernible. Nevertheless, such large uncertainties should not prevent the use of MCTP because we demonstrated that MCTP still allows the capture of differences in performance of products with different temporal emission profiles.

We recall that the availability of time differentiated emission inventories of the assessed products is necessary for a meaningful use of the set of emission-year-specific MCTPs provided here (Supporting Information). The main implications for life cycle inventory (LCI) modelers is the need to focus on modeling and the reporting of emission inventories in temporarily disaggregated forms. The main implication for LCA software developers is the need to develop modules that can calculate impact scores using temporarily disaggregated inventories and time-dependent characterization factors. The same challenges are still relevant for dynamic methods, including the dynamic GWP approach.<sup>29</sup> We expect that potential take up of climate tipping as an impact category in LCA will make it attractive to increase the availability of

temporarily differentiated emission inventories and their handling in LCA software. Until then, dynamic approaches, including our MCTP, have to be used offline.

The reader should note, however, that the iterative nature of LCA allows using our MCTP factors even if a full timedifferentiated inventory is not available for all processes in a given life cycle. In this case, the ideal would be to identify processes where time-differentiation of emissions is relevant and is expected to really matter for the LCA results (such as end-of-life processes, biomass growth, or deforestation) and obtain a time-differentiated inventory for these processes only. This can be done with a sensitivity analysis. The MCTP impact score for these processes can then be calculated offline using eq 5. The impact score for all the remaining processes not associated with a time-differentiated inventory, or for those processes which do not matter for the LCA results (small contribution to total impact), can be calculated by multiplying the total amount of CO2, CH4, and N2O emissions from these processes by the corresponding MCTP factor relative to the year when their emission is expected to take place. The sum of the two impact scores returns the final MCTP results.

The new metric is expected to be particularly valuable in the life cycle assessments of biodegradable plastics, deteriorating wooden products, or engineered chars used for temporary carbon storage.<sup>35,39</sup> We recommend the presenting of results for all three considered RCP scenarios to show if, and how, the choice of future uncertain emission pathways could influence conclusions of the study of interest. Our MCTPs are expected to add less value in the comparative LCA context when emissions occur all at once, such as the incineration scenario in our case study, or when there are large differences in the emitted amount of GHGs (e.g., very slow degradation scenario). Further, although emissions do not influence the background emission path, the MCTPs are not directly applicable in the assessment of large-scale systems, like GWP and GTPs, are better suited for this purpose.

The MCTP is proposed as a method for climate change impacts at the midpoint level; therefore, the interest here is to cover only climate change impacts at the midpoint level. If crossing a tipping point leads to loss of species (directly by, e.g., loss of habitat when ice melts, or indirectly via temperature increase), then this should be accounted for at the damage level.

#### ASSOCIATED CONTENT

#### Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.est.0c02928.

Emission-year specific MCTP values (XLSX)

Methods and results (PDF)

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#### Notes

The authors declare no competing financial interest.

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# **Supporting Information-1**

# Multiple climate tipping points metrics for improved sustainability assessment of products and services

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# **S3. References**

# S1. Supplementary methods

This section includes (i) review and selection of climate tipping elements, (ii) methods for calculation of *impact of the emission*, capacity and effects from crossing tipping points (including justifications when effects from tipping were not modelled), (iii) reasoning for setting a capacity cutoff, (iv) an example of MCTP calculation with two tipping points, (v) details of the two illustrative simulations presented in the main article and (vi) equations for calculation of impact scores with MCTP and the other metrics used in the case study.

### S1.1 Review and selection of climate tipping elements

The following three criteria were used to select relevant tipping elements in this study:

Criterion 1: There is an evidence of a critical threshold beyond which a small change in one variable controlling the system (control variable) causes a large qualitative change in the system (that is, the system exhibits threshold behavior). The change may be abrupt and occur immediately after the cause or gradual and spanning over longer timescales. This criterion excludes those tipping elements for which the transition to a new state is a continuous process without strong nonlinearity or threshold behavior. To ensure that there is minimum understanding of the tipping dynamics supported by scientific evidence we considered only those tipping points, which are described in at least two studies published by different groups in peer-reviewed journals. In cases where there were more studies but the evidence of threshold behavior was debated between them, we conservatively assumed that the potential tipping element does exhibit threshold behavior, thus meeting the criterion.

*Criterion 2: There is an evidence that the system's critical control variable that may pass a threshold is influenced by changes in atmospheric CO*<sub>2</sub>*-equivalent GHGs concentration.* This influence is typically indirect, meaning that a change in GHG

concentrations affects certain parameters that in turn have an influence on the control variable of the system (e.g. GHG concentrations affect atmospheric temperature, which, in turn, influences the freshwater and heat inputs that control the thermohaline circulation in the North Atlantic). This criterion is chosen because climate tipping characterization factors (CF) are for greenhouse gas emissions. Thus, those tipping points that cannot be related to GHG concentrations, but are influenced by e.g. aerosol pollution, are not relevant and are therefore excluded.

*Criterion 3: Tipping threshold estimates and their relative uncertainties can be expressed as global mean temperature change above pre-industrial levels.* Despite relatively uncertain link between global mean temperature and the actual control variable of a tipping element<sup>1</sup>, global mean temperature change is used here as indicator of threshold levels because it was found to be the most common way of reporting critical thresholds among studies (see references in Table S1). Thus, we excluded tipping elements for which threshold estimations are only given based on local physical parameters, e.g. sea ice extent/thickness, rate of ocean current or precipitation rate, for which the calculation of the corresponding level of atmospheric GHGs concentration equivalents (i.e. the concentration necessary to calculate the remaining capacity) is either not possible or highly uncertain.

An overview of all potential tipping elements is given in Table S1. Table S2 provides an overview of potential occurrence of the 13 selected tipping elements under the considered Representative Concentration Pathways (RCP).

1 **Table S1**: Overview of potential tipping elements from the literature and their fulfilment of the selection criteria (1, 2 and 3) in this study. Selected tipping

2 points that meet all criteria are highlighted in bold. When available, ranking based on likelihood is shown for illustrative purposes even though it was not used

3 as a criterion. Fulfilment of selection criteria is indicated with 'y' = yes; 'n' = no; 'un' = uncertain.

Tipping element	Critical tipping threshold <sup>a</sup> (global mean temperature above pre-industrial in °C, unless differently indicated)		Climatic triggering and main feedback mechanism	Transition period <sup>b</sup> (yr)		Likelihood		Fulfilled selection criteria		
		Reference			Reference	<b>Relative</b> likelihood <sup>2</sup>	Likelihood with increasing global warming <sup>3</sup>	1	2	3
Arctic summer sea ice loss	$1.2 - 2.7^{\circ}$	4	Melting of sea exposes larger areas of ocean surface to solar radiation, decreasing the albedo and increasing heat absorption by the ocean, thus amplify the warming. This loss of sea ice could lead to ice cap melting beyond certain size/thickness at which complete melting is likely to occur	10	4	1	1	У	У	У
(AS)	1 – 3	5								
	$1.5 - 2^{d}$	6, 7								
	2.2 – 2.7 (2.5)	8								
Greenland ice sheet melt (GI)	$1.7 - 2.7^{\circ}$	4	Increased air temperatures cause surface	300 - 7500	10	2	2	у	у	у
	1 - 3	5	ice melting, which lowers ice altitude and increases surface temperature (due to higher temperatures at lower elevation) causing further warming and melting (melt elevation feedback) to a point	(1500) <sup>c</sup>						
	$0.8 - 3.2 (1.6)^{e}$	11								
	$1.9 - 5.1 (3.1)^{e}$	12								
	2 - 3	15								
	2-4	1+	beyond which there is net mass loss and GI shrinks radically <sup>9</sup> .							
West Antarctic ice sheet	$3.7 - 5.7^{\circ}$	4	The collapse is due to the combination of (i) surface melting (see GI) and (ii) the retreat of the submerged grounding line caused by the intrusion of warmer ocean water, which increases the ice flux and induces further retreat <sup>3.9</sup> .	100 - 2500	10	3	4	у	у	у
collapse (AI)	1 – 3	5		(500) <sup>c</sup>				-	-	-
	4 <sup>f</sup>	15								
	1-5.7	16								
Amazon rainforest dieback	$3.7 - 4.7^{\circ}$	4	Warmer temperatures cause reduction in	50 - 250	10	3	3	у	у	у
( <b>AF</b> )	3-5	5	precipitations, lengthening of the dry season and directly affect vegetation	(50) <sup>c</sup>					•	
	2.5, 6.2 <sup>g</sup>	18								
	2, 3, 4 <sup>h</sup>	17	productivity, leading to forest dieback, which in turn further reduces precipitations <sup>17</sup> .							
Sahara/Sahel and West	$3.7 - 4.7^{\circ}$	4	Warming of sea surface temperature	10	4	4	6	у	у	у
African monsoon shift (AM)	3-5	5	influences the direction of the West					-	-	
	2.1, 2.8, 3.5 <sup>i</sup>	18	African monsoon, which in turn affects rainfall in the Sahara/Sahel region. It is uncertain whether WAS will shift northward (leading to increased rainfall) or southward (leading to further drying of the Sahel) <sup>3</sup> .							

Boreal forest dieback (BF)	$3.7 - 5.7^{\circ}$	4	Increased water stress, peak summer heat	50	4	5	4	v	v	v
	3-5	5	stress, vulnerability to disease and fire					5	2	5
			frequency due to higher temperatures							
			cause boreal forest dieback and transition							
			to open woodlands or grasslands, which in							
			turn would amplify summer heat stress,							
			drying and fire frequency <sup>3</sup> .							
El Niño-Southern Oscillation	$3.7 - 6.7^{\circ}$	4	Increased heat uptake in the equatorial	100	4	5	5	y	y	y
change in amplitude (EN)	3-5	5	Pacific could lead to a permanent					2	2	, in the second
			deepening of the thermocline, which could							
			result in more persistent El Niño-like							
			conditions. However, it is not excluded							
			that stronger warming of the west							
			Equatorial Pacific than the east could lead							
			to more persistent La Niña-like							
			conditions <sup>4</sup> . Complex and uncertain							
			mechanism.							
Atlantic thermohaline	$3.7 - 5.7^{\circ}$	4	Addition of freshwater in the North	10 - 250	10	5	5	y	y	y
circulation shutoff (TC)	2 5	5	Atlantic (due to sea ice and Greenland ice	(50) <sup>c</sup>				2	2	2
	3 - 3		sheet melting, river inputs and ocean	. ,						
	$1.4, 1.6, 1.9^{i}$	18	precipitation) may reduce the density-							
	6-8 <sup>j</sup>	20	driven sinking of North Atlantic waters							
	0 0		until the Atlantic thermohaline circulation							
	1.1.1.6.2.2	21	is significantly slowed down or even							
	1.4, 1.6, 2.2,	21	stopped <sup>19</sup> .							
	2.5		**							
Permafrost loss (P)	5.6	18	Thawing of permafrost (highly rich in	<100	4	Not	7	У	У	у
			organic carbon) in the northeastern Siberia			assessed				
			organie europhy in the normeustern Stoerna							
	> 5	5	(Yedoma) triggers biochemical							
	> 5	5	(Yedoma) triggers biochemical decomposition of the organic matter,							
	> 5 > 5	5	(Yedoma) triggers biochemical decomposition of the organic matter, which generates heat that further increases							
	> 5 > 5	5	(Yedoma) triggers biochemical decomposition of the organic matter, which generates heat that further increases warming and melting.							
Indian summer monsoon	> 5 > 5 3 - 5	5 16 5 5	(Yedoma) triggers biochemical decomposition of the organic matter, which generates heat that further increases warming and melting. Monsoon dynamics depend on heat and	1	4	Not	Not assessed	у	n	у
Indian summer monsoon collapse	> 5 > 5 3 - 5	5 16 5	(Yedoma) triggers biochemical decomposition of the organic matter, which generates heat that further increases warming and melting. Monsoon dynamics depend on heat and pressure differences between land and	1	4	Not assessed	Not assessed	у	n	у
Indian summer monsoon collapse	> 5 > 5 3 - 5	5           16           5           5	<ul> <li>(Yedoma) triggers biochemical</li> <li>decomposition of the organic matter,</li> <li>which generates heat that further increases</li> <li>warming and melting.</li> <li>Monsoon dynamics depend on heat and</li> <li>pressure differences between land and</li> <li>ocean. Black carbon and aerosol emissions</li> </ul>	1	4	Not assessed	Not assessed	у	n	у
Indian summer monsoon collapse	> 5 > 5 3 - 5	5 16 5	<ul> <li>(Yedoma) triggers biochemical decomposition of the organic matter, which generates heat that further increases warming and melting.</li> <li>Monsoon dynamics depend on heat and pressure differences between land and ocean. Black carbon and aerosol emissions on land reduce land-absorbed solar</li> </ul>	1	4	Not assessed	Not assessed	у	n	у
Indian summer monsoon collapse	> 5 > 5 3 - 5	5 16 5 5	<ul> <li>(Yedoma) triggers biochemical decomposition of the organic matter, which generates heat that further increases warming and melting.</li> <li>Monsoon dynamics depend on heat and pressure differences between land and ocean. Black carbon and aerosol emissions on land reduce land-absorbed solar radiation and the resulting lower warming</li> </ul>	1	4	Not assessed	Not assessed	у	n	у
Indian summer monsoon collapse	> 5 > 5 3 - 5	5 16 5 5	<ul> <li>(Yedoma) triggers biochemical</li> <li>decomposition of the organic matter,</li> <li>which generates heat that further increases</li> <li>warming and melting.</li> <li>Monsoon dynamics depend on heat and</li> <li>pressure differences between land and</li> <li>ocean. Black carbon and aerosol emissions</li> <li>on land reduce land-absorbed solar</li> <li>radiation and the resulting lower warming</li> <li>of the land compared to the ocean weakens</li> </ul>	1	4	Not assessed	Not assessed	у	n	у
Indian summer monsoon collapse	> 5 > 5 3 - 5	5	<ul> <li>(Yedoma) triggers biochemical</li> <li>decomposition of the organic matter,</li> <li>which generates heat that further increases</li> <li>warming and melting.</li> <li>Monsoon dynamics depend on heat and</li> <li>pressure differences between land and</li> <li>ocean. Black carbon and aerosol emissions</li> <li>on land reduce land-absorbed solar</li> <li>radiation and the resulting lower warming</li> <li>of the land compared to the ocean weakens</li> <li>the monsoon to its eventual collapse. On</li> </ul>	1	4	Not assessed	Not assessed	у	n	у
Indian summer monsoon collapse	>5 >5 3-5	5	<ul> <li>(Yedoma) triggers biochemical</li> <li>(Yedoma) triggers biochemical</li> <li>decomposition of the organic matter,</li> <li>which generates heat that further increases</li> <li>warming and melting.</li> <li>Monsoon dynamics depend on heat and</li> <li>pressure differences between land and</li> <li>ocean. Black carbon and aerosol emissions</li> <li>on land reduce land-absorbed solar</li> <li>radiation and the resulting lower warming</li> <li>of the land compared to the ocean weakens</li> <li>the monsoon to its eventual collapse. On</li> <li>the contrary, increased warming over land</li> </ul>	1	4	Not assessed	Not assessed	y	n	У
Indian summer monsoon collapse	>5 >5 3-5	5	<ul> <li>(Yedoma) triggers biochemical decomposition of the organic matter, which generates heat that further increases warming and melting.</li> <li>Monsoon dynamics depend on heat and pressure differences between land and ocean. Black carbon and aerosol emissions on land reduce land-absorbed solar radiation and the resulting lower warming of the land compared to the ocean weakens the monsoon to its eventual collapse. On the contrary, increased warming over land due to GHG emissions generally</li> </ul>	1	4	Not assessed	Not assessed	y	n	У
Indian summer monsoon collapse	>5 >5 3-5	5	(Yedoma) triggers biochemical decomposition of the organic matter, which generates heat that further increases warming and melting. Monsoon dynamics depend on heat and pressure differences between land and ocean. Black carbon and aerosol emissions on land reduce land-absorbed solar radiation and the resulting lower warming of the land compared to the ocean weakens the monsoon to its eventual collapse. On the contrary, increased warming over land due to GHG emissions generally strengthens the monsoon. Increasing	1	4	Not assessed	Not assessed	у	n	У
Indian summer monsoon collapse	>5 >5 3-5	5	<ul> <li>(Yedoma) triggers biochemical decomposition of the organic matter, which generates heat that further increases warming and melting.</li> <li>Monsoon dynamics depend on heat and pressure differences between land and ocean. Black carbon and aerosol emissions on land reduce land-absorbed solar radiation and the resulting lower warming of the land compared to the ocean weakens the monsoon to its eventual collapse. On the contrary, increased warming over land due to GHG emissions generally strengthens the monsoon. Increasing global average temperature influences the</li> </ul>	1	4	Not assessed	Not assessed	У	n	У
Indian summer monsoon collapse	>5 >5 3-5	5	<ul> <li>(Yedoma) triggers biochemical decomposition of the organic matter, which generates heat that further increases warming and melting.</li> <li>Monsoon dynamics depend on heat and pressure differences between land and ocean. Black carbon and aerosol emissions on land reduce land-absorbed solar radiation and the resulting lower warming of the land compared to the ocean weakens the monsoon to its eventual collapse. On the contrary, increased warming over land due to GHG emissions generally strengthens the monsoon. Increasing global average temperature influences the monsoon but does not lead to its</li> </ul>	1	4	Not assessed	Not assessed	у	n	У
Indian summer monsoon collapse	>5	5	(Yedoma) triggers biochemical decomposition of the organic matter, which generates heat that further increases warming and melting. Monsoon dynamics depend on heat and pressure differences between land and ocean. Black carbon and aerosol emissions on land reduce land-absorbed solar radiation and the resulting lower warming of the land compared to the ocean weakens the monsoon to its eventual collapse. On the contrary, increased warming over land due to GHG emissions generally strengthens the monsoon. Increasing global average temperature influences the monsoon but does not lead to its collapse <sup>19</sup> .	1	4	Not assessed	Not assessed	у	n	У
Indian summer monsoon collapse Tundra loss	> 5 > 5 3 - 5 7.2	5 16 5 18	<ul> <li>(Yedoma) triggers biochemical decomposition of the organic matter, which generates heat that further increases warming and melting.</li> <li>Monsoon dynamics depend on heat and pressure differences between land and ocean. Black carbon and aerosol emissions on land reduce land-absorbed solar radiation and the resulting lower warming of the land compared to the ocean weakens the monsoon to its eventual collapse. On the contrary, increased warming over land due to GHG emissions generally strengthens the monsoon. Increasing global average temperature influences the monsoon but does not lead to its collapse<sup>19</sup>.</li> <li>Warmer temperatures enable northward</li> </ul>	1	4	Not assessed	Not assessed	y	n y	y
Indian summer monsoon collapse	> 5 > 5 3 - 5 7.2	5	<ul> <li>(Yedoma) triggers biochemical decomposition of the organic matter, which generates heat that further increases warming and melting.</li> <li>Monsoon dynamics depend on heat and pressure differences between land and ocean. Black carbon and aerosol emissions on land reduce land-absorbed solar radiation and the resulting lower warming of the land compared to the ocean weakens the monsoon to its eventual collapse. On the contrary, increased warming over land due to GHG emissions generally strengthens the monsoon. Increasing global average temperature influences the monsoon but does not lead to its collapse<sup>19</sup>.</li> <li>Warmer temperatures enable northward expansion of boreal forest in replacement</li> </ul>	1	4	Not assessed Not assessed	Not assessed	y y	n y	y n

			snow-albedo feedback where the darker surface covered with trees reduces snow albedo and amplifies warming.							
Marine methane hydrates release	-	-	Warmer ocean temperatures could melt the large amount of frozen methane hydrates and the gas bubbles they trap beneath sediments in the ocean floor, which would then be released in the atmosphere causing further warming <sup>3</sup> .	1000 - 100,000	4	Not assessed	Not assessed	У	у	n
Ocean anoxia	-	-	Warmer ocean temperatures decrease ventilation of deep water and solubility of $O_2$ in surface water leading to widespread oceanic anoxic conditions. Low oxygen levels in the ocean increment the nitrous oxide emissions <sup>22</sup> and may have other consequences that could reduce ocean's $CO_2$ absorption capacity <sup>23</sup> .	10,000	4	Not assessed	Not assessed	у	у	n
Arctic ozone loss	-	-	"Global warming implies global cooling of the stratosphere that supports formation of ice clouds, which in turn provide a catalyst for stratospheric ozone destruction" <sup>24</sup>	1	4	Not assessed	Not assessed	un	у	n
Antarctic bottom water formation collapse	-	-	Increased precipitations at high latitudes resulting from global warming cause surface water freshening around Antarctica, which suppresses ocean convection and so bottom water formation <sup>25</sup>	≈ 100	4	Not assessed	Not assessed	un	у	n
Alpine glaciers loss (AG)	2 1-3	26 5	Increased temperatures cause reduction in snow and ice cover, originating a positive ice-albedo feedback, and prolongation of the melting season, which destabilizes the glacier mass balance towards glacier thinning and disintegration <sup>26</sup>	100	26	Not assessed	Not assessed	у	у	у
Coral reefs deterioration (CR)	$\frac{450 - 500 \text{ ppm}}{[CO_2]_{atm}}$ $1 - 3$ $1.25 - 2^k$	27 5 29	Increased sea temperature due to global warming results in coral bleaching (breakdown of symbiosis between corals and the algae that live inside their tissues) and mortality. Moreover, increased atmospheric $CO_2$ concentration means higher uptake by oceans, where $CO_2$ reacts to form carbonic acid, which reduces the availability of carbonate ions and the rate of calcification of corals ultimately favoring erosion. Both processes trigger multiple ecological feedback loops that eventually drive reefs to a non-coral dominated state <sup>27</sup>	few years to decades (<100)	28	Not assessed	Not assessed	У	у	У

East Antarctic ice sheet collapse	>5	16, 5	Same dynamics as AI	200 - 800	30	Not assessed	Not assessed	un	у	у
Arctic winter sea ice loss (AW)	4.5, 5.2, 6.2, 7.4, 8.2 <sup>g</sup> >5	18	Besides ice-albedo feedback (see Arctic summer sea ice) also reduced ice thickness creates a positive feedback that leads to complete ice loss.	10	18	Not assessed	Not assessed	У	у	у
North Atlantic subpolar gyre convection collapse (SG)	1.1, 1.4, 1.6, 1.7, 1.9, 2.0, 3.8 <sup>1</sup>	21	Warming and freshening of the North Atlantic subpolar gyre (an area of cyclonic ocean circulation in the Northwest Atlantic) leads to stratification (as consequence of lower surface density), that weakens the local deep convection, which in turn amplifies the stratification (because of reduced inflow of saltier water from the surroundings), eventually leading to permanent convection collapse. This collapse involves only the subpolar gyre (which is part of the TC) and not the whole North Atlantic TC.	10	18 21	Not assessed	Not assessed	у	у	у
West tropical Indian oceanic bloom	10.9	18	"This event features an increase in equatorial upwelling, which is due to a general increase in oceanic velocity and divergence at the equator associated with enhanced wind stress at the surface linked to changes in monsoon regime. As a consequence of this increased divergence in the equatorial area, the upwelling increases, bringing a large amount of nutrients to the surface that are then advected toward the coast of Somalia, where the bloom is maximal" <sup>18</sup> .	~ 10	18	Not assessed	Not assessed	n	un	n
Abrupt sea ice increase in Southern Ocean	1.6	18	Warming causes deep ocean convection to stop in the Indian sector of the Southern Ocean, which enables the formation of a fresh surface layer and hence of sea ice.	≈ 10	18	Not assessed	Not assessed	n	у	n
Abrupt Tibetan snow melt	1.4 - 2.2	18	Rising temperature "drives the system into a regime where the annual mass flux balance becomes negative and snow becomes a seasonal phenomenon" leading to a sudden loss of snow <sup>18</sup> .	≈ 10	18	Not assessed	Not assessed	n	у	у

<sup>a</sup> Estimates are given as either intervals or single data points.

<sup>b</sup> Time required for the full effect to unfold.

4 5 6 7 8 9 10 11 <sup>c</sup> Data from Lenton et al.<sup>4</sup> has been converted from 1980-1999 to 1850-1900 (pre-industrial) reference period by adding the average temperature change difference (0.7°C) between 1850-1900 and 1986-2005 periods found in the literature<sup>14,31</sup> (Berkeley Earth global land and ocean data), assuming that the mean of 1980-1999 and 1986-2005 periods are not significantly different.

<sup>d</sup> Projections do not refer to the range of global warming after which every Arctic summer will be ice free, but they represent the range of warming after which there is 30% (under 1.5°C) to 100% (under 2°C)

probability of occurrence of at least an ice free summer by 2100. For example, at 2 degrees there is 100% probability that an ice-free summer will occur before 2100, but it is not a yearly recurring event. Thus, the

value does not indicate whether a shift to a different state (an ice-free state) has occurred.

<sup>e</sup> Best estimate in brackets.

- <sup>f</sup> Above 4°C it is more likely than not that the AI will collapse. <sup>g</sup> Separate values obtained from different climate models under RCP8.5 assumptions. <sup>h</sup> Thresholds above which around 20, 70 and 80% of dieback is inevitable, respectively.
  - <sup>i</sup> Separate values obtained with the same model under different RCP assumptions.
  - <sup>j</sup> Probability of TC collapse increases from 11% at 6°C warming to 30% at 8°C warming.
  - <sup>k</sup> Range at which more than 90% of reef cells are at risk of long-term degradation depending on the thermal tolerance of coral reefs.
  - <sup>1</sup> Separate values obtained from different climate models and emission scenario

*Arctic summer sea ice loss*: Future loss of Arctic summer sea ice has been extensively studied in the literature (see for instance references <sup>32,33,34</sup>). Some authors argue that abrupt transition to summer ice-free conditions is not likely based on the fact that the loss is in principle reversible<sup>35,36</sup>. Others affirm that irreversibility is not a prerequisite for being a tipping point and consider Arctic summer sea ice loss as one of the first tipping points to be triggered as global temperature increases<sup>3,37,38</sup>. Despite this uncertainty, Arctic summer sea ice is conservatively assumed to be a tipping point in this study.

*West Antarctic ice sheet collapse*: Initial estimations place a potential threshold for AI collapse at around 4°C warming or above. However, more recent studies highlight that AI might have already started tipping<sup>39,40</sup> even though no clear threshold range is indicated. Based on this, recent review studies expanded the range with a potential threshold already at  $1^{\circ}C^{5,16}$ . All three criteria are met for this tipping element.

*Permafrost loss*: Initial projections of permafrost melt did not show evidence of a critical threshold, however recent work has suggested that at least one large area of permafrost could exhibit coherent threshold behavior<sup>41–43</sup>. Based on this, criterion 1 is met.

*Indian summer monsoon collapse*: Increasing global average temperature influences the monsoon but does not lead to its collapse<sup>19</sup>, therefore the second criterion is not met.

*Tundra loss*: According to Lenton et al.<sup>4</sup> tundra loss is not considered a tipping point because "the transition from tundra to boreal forest is a continuous process without strong non-linearity or threshold behavior". However, a more recent study finds abrupt loss of tundra (in terms of roughly 70% boreal forest northward expansion in 100 years) at 7.2°C above pre-industrial, despite it is acknowledged that tundra loss is a gradual transition<sup>18</sup>. Also Scheffer et al.<sup>44</sup> support the fact that "climate change may invoke massive nonlinear shifts in boreal biomes" including tundra loss. Despite the contrasting findings, it is

conservatively decided that tundra loss does exhibit threshold behavior and thus meets the first criterion. Threshold estimations in terms of global temperature change above pre-industrial levels were found to be limited to the single value reported by ref. <sup>18</sup>, with no information about uncertainty. Due to this lack of uncertainty estimations, criterion three is not met.

*Marine methane hydrates release*: The release of methane via gas hydrate degradation is considered a 'slow' tipping point leading to a long-term chronic release of methane on timescales of millennia and longer<sup>45</sup>. Due the length of the transition, this potential tipping point does not meet the definition of ref. <sup>4</sup> because it is unlikely that qualitative changes in this Earth system will occur within this millennium. Despite this, critical thresholds have been proposed suggesting that there is potential for threshold behavior<sup>45</sup>, thus meeting the first selection criterion. However, estimations are only based on local parameters such as ocean temperature increase, thus criterion no. 3 is not met. In addition, it is uncertain whether the released methane will actually reach the atmosphere in such amounts as to significantly influence global GHGs concentration. Many biogeochemical sinks and physical processes could prevent much of the gas from reaching the sea-air interface and being injected into the atmosphere<sup>46</sup>, with implications on quantification of effects on the global climate system.

*Ocean anoxia*: Whether ocean anoxia represents an actual tipping point is still debated. While some believe that anoxia events can lead to major regime shifts in relatively rapid time<sup>47</sup>, others claim that a shift to anoxic state requires too long periods (around 10000 years) for being considered a tipping point<sup>4</sup>. Ocean anoxia is not considered an immediate climate change concern, however it is not excluded that human-induced warming could increase nutrient weathering rates, which could cause ocean anoxia (past ocean anoxia events are thought to be caused by global warming)<sup>48</sup>. Even if considering the phenomenon as a tipping point, criterion three is not met due to lack of threshold estimations.

*Arctic ozone loss*: It is currently unclear whether a tipping point exists for Arctic ozone<sup>24,26</sup>. Feedback mechanisms on the climate system due to a large-scale depletion of Arctic ozone are also poorly described in the reviewed literature. According to Baldwin et al.<sup>49</sup>, there are interactions between the climate and the state of the ozone layer, e.g. as ozone is a greenhouse gas, its depletion could cause cooling of the lower stratosphere. Overall, there is lack of evidence supporting that Arctic ozone loss is a tipping element and no threshold estimations are reported (criterion 1 and 2 not met).

*Antarctic bottom water formation collapse*: There is evidence that bottom water formation decreases under climate change scenario simulations<sup>25,50–52</sup>, however it is still not clear whether the phenomenon has threshold behavior. As no threshold estimations were found, this potential tipping element does not meet criterion 3.

*Alpine glaciers loss*: Different model simulations of Alpine glacier extent demonstrate that an increase in global mean air temperature of 2°C leads to an almost complete loss of glaciers in the Alps<sup>53–55</sup>. Thus, Alpine glacier loss is selected as tipping element in our study.

*Coral reefs deterioration*: There is agreement that rapid climate change and ocean acidification could lead coral to the functional collapse of coral reefs<sup>16,27–29,56</sup>. Despite this, some argue that it is still unclear whether there is a large-scale tipping point<sup>41</sup>. Due to this uncertainty, coral reefs deterioration is conservatively assumed to be a tipping element.
*East Antarctic ice sheet collapse*: Not enough evidence was found to conclude that the collapse of East Antarctic ice sheet could show threshold behavior. More research is needed to understand and quantify the potential as a major tipping element in the Earth's climate system<sup>57</sup>.

*Arctic winter sea ice loss*: According to Kopp et al.<sup>58</sup>, "the evidence that winter Arctic sea ice is a tipping element is stronger than for summer Arctic sea ice" and other authors found abrupt year-round ice loss in their simulations<sup>18</sup> (meeting criterion 1).

*North Atlantic Subpolar Gyre convection collapse*: Some models forecast a collapse of the SG, where the deep convection in the Labrador sea shuts off in response to climatic conditions<sup>59–61</sup>. In addition, two recent studies have identified the potential existence of a tipping point for the collapse of the SG<sup>18,21</sup>. All three criteria are met for this element.

*West tropical Indian oceanic bloom; Abrupt sea ice increase in Southern Ocean; Abrupt Tibetan snow melt*: these potential abrupt events are described by only one of the reviewed studies<sup>18</sup>, hence the first selection criterion is not met. In addition, no uncertainty of threshold estimations are found for the first two candidates.

Selected tipping Temperature threshold range <sup>†</sup> element (global mean temperature above		Occurrence		
	pre-industrial level in °C)	RCP4.5	RCP6	RCP8.5
Arctic summer sea ice loss (AS)	1.5 – 2.6	Expected	Expected	Expected
Greenland ice sheet melt (GI)	1.6 - 3.5	Potential	Expected	Expected
West Antarctic ice sheet collapse (AI)	1.9 – 4.8	Potential	Potential	Expected

**Table S2:** Overview of selected tipping elements with relative temperature threshold intervals and their occurrence under the chosen RCP pathways.

Amazon rainforest dieback (AF)	2.8-5.0	Potential	Potential	Expected
Boreal forest dieback (BF)	3.4 – 5.4	Not expected	Potential	Expected
El Niño-Southern Oscillation change in amplitude (EN)	3.4 - 5.9	Not expected	Potential	Expected
Permafrost loss (P)	$5 - 8.5^{\ddagger}$	Not expected	Not expected	Expected
Arctic winter sea ice loss (AW)	4.8 - 8.2	Not expected	Not expected	Expected
Atlantic thermohaline circulation shutoff (TC)	3.1 - 4.6	Not expected	Potential	Expected
North Atlantic subpolar gyre convection collapse (SG)	1.2 <sup>§</sup> - 3.8	Potential	Expected	Expected
Sahara/Sahel and West African monsoon shift (AM)	2.9 – 4.4	Potential	Potential	Expected
Alpine glaciers loss (AG)	$1.2^{\$} - 3.0$	Expected	Expected	Expected
Coral reefs deterioration (CR)	1.2 <sup>§</sup> -2.5	Expected	Expected	Expected

<sup>†</sup> Assigned by taking the mean of the lower and upper bounds of available intervals following the approach in ref. <sup>62</sup>, if not differently specified.

<sup>§</sup> Literature data reports lower bounds (see Table S1), however 1.2°C was chosen arbitrarily to exclude the possibility that a tipping has already been crossed.

<sup>‡</sup> As no specific upper bound is found (see Table S1), 8.5°C was chosen because it corresponds to the maximum temperature possibly reachable under the selected RCP pathways within year 2500.

### S1.2 Calculation of the *impact of the emission*, $I_{\text{emission},i,j}(T_{\text{emission}})$

Recall, that the *impact of the emission* for a chosen tipping point is calculated following the approach in ref. <sup>63</sup>, and is renamed to the absolute climate tipping potential of gas *i* integrated between the emission year  $T_{\text{emission}}$  and the year of tipping  $T_{\text{tipping},j}$ (*ACTP*<sub>*i*,*j*</sub>( $T_{\text{emission}}$ )) divided by the radiative efficiency of 1 ppm CO<sub>2</sub> ( $RE_{\text{CO}_2}$ ):

$$I_{\text{emission},i,j}(T_{\text{emission}}) = \frac{ACTP_{i,j}(T_{\text{emission}})}{RE_{\text{CO}_2}} = \frac{\sum_{k=1}^{n} RF_i(T_{k-1}) \cdot \Delta T}{RE_{\text{CO}_2}}$$
(S1)

Where *j* indicates the *j*th tipping point occurring after the emission year and  $RF_i$  is the radiative forcing of gas *i*. The radiative forcing is usually expressed (as a function of

continuous time t) as the product of the radiative efficiency of gas i ( $A_i$ ) and the impulse response function (*IRF*), which for most non-CO<sub>2</sub> GHGs is represented with a single exponential decay (eq. S2) and for CO<sub>2</sub> with a sum of l exponentials (eq. S3)<sup>64</sup>:

$$RF_i(t) = A_i \cdot IRF_i(t) = A_i \left[ e^{-\frac{t}{\tau_i}} \right]$$
(S2)

$$RF_{CO_2}(t) = A_{CO_2} \cdot IRF_{CO_2}(t) = A_{CO_2} \left[ a_0 + \sum_l a_l e^{-\frac{t}{\tau_l}} \right]$$
(S3)

The *IRF* describes the decay with continuous (and relative) time *t* of a perturbation in atmospheric concentration of gas *i* after a pulse emission considering how quick the substance is removed from the atmosphere. A summary of the different terms and parameters for calculation of the *impact of the emission* is found in Tables S3, S4 and S5.

Radiative forcing function which was expressed as Riemann sum in eq. S1, can also be solved analytically (eq. S4 for a non-CO<sub>2</sub> gas *i* and eq. S5 for CO<sub>2</sub>):

$$I_{\text{emission},i,j}(T_{\text{emission}}) = \frac{A_i \tau_i \left[1 - e^{-\frac{(T_{\text{tipping},j} - T_{\text{emission}})}{\tau_i}}\right]}{RE_{\text{CO}_2}}$$
(S4)  
$$I_{\text{emission},\text{CO}_2,j}(T_{\text{emission}}) = \frac{A_{\text{CO}_2} \left[a_0(T_{\text{tipping},j} - T_{\text{emission}}) + \sum_l a_l \tau_l (1 - e^{-\frac{(T_{\text{tipping},j} - T_{\text{emission}})}{\tau_l}}\right]}{RE_{\text{CO}_2}}$$
(S5)

As can be seen, for gas *i* the *impact of the emissions* occurring at different times is different as it depends on the distance between the emission year and the year of tipping.

Parameter Definition Name Unit Note Impact of the Time-integrated  $I_{\text{emission},i,j}(T_{\text{emission}})$ ppm emission of gas i CO2e · change in atmospheric  $yr \cdot kg_i^{-1}$ emitted at CO<sub>2</sub>-equivalent  $T_{\rm emission}$  for the concentration due to a pulse emission of gas *i*th tipping point *i* from  $T_{\text{emission}}$  to T<sub>tipping,j</sub>  $W \cdot m^{-2} \cdot$ Time-integrated  $ACTP_{i,i}(T_{emission})$ Absolute Climate Tipping  $yr \cdot kg_i^{-1}$ radiative forcing due Potential of gas i to a pulse emission of gas *i* from  $T_{\text{emission}}$  to T<sub>tipping, i</sub> Index for the An index taking j \_ \_ numerical values was sequence of occurring tipping points in a preferred rather than a given iteration qualifier for the subscript *j*, because the order of occurrence of tipping points can be different in different simulations Emission year Any year starting See Table S7 Temission vr (*interval* time) from 2021 in which an emission can occur. T<sub>emission</sub> indicates a specific time interval of 1 year. See Table S7 Generic time Continuous, point t yr (point in time) time expressed with real numbers Number of time steps Equal to the difference п \_ between the year of tipping  $T_{\text{tipping},j}$  (i.e. the year when the *j*th tipping point is exceeded) and the year of emission, T<sub>emission</sub>.  $W \cdot m^{-2} \cdot$ Radiative forcing Radiative forcing due  $RF_i/CO_2$ to a pulse emission of  $kg_{i/CO_2}^{-1}$ gas *i*/CO<sub>2</sub>  $W \cdot m^{-2}$ Radiative Radiative forcing of 1 Reference value:  $RE_{CO_2}$ 1.31.10<sup>-2</sup> (calculated efficiency per · ppm ppm CO<sub>2</sub> with a ppm CO<sub>2</sub>  $CO_{2}^{-1}$ current background based on ref. 65). concentration of 409<sup>a</sup> ppm

**Table S3:** Overview of terms used in the calculation of  $I_{\text{emission},i,j}(T_{\text{emission}})$ .

IRFi/co <sub>2</sub>	Impulse Response Function	unitless	Fraction of gas <i>i</i> /CO <sub>2</sub> remaining in the atmosphere at time <i>t</i>	
			after a pulse emission	
$A_{i/\text{CO}_2}$	Radiative efficiency of gas	$W \cdot m^{-2} \cdot$	Radiative forcing per unit mass increase in	See Table S4.
	i/CO <sub>2</sub>	kg <i>i</i> / co <sub>2</sub> <sup>-1</sup>	atmospheric	
			abundance of gas $i/CO_2$	
τι	Atmospheric lifetime (or adjustment time)	yr	Time scale characterizing the decay of a pulse emission input into the atmosphere <sup>66</sup>	Different from the lifetime of a gas, as it accounts for the effects of feedbacks resulting from a pulse emission <sup>67</sup> . See Table S4.
$a_l \{l=0,1,2,3\}$	-	unitless	Weight of each exponential	See Table S5.
$[\tau_l \\ \{l=1,2,3\}$	-	yr	Decay times of each exponential	See Table S5.
l	-	-	Number of exponentials	Up to 4

<sup>a</sup> Annual average of CO<sub>2</sub> in situ air measurements (February 2018 - January 2019) from Mauna Loa Observatory, Hawaii<sup>68</sup>.

**Table S4:** Radiative efficiency  $(A_i)$  and atmospheric lifetime  $(\tau_i)$  for CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub>O<sup>66</sup>.  $A_i$  values are converted from W · m<sup>-2</sup> · ppbv<sub>i</sub><sup>-1</sup> to W · m<sup>-2</sup> · kg<sub>i</sub><sup>-1</sup> using previous methods<sup>64</sup>.

	$A_i (\mathbf{W} \cdot \mathbf{m}^{-2} \cdot \mathbf{kg}_i)$	$\tau_i (\mathbf{yr})$
CO <sub>2</sub>	1.67E-15 <sup>a</sup>	-
CH <sub>4</sub>	1.82E-13 <sup>b</sup>	12
N <sub>2</sub> O	3.87E-13	114

<sup>a</sup> Obtained using the updated radiative efficiency per ppm of CO<sub>2</sub> ( $RE_{CO_2}$ ) presented in Table S3 (1.31·10<sup>-2</sup> W m<sup>-2</sup>· ppm CO<sub>2</sub><sup>-1</sup>).

<sup>b</sup> The calculation includes multiplication by a factor 1.4 to account for indirect radiative effects of methane emissions<sup>66</sup>.

Table S5: Constant parameter values for calculation of radiative forcing of CO<sub>2</sub> from ref.<sup>69</sup>.

Parameter	1 <sup>st</sup> term ( <i>l</i> =0)	2 <sup>nd</sup> term ( <i>l</i> =1)	3 <sup>rd</sup> term ( <i>l</i> =2)	4 <sup>th</sup> term ( <i>l</i> =3)
$a_l$ (unitless)	2.123E-01 (a <sub>0</sub> )	2.444E-01	3.360E-01	2.073E-01
$\tau_l$ (yr)	-	3.364E+02	2.789E+01	4.055E+00

#### S1.3 Calculation of capacity, $CAP_i(T_{\text{emission}})$

Recall, that the  $CAP_i(T_{\text{emission}})$  (ppm CO<sub>2</sub>e · yr) is given:

$$CAP_{j}(T_{\text{emission}}) = C(T_{\text{tipping},j}) \cdot (T_{\text{tipping},j} - T_{\text{emission}}) - \sum_{k=1}^{n} [C(T_{k-1}) + C_{\text{tip}}(T_{k-1})] \cdot \Delta T$$
(S6)

where,  $C(T_{\text{tipping},j})$  is the atmospheric CO<sub>2</sub>-equivalent concentration at the year of tipping  $T_{\text{tipping},j}$ , C(T) is the CO<sub>2</sub>-equivalent concentration from background emissions at time T and  $C_{\text{tip}}(T)$  is the change in CO<sub>2</sub>-equivalent concentration at time T caused by all tipping points occurred before  $T_{\text{emission}}$  (all terms expressed in ppm CO<sub>2</sub>e). Determination of  $C(T_{\text{tipping},j})$  and C(T) depends on the background development of GHG emissions as predicted by the RCP pathways. Differences in the relationship between projected GHGs concentration and the corresponding equilibrium temperature between the pathways (Figure S1) results in different remaining capacity to the same tipping point when calculated with the three RCPs.



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**Figure S1:** Relationship between projected GHGs concentration and temperature change in the chosen RCP pathways.

#### S1.3.1 Calculation of effects from tipping, $C_{tip}(T)$

 $C_{\text{tip}}(T_{\text{effect}})$  is defined as the sum of the change in CO<sub>2</sub>-equivalent concentration caused by all tipping points occurred before the emission year  $T_{\text{emission}}$ .  $T_{\text{effect}}$  is used here (rather than generic year *T*) to represent the year in which effects caused by all these tipping points unfold. The resulting overall effect from tipping is therefore expressed as a sum of effects of each tipping element (eq S7):

$$C_{\rm tip}(T_{\rm effect}) = \sum_{a} C_{\rm tip,a}(T_{\rm effect})$$
(S7)

where *a* indicates a concrete tipping element that passed its tipping point before  $T_{\text{emission}}$ , and  $C_{\text{tip},a}$  is the CO<sub>2</sub>-equivalent concentration increase caused by crossing the tipping point of the tipping element *a*. Here we use subscript *a* indicating a specific tipping element (e.g. *a* = Arctic summer sea ice loss), rather than subscript *j* because the effect from tipping depends on the tipping element being crossed and not on its order of occurrence.

For Arctic summer and winter sea ice loss (AS and AW), the effect from tipping is calculated based on the RF change due to reduced sea ice albedo (Table S6), which is then converted to annual concentration increase using the radiative efficiency of CO<sub>2</sub> per 1 ppm (found in Table S3). This effect is assumed to unfold completely from the year after tipping and to remain constant over the years, as the evolution of radiative forcing changes after tipping is unknown. Thus, at any year after tipping ( $T_{effect}$ ),  $C_{tip,AS}$  and  $C_{tip,AW}$  are found to be 22.2 and 52.0 ppm CO<sub>2</sub>e (Figure S2). For Greenland ice sheet melt (GI), West Antarctic ice sheet collapse (AI), El Niño-Southern Oscillation change in amplitude (EN), Permafrost loss (P), Amazon (AF) and Boreal forest (BF) tipping points, a dynamic (i.e. changing over time) effect (in terms of equivalent GHG concentration increase) was calculated by adapting the method used in Levasseur et al.<sup>70</sup>. Estimates of carbon emissions that could be released after tipping (shown in Table S6) were used to calculate the dynamic effects, considering that all emitted carbon is in the form of CO<sub>2</sub>, except for emissions from permafrost thawing or flooding, which are in the form of methane (CH<sub>4</sub>). Considering the residence time of CO<sub>2</sub> and methane in the atmosphere, the instantaneous value of the dynamic characterization factor (expressed as time-integrated increase in CO<sub>2</sub>-equivalent concentration) of a pulse emission at any year *T* after the emission was calculated as:

$$DCF_{\text{inst},i}(T) = \int_{t_{\text{ini}}-1}^{t_{\text{ini}}} \Delta C_i \cdot IRF_i(t) \cdot \frac{RE_i}{RE_{\text{CO}_2}} dt \text{ for } T = 1,2,3,...$$
(S8)

where  $DCF_{\text{inst},i}(T)$  is the instantaneous dynamic characterization factor of gas *i* computed for *intervals* of 1-year length (i.e. T = year 1, year 2, etc.), where the relative time interval *T* is defined within  $T = [t_{\text{ini}}, t_{\text{end}}]$ , and where time *t* is relative and continuous. The  $\Delta C_i$  (ppm<sub>i</sub> · kg<sub>i</sub><sup>-1</sup>) is the change in atmospheric GHG concentration due to a unit emission of gas *i*;  $IRF_i(t)$  is the impulse response function of gas *i* representing the decay of the gas after a pulse emission (defined as in eq. S2, for non-CO<sub>2</sub> gasses, and eq. S3, for CO<sub>2</sub>);  $RE_i$  is the radiative efficiency per ppm of gas *i* (0.37 W · m<sup>-2</sup> · ppm<sup>-1</sup> for methane<sup>71</sup>) and  $RE_{CO_2}$  is the radiative efficiency per ppm CO<sub>2</sub> (see Table S3). Note that  $DCF_{\text{inst},i}$  is expressed as time-integrated increase in CO<sub>2</sub>-equivalent concentration (ppm CO<sub>2</sub>e · yr · kg<sub>i</sub><sup>-1</sup>) and thus it deviates from the *DCF* expressed as time-integrated radiative forcing increase (W · m<sup>-2</sup> · yr · kg<sub>i</sub><sup>-1</sup>) calculated in Levasseur et al.<sup>70</sup>. The  $\Delta C_i$  was calculated as:

$$\Delta C_i = \frac{1 \cdot 10^6 / M_i}{m_{\text{air}} / M_{\text{air}}} \cdot 1 \cdot 10^3 \tag{S9}$$

Where  $M_i$  is the molar mass of gas i (16 and 44 g · mol<sup>-1</sup> for CH<sub>4</sub> and CO<sub>2</sub> respectively);  $m_{air}$  (5.14·10<sup>21</sup> g) and  $M_{air}$  (28.9 g · mol<sup>-1</sup>) are the total mass and the molar mass of air in the atmosphere respectively<sup>71</sup>, 1·10<sup>6</sup> (ppm) and 1·10<sup>3</sup> (g · kg<sup>-1</sup>) are conversion factors. The instantaneous dynamic characterization factor represents the annual value of the characterization factor of a pulse emission, where the pulse emission is the annual amount of CO<sub>2</sub> or methane emissions caused by crossing a tipping point. By combining the instantaneous dynamic characterization factor of one annual release with the evolution of this annual release over the years, the dynamic effect at year  $T_{effect}$  was obtained:

$$C_{\text{tip},a}(T_{\text{effect}}) = \sum_{i} \sum_{T=T_a+1}^{T_{\text{effect}}} e_i(T) \cdot DCF_{\text{inst},i}(T_{\text{effect}} - T)$$
(S10)

Where  $T_a$  is the year of tipping of the element *a*,  $e_i(T)$  (kg<sub>i</sub> · yr<sup>-1</sup>) is the annual release of gas *i* (either CO<sub>2</sub> or methane depending on the tipping point) at year *T*, i.e. at any year before the year of calculation of the dynamic effect ( $T_{effect}$ ) since the year following the tipping ( $T_a + 1$ ). The  $e_i(T)$  is determined by equally subdividing the estimated total carbon release after tipping (shown in Table S6) over the transition period of the tipping event (i.e. time required for the full effect to unfold found in Table S1). In this way, the time evolution of the annual release is assumed to be constant, meaning that the same amount of emissions is released every year over the transition period. In the case of GI, AI and Amazon forest, the transition period was also considered to calculate for how long this annual release lasts (e.g. for Amazon tipping point annual release ceases after 50 years). For EN the estimated release is basically permanent<sup>10</sup>, while for permafrost and Boreal forest 80 years of release are assumed given that the figures used from ref. <sup>5</sup> refer to emissions from present day to 2100 ( $\approx$  80 years)<sup>5</sup>.

At any year after tipping ( $T_{effect}$ ), the dynamic effect calculated through eq. S10 is the result of the emissions released at year  $T_{effect}$  and the non-decayed fraction of emissions that occurred in all previous years (*T*) since the year of tipping. The result provides the cumulative increase in CO<sub>2</sub>-equivalent concentration at time  $T_{effect}$  caused by every discrete annual release occurred since the year after the tipping event until  $T_{effect}$ . Dynamic and constant (for Arctic summer and winter sea ice loss) effects from tipping used in this study are presented in Figure S2.

Selected tipping element	Estimated consequences from tipping		
	Amount	Unit	Definition
Arctic summer sea ice loss (AS)	0.29	$W \cdot m^{-2} \cdot yr^{-1}$	Total annual radiative forcing caused by one month of ice-free conditions, calculated from reduced sea-ice albedo effect <sup>72</sup> . In this study, the effect is assumed to unfold completely the year after tipping and to remain constant over time.
Greenland ice sheet melt (GI)	100	Gt C	Total carbon emissions, released over the transition period (best estimate 1500 years), from flooding of large areas of low-lying permafrost <sup>10</sup> .
West Antarctic ice sheet collapse (AI)	100	Gt C	Total carbon emissions, released over the transition period (best estimate 500 years), from flooding of large areas of low-lying permafrost <sup>10</sup> .
Amazon rainforest dieback (AF)	50	Gt C	Total carbon emissions, released over the transition period (best estimate 50 years), from forest dieback <sup>10</sup> .
Boreal forest dieback (BF)	10-40 (30)	Gt C	Estimated carbon emissions by 2100 <sup>5</sup> . In this study, it is assumed to be the total effect from tipping occurring over a transition period of 80 years.
El Niño-Southern Oscillation change in amplitude (EN)	0.2	Gt C · yr <sup>-1</sup>	Total annual carbon emissions released from anomalous fire events caused by stronger El Niño events. Assumed to be a permanent effect <sup>10</sup> .
Permafrost loss (P)	20-80 (45)	Gt C	Estimated carbon emissions by 2100 <sup>5</sup> . In this study, it is assumed to be the total effect from tipping occurring over transition period of 80 years.
Arctic winter sea ice loss (AW)	0.68	$W \cdot m^{-2} \cdot yr^{-1}$	Total annual radiative forcing caused by year-round ice- free conditions, calculated from reduced sea-ice albedo effect <sup>72</sup> . This effect is assumed to unfold completely the year after tipping and to remain constant over time.

**Table S6**: Best available estimated consequences from tipping found in the literature used to calculate  $C_{\text{tip}}$  for 8 tipping elements (no effect was modelled for the other tipping elements).



**Figure S2**: Temporal evolution of CO<sub>2</sub>-equivalent concentration increase caused by crossing eight of the selected tipping elements as modelled in this study. Uncertainty surrounding these results is undefined and thus not considered. AS = Arctic summer sea ice loss, GI = Greenland ice sheet melt, BF = Boreal forest dieback, EN = El Niño-Southern Oscillation change in amplitude, AW = Arctic winter sea ice loss, P = Permafrost loss, AI = West Antarctic ice sheet collapse, AF = Amazon rainforest dieback.

#### S1.3.2 Notes on tipping elements for which C<sub>tip</sub> was not modelled

Sahara/Sahel and West African monsoon shift (AM): It is uncertain whether AM will shift northward (leading to increased rainfall) or southward (leading to further drying of the Sahel)<sup>3</sup>. In either cases, modelling the consequences of a local change in rainfall on the global climate system remains challenging and no estimate allowing expressing the effect as a change in  $CO_2$ -equivalent concentration was found. Therefore, the effect from crossing this climate tipping point was not modelled.

Atlantic thermohaline circulation shutoff (TC) and North Atlantic Subpolar Gyre convection collapse (SG): The main expected consequences of a potential Atlantic thermohaline circulation shutoff are cooling of the northern hemisphere and warming of the southern hemisphere<sup>21,73,74</sup>. A collapse of the subpolar gyre convection would cause local cooling over the North Atlantic and, to a minor extent, over Western Europe and North American coast<sup>21</sup>. Some studies found that a collapse of both TC and SG would cause a reduction of the global mean temperature, leading to an overall cooling of the planet contrasting the global warming trend<sup>21,75</sup>. However, no clear evidence of the underlying mechanism emerges from the studies and the same authors highlight that the observed cooling might be the result of factors such as the climate sensitivity parameter used in the models<sup>21</sup>. For this reason, no effect from these two tipping points is assumed in our model.

Alpine glaciers loss (AG): Shrinkage of Alpine glaciers and snow cover is expected to have mainly local effects, reducing surface reflectivity and thus leading to amplified temperature increase in the region<sup>26</sup>. However, no estimate allowing expressing the effect as a change in global  $CO_2$ -equivalent concentration was found; therefore the effect from crossing this climate tipping point was not modelled.

*Coral reefs deterioration (CR)*: Deterioration of coral reefs damages local marine habitats and species, causing loss of biodiversity<sup>27</sup>, however it does not have direct or measurable consequences on the climate system, such as temperature increase due to positive feedbacks. Thus, the effect from crossing this climate tipping point was not accounted for.

#### S1.3.3 Atmospheric capacity cutoff

To define a meaningful minimum value for the atmospheric capacity (i.e. the value below which the difference between  $CO_2$ -equivalent concentrations is considered too small), the uncertainty surrounding the calculation of the capacity shall be quantified. The annual variability of atmospheric  $CO_2$  concentrations, based on average in situ air measurements between 1959 – 2018 from Mauna Loa Observatory, Hawaii<sup>68</sup>, was used as a proxy. The

average difference in annual  $CO_2$  concentrations was found to be 5.89 ppm  $CO_2$ , which was rounded to 6 ppm  $CO_2$  because differences in annual measurements were not detected at decimal level. The cutoff was then applied to the difference between the concentration at the year of tipping and the concentration at year *T* when calculating the capacity as in eq. 4 in the main article.

Ideally, the uncertainty of future projections of GHGs concentrations should be used, as the capacity depends mainly on this parameter. However, when calculated from IPCC's temperature projections uncertainties<sup>76</sup>, we found cutoff values between 43 - 70 ppm CO<sub>2</sub> equivalents, depending on the RCP pathway, which are deemed too high and were therefore not used. As a measure of the variability of GHGs concentration within the yearly time step used in the model, CO<sub>2</sub> was taken as a proxy because it is the most abundant anthropogenic greenhouse gas in the atmosphere.

#### S1.4 Consideration of time as a variable

Symbol	Meaning	Where it is used
т	Interval-like time variable indicating generic years that	In eq. 2, 3, 4, S1, S6, S8, S10.
1	can be either <i>absolute</i> or <i>relative</i> .	
	<i>Point-like</i> time variable indicating continuous time that	In the standard definition of RF
	can be either <i>absolute</i> or <i>relative</i> .	(eq. S2, S3) and as integration
t		variable in eq. S8. Used also in
		Figure 1 as <i>absolute</i> variable.
	Interval-like and absolute time variable used to	In all situations where the
	indicate emission years.	dependent variable is a function
T		of the emission year and where
<sup>2</sup> emission		years are intended as time
		intervals (eq. 1-4, S1 and S4-S6).
<i>T.</i>	Interval-like and absolute time variable indicating the	In eq. 3, 4, S4-S6.
<sup>1</sup> tipping, j	year of tipping of the <i>j</i> th expected tipping point.	

Table S7: Summary of the symbols used to indicate the time variable in this paper.

T <sub>effect</sub>	<i>Interval-like</i> and <i>absolute</i> time variable used to indicate the years after crossing tipping points, when <i>effects</i> of tipping unfold.	For calculation of the concentration increase from tipping $C_{tip}$ (eq. S7 and S10).
T <sub>tipping</sub> ,j <sub>last</sub>	Interval-like and absolute time variable indicating the year of tipping of the last $(j_{last})$ expected tipping point across 10,000 Monte Carlo simulations.	As upper bound of the summation sign in eq. 5.
T <sub>a</sub>	<i>Interval-like</i> and <i>absolute</i> time variable indicating the year of tipping of tipping element <i>a</i> (used for calculation of the effect from tipping). Subscript <i>a</i> is used rather than subscript <i>j</i> (as in $T_{\text{tipping},j}$ ), because the effect from tipping depends on the tipping element being crossed and not on its order of occurrence.	Used to define the lower bound of the summation in eq. S10

#### S1.5 Example calculation of MCTP with two tipping points

Figure 1 in the main article illustrates how the MCTP framework can be applied with two tipping points. When considering the first tipping point (j = 1) occurring at year  $T_{\text{tipping,1}}$ , every emission at  $T_{\text{emission}} < T_{\text{tipping,1}}$  (before  $T_{\text{tipping,1}}$ ) takes up a certain part of the atmospheric capacity available before reaching the concentration at the year of tipping  $T_{\text{tipping,1}}$  ( $C(T_{\text{tipping,1}})$ ). However, when considering a second tipping point (j = 2) at year  $T_{\text{tipping,2}}$ , the same emission  $T_{\text{emission}} < T_{\text{tipping,1}}$  will now take up also the capacity left before reaching the concentration at the second year of tipping  $T_{\text{tipping,2}}$  ( $C(T_{\text{tipping,2}})$ ). Therefore, the total MCTP of gas i emitted at year  $T_{\text{emission}} < T_{\text{tipping,1}}$  is given by the sum of the MCTPs for the first and the second tipping point (first and second term in eq. S11 respectively). Assuming, hypothetically,  $T_{\text{tipping,1}} = 2030$ ,  $T_{\text{tipping,2}} = 2043$  and  $T_{\text{emission}} < T_{\text{tipping,1}} = 2025$ :

$$MCTP_{i}(2025) = \frac{I_{\text{emission},i,1}(2025)}{CAP_{1}(2025)} + \frac{I_{\text{emission},i,2}(2025)}{CAP_{2}(2025)} = \frac{\left\{\frac{A_{i}\tau_{i}\left[1-e^{-\frac{(2030-2025)}{\tau_{i}}}\right]}{\frac{RE_{CO_{2}}}{C(2030)\cdot(2030-2025)-\sum_{k=1}^{5}[C(T_{k-1})]\cdot 1} + \frac{\left\{\frac{A_{i}\tau_{i}\left[1-e^{-\frac{(2043-2025)}{\tau_{i}}}\right]}{\frac{RE_{CO_{2}}}{C(2043)\cdot(2043-2025)-\sum_{k=1}^{18}[C(T_{k-1})]\cdot 1}\right\}}{(S11)}$$

where, each term of the sum is the ratio between the *impact of the emission* for either the first or the second tipping point and the corresponding remaining capacity;  $A_i$  is the radiative efficiency of gas  $i [W \cdot m^{-2} \cdot kg_i^{-1}]$ ;  $\tau_i$  is the atmospheric lifetime of gas i [yr] and  $RE_{CO_2}$  is the radiative efficiency per ppm CO<sub>2</sub> [W  $\cdot m^{-2} \cdot ppm CO_2^{-1}$ ]. Note, that the  $C_{tip}(T)$  term is not included in eq. S11 because no tipping point has been crossed yet in this case.

For an emission at  $T_{\text{emission}} > T_{\text{tipping,1}}$  (after  $T_{\text{tipping,1}}$ ), which will also take up part of the capacity left before  $T_{\text{tipping,2}}$ , but has no influence on  $T_{\text{tipping,1}}$ , the total MCTP is given only by the contribution to exceed the second tipping point (assuming  $T_{\text{emission}} > T_{\text{tipping,1}} = 2035$ ):

$$MCTP_{i}(2035) = \frac{I_{\text{emission},i,2}(2035)}{CAP_{2}(2035)} = \frac{\left\{ \underbrace{A_{i}\tau_{i} \left[ 1 - e^{-\frac{(2040 - 2035)}{\tau_{i}}} \right]}_{(2040) \cdot (2040 - 2035) - \sum_{k=1}^{5} \left[ C(T_{k-1}) + C_{\text{tip}}(T_{k-1}) \right] \cdot 1} \right\}}$$
(S12)

Here, the tipping point occurring at  $T_{\text{tipping},1}$  has an effect on the climate system ( $C_{\text{tip}}$ ) that further reduces the remaining capacity up to the following year of tipping and anticipating tipping from 2043 to 2040 (so that  $T_{\text{tipping},2} = 2040$ ). This is also accounted for in the calculation of the capacity.

While for both emissions at  $T_{\text{emission}} < T_{\text{tipping,1}}$  and  $T_{\text{emission}} > T_{\text{tipping,1}}$  the *impact of the emission* depends on the residence time of the gas in the atmosphere and the difference between the emission year and the year of tipping, the capacity varies depending on i) the difference in atmospheric CO<sub>2</sub>-equivalent concentration between the emission year and the year of tipping and ii) on timing of emissions. For emissions at  $T_{\text{emission}} < T_{\text{tipping,1}}$  (eq. S11), the effect from tipping ( $C_{\text{tip}}$ ) is equal to zero as no tipping points have been crossed yet and therefore the total remaining capacity for these

emissions is not affected. On the contrary, for emissions at  $T_{\text{emission}} > T_{\text{tipping,1}}$  (eq. S12), the remaining capacity is influenced by the  $C_{\text{tip}}$  from the crossed level.

#### S1.6 Details of two illustrative simulations

This section gives an overview on occurrence of tipping points in the two illustrative simulations presented in the main article and shows typical trends for *impacts of the emission* and remaining capacities in the calculation of MCTPs (taking as example simulation 1).

	Triggered tipping points (from first to last)	Threshold temperature (°C above pre- industrial)	Concentration at year of tipping (ppm CO <sub>2</sub> e)	Anticipated year of tipping (year)	Year of tipping without C <sub>tip</sub> (year)
Simulation 1	Arctic summer sea ice loss	1.62	484	2042	2042
	West African monsoon shift	1.87	523	2047	2054
	North Atlantic subpolar gyre convection collapse	2.17	576	2060	2065
	West Antarctic ice sheet collapse	2.59	652	2074	2078
	Greenland ice sheet melt	2.95	711	2081	2092
	Amazon rainforest dieback	3.23	755	2089	2107
	Permafrost loss	3.41	784	2095	2119
	Arctic winter sea ice loss	3.42	786	2096	2120
	Atlantic thermohaline circulation shutoff	3.75	814	2103	2165
Simulation 2	Arctic summer sea ice loss	1.95	535	2056	2056
	West African monsoon shift	2.17	576	2060	2065

**Table S8**: Data on tipping points triggered in simulation 1 and simulation 2.

	Greenland ice sheet melt	2.30	600	2065	2069
	North Atlantic subpolar gyre convection collapse	2.40	617	2067	2072
	Arctic winter sea ice loss	2.59	652	2073	2078
	Atlantic thermohaline circulation shutoff	3.34	773	2100	2114
	Permafrost loss	4.02	814	2116	2298



**Figure S3**: (a) *Impact of the emission* of 1 kg  $CO_2$  and (b) remaining atmospheric capacity relative to each of the 9 tipping points triggered in simulation 1. Both *impacts* and remaining capacities decrease over time, but capacities decrease faster than the *impacts*, explaining why MCTPs

increase while approaching a tipping point. AS = Arctic summer sea ice loss, AM = West African monsoon shift, SG = North Atlantic subpolar gyre convection collapse, AI = West Antarctic ice sheet collapse, GI = Greenland ice sheet melt, AF = Amazon rainforest dieback, P = Permafrost loss, AW = Arctic winter sea ice loss, TC = Atlantic thermohaline circulation shutoff.

#### S1.7 Calculation of impact scores for the case study

**Table S9**: Overview of equations used for calculation of impact scores (*IS*) with all metrics used in this study. For all metrics, *i* denotes a specific GHG and  $T_{\text{emission}}$  the emission year. Note that the original notation for the time variable of the GWP-based and GTP CFs was harmonized with the notation used in this paper.

	Impact score calculation	Symbols
MCTP [ppt <sub>rc</sub> /kg plastic]	$IS_{\text{MCTP}} = \sum_{i} \sum_{T_{\text{emission}}=2021}^{T_{\text{tipping}, j_{\text{last}}}} m_i(T_{\text{emission}})$ $\cdot MCTP_i(T_{\text{emission}})$	$T_{\text{tipping},j_{\text{last}}} = \text{year of last}$ tipping point; $m_i(T_{\text{emission}})$ = mass of gas <i>i</i> emitted at year $T_{\text{emission}}$ [kg]; $MCTP_i(T_{\text{emission}}) = \text{MCTP}$ for gas <i>i</i> and emission year $T_{\text{emission}}$ [ppt <sub>rc</sub> · kg <sub>i</sub> <sup>-1</sup> ]
GWP20 [kg CO <sub>2</sub> eq/kg plastic]	$IS_{\rm GWP20} = \sum_{i} M_i \cdot GWP20_i$	$M_i = \text{total mass of gas } i$ emitted in 20 years [kg]; $GWP20_i = \text{GWP20 of gas } i$ [kg CO <sub>2</sub> eq · kg <sub>i</sub> <sup>-1</sup> ]
GWP100 [kg CO <sub>2</sub> eq/kg plastic]	$IS_{\rm GWP100} = \sum_{i} M_i \cdot GWP100_i$	$M_i = \text{total mass of gas } i$ emitted in 100 years [kg]; $GWP100_i = \text{GWP100 of gas}$ $i [kg CO_2 \text{eq} \cdot kg_i^{-1}]$
GWP100 <sub>ILCD</sub> [kg CO <sub>2</sub> eq/kg plastic]	$IS_{\text{GWP100}_{\text{ILCD}}} = \sum_{i} M_{i} \cdot GWP100_{i} - Credit_{i}$ $Credit_{i} = \sum_{T=2}^{100} m_{i}(T) \cdot T \cdot EQ_{i}$	<i>Credit</i> <sub>i</sub> = ILCD credit for carbon storage; $m_i(T) =$ mass of gas <i>i</i> emitted at relative time <i>T</i> ; $EQ_i =$ equivalency factor for gas <i>i</i> (0.01, 0.34 and 0.36 [kg CO <sub>2</sub> eq · kg <sub>i</sub> <sup>-1</sup> · yr <sup>-1</sup> ] for CO <sub>2</sub> ,

		biogenic and fossil CH <sub>4</sub> respectively <sup>77,78</sup> )
Dynamic GWP100 [kg CO <sub>2</sub> eq/kg plastic]	$IS_{\rm dynGWP100} = \frac{GWI_{\rm cum}(100)}{\int_0^{100} A_{\rm CO_2} \cdot C(t)_{\rm CO_2} dt}$ $GWI_{\rm cum}(100) = \sum_{T=0}^{100} GWI_{\rm inst}(T)$ $GWI_{\rm inst}(100) = \sum_i \sum_{T=0}^{100} m_i(T) \cdot DFC_i(100)$ $-T)$ $DFC_i(100) = \int_{t-1}^{100} A_i \cdot C(t)_i dt$	$GWI_{cum}(100) = cumulative$ global warming impact in 100 years [W · m <sup>-2</sup> · yr · kg <sub>i</sub> <sup>-1</sup> ]; $A_{i/CO_2}$ = radiative efficiency per unit mass gas $i/CO_2$ increase [W · m <sup>-2</sup> · kg <sub>i</sub> <sup>-1</sup> ]; $T$ = relative <i>interval</i> time [yr]; $t$ = relative <i>point in time</i> [yr]; $C(t)_{i/CO_2}$ = atmospheric load of gas $i/CO_2$ at time $t$ after emission [kg]; $GWI_{inst}(100)$ = instantaneous global warming impact in 100 years [W · m <sup>-2</sup> · yr · kg <sub>i</sub> <sup>-1</sup> ]; $DFC_i$ = dynamic characterization factor of gas $i$ [W · m <sup>-2</sup> · yr]; (see equations 1-4 in Levasseur et al. <sup>79</sup> )
GTP100 [kg CO <sub>2</sub> eq/kg plastic]	$IS_{\rm GTP100} = \sum_{i} M_i \cdot GTP100_i$	$M_i = \text{total mass of gas } i$ emitted over 100 years [kg]; $GTP100_i = \text{GTP100 of gas } i$ [kg CO <sub>2</sub> eq · kg <sub>i</sub> <sup>-1</sup> ]

## S2. Supplementary results

Sub-section S2.1 contains additional figures comparing average MCTP results for the three major anthropogenic GHGs (carbon dioxide ( $CO_2$ ), methane ( $CH_4$ ) and nitrous oxide ( $N_2O$ )) and without considering the effects from tipping. In sub-section S2.2, we show details on the case study, comparing emission profiles with MCTP values and presenting MCTP impact scores calculated under different RCP pathways.

#### **S2.1 Supplementary MCTP results**



**Figure S4**: Average (geometric mean) multiple climate tipping points potential (MCTP) of  $CO_2$ ,  $CH_4$  and  $N_2O$  at different emission years under RCP6 pathway. Note that results for  $CO_2$  are given for 10 kg rather than 1 kg.



**Figure S5:** Average (geometric mean) multiple climate tipping points potential (MCTP) of 1 kg CO<sub>2</sub> under RCP6 considering effects from crossing tipping points (black solid line) and without considering such effects (green dashed line).



S2.2 Details and supplementary results for the case study

**Figure S6:** CO<sub>2</sub> emission profile for fast, medium and slow degrading plastics under anaerobic conditions (left axis) and multiple climate tipping points potential (MCTP) per unit CO<sub>2</sub> emission (right axis).

**Table S10:** Climate tipping impact scores for different end-of-life degradation scenarios of plastic polymers calculated assuming background concentration pathways RCP4.5, RCP6 and RCP8.5. Ranking between scenarios 1 - 7 is illustrated within each column with different colors. Red shading indicates the highest impact scores and green the lowest impact scores.

End-of-life	MCTP - under	MCTP - under RCP6	MCTP - under
degradation scenario	RCP4.5	(ppt <sub>rc</sub> /kg plastic)	RCP8.5
	(ppt <sub>rc</sub> /kg plastic)		(ppt <sub>rc</sub> /kg plastic)
1. Incineration <sup>a</sup>	0.015	0.014	0.014
Plastic degradation			
rate <sup>b</sup>			
2. Fast <sup>c</sup>	0.12	0.089	0.11
3. Medium <sup>d</sup>	0.22	0.14	0.17
4. Slow <sup>e</sup>	0.25	0.16	0.13
5. Very slow <sup>f</sup>	0.0027	0.0020	0.0011
Delayed			
degradation <sup>g</sup>			
6. After 20 years	0.21	0.21	0.24
(fast rate)	0.51	0.21	0.24
7. After 50 years	0.45	0.16	0.15
(fast rate)	0.45	0.10	0.15

<sup>a</sup>Incineration of fossil-based plastic where all carbon is emitted as CO<sub>2</sub> in the first year. <sup>b</sup>Degradation under anaerobic conditions. <sup>e90%</sup> degradation of polycaprolactone (PCL) in 2 years<sup>80</sup>. <sup>d</sup>90% degradation of polybutylene succinate (PBS) in 31 years<sup>81</sup>. <sup>e90%</sup> degradation of polystyrene (PS) in 105 years<sup>82</sup>. <sup>f</sup>1% degradation of bio-based PLA in 100 years<sup>83</sup>. <sup>g</sup>Potential short (20 years) and long (50 years) lag phase in degradation based on ref. <sup>83</sup>.

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## **Supporting Information-2**

# Multiple climate tipping points metrics for improved sustainability assessment of products and services

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Supporting information 2 is an Excel file providing multiple climate tipping point potential (MCTP) values at midpoint for 1 kg CO<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub>O and for three Representative concentration pathways (RCP).
# Article II

# Development of metrics for climate tipping in life cycle assessment based on damage to ecosystems

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Manuscript in preparation intended for submission to Ecological Indicators.

# Development of metrics for climate tipping in life cycle assessment based on damage to ecosystems

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# Abstract

Climate tipping is a category of impact that addresses the contribution of greenhouse gas emissions to disturb those processes in the Earth system, which could pass a tipping point and thereby trigger large, abrupt and potentially irreversible changes. Recent efforts toward including climate tipping as an impact category in life cycle assessment (LCA) include the development of the multiple climate tipping points potential (MCTP) metric, which considers up to 13 projected tipping points, incorporate the effect that the crossing of a given tipping point has on accelerating the crossing of other tipping points, and address uncertainties in the temperature thresholds that correspond to the tipping points. Here, we further develop these midpoint metrics by linking them to losses of terrestrial species biodiversity at either local or global scales. The resulting damage MCTPs range from  $2.3 \cdot 10^{-17}$  to  $1.1 \cdot 10^{-15}$  PDF (potentially disappeared fraction of species at global level) per 1 kg of CO<sub>2</sub> emitted. They are time-dependent, and the largest values are found for emissions occurring between 2030-2045, generally declining for emissions occurring toward the end of the century. Differences in how time is treated in MCTP as opposed to other damage metrics used in LCA warrant further harmonization efforts.

## **1. Introduction**

Life cycle assessment (LCA) aims at quantifying the potential environmental impacts of a product or service over its full life cycle, from extraction of raw materials, through manufacturing and use, to end-of-life (Bjørn et al., 2018). During the life cycle impact assessment (LCIA) phase of an LCA, exchanges between environment and the product system (like emissions of greenhouse gases, GHG) are translated into potential environmental impacts using characterization factors (CF). These represent the potency of an emission to affect an indicator of the state of the environment that is chosen to represent the environmental impact in question (like radiative forcing in the case of the greenhouse effect) (Hauschild and Huijbregts, 2015). CFs are calculated using a model of the underlying impact that connects emissions to environmental damage. The indicator

may be chosen at any point between emissions and damage to the functioning of ecosystems or human health. Characterization factors modelled at the damage level allow for translating an emission into potential damage to exposed ecosystems. For example, damage-oriented global warming potentials (GWP) of GHG emissions combine timeintegrated change in radiative forcing (the indicator chosen for computing midpoint GWP, as proposed by the IPCC), with the resulting time-integrated change in temperature increase, and link that to the resulting damage to either terrestrial or freshwater ecosystems (e.g. ReCiPe 2016, Huijbregts et al., 2017).

Climate tipping is a relatively new impact category in LCIA (Fabbri et al., 2021; Jørgensen et al., 2014). It offers a complementary perspective to the climate change impact category represented by the time-integrated radiative forcing of the GWPs. Indicators of climate tipping, the multiple climate tipping points potentials (MCTP), represent the contribution of a GHG emission to crossing climatic tipping points (observed for processes of the Earth system which may pass a threshold that triggers large abrupt, potentially irreversible changes like change in surface albedo resulting from loss of Artic Summer see ice) (Lenton et al., 2008). In the MCTP approach, the impact of a GHG emission represents the time-integrated change in atmospheric CO<sub>2</sub>-equivalent concentration resulting from a unit emission of a greenhouse gas. This integration is from the emission year to the year where the next tipping point is predicted to occur according to the assumed background emission pathway (rather than over a fixed time horizon, like in the GWP). This impact is then expressed as the occupied fraction of the remaining capacity of the atmosphere to absorb the GHG impact without crossing a tipping point (rather than expressing it in unit emissions of a reference gas like CO<sub>2</sub>, as done in GWP). The remaining capacity is also expressed in atmospheric CO<sub>2</sub>-equivalent concentration, and the resulting MCTP characterization factors are therefore expressed in parts per trillion of remaining capacity per unit of GHG emission (Fabbri et al., 2021). Further developments are, however, necessary to link these MCTPs to damage to terrestrial ecosystems.

In LCIA, damage modelling for ecosystems traditionally focuses on species biodiversity, and the potentially disappeared fraction of species (PDF) is the most common metric (Curran et al., 2011; Woods et al., 2018). As explained in (Verones et al., 2020), exposure duration is also included in the unit of ecosystem damage, so resulting ecosystem damage is expressed as PDF·yr. It can be also expressed as species yr, when species density and area of exposed ecosystem are known. As argued in (Verones et al., 2020), damage scores in LCA should be interpreted as "an increase in global extinction risk over a certain exposure period of time and not so much as an instantaneous global species loss". Current damage oriented characterization factors express biodiversity loss at either local, or regional or global scales, and these are frequently mixed in LCIA methods (Verones et al., 2020). A local (or regional) loss of species occurs within a spatially delimited area can be reverted through repopulation. Global loss means that the species becomes extinct across the whole planet, and it is thus irreversible. This difference implies that a metric based on local species loss cannot be directly compared

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with one based on global losses. To avoid comparability issues, it is essential to clearly report at which level new metrics are developed (Jolliet et al., 2018). Local assessments are important to ensure ecosystem functionality while global assessments are necessary to avoid irreversible extinction of species. Thus, the two measures complement each other and it has been argued that characterization factors addressing both scales should be developed for all impact categories (Jolliet et al., 2018; Purvis, 2020; Verones et al., 2020).

The aim of this paper is to present a framework for calculating the multiple climate tipping points potential (MCTP) at endpoint (damage) level for three greenhouse gases (carbon dioxide (CO<sub>2</sub>), methane (CH<sub>4</sub>) and nitrous oxide (N<sub>2</sub>O)) at either local or global scale. The resulting characterization factors, referred to as  $MCTP_{endpoint}$ , quantify potential damage to terrestrial ecosystems considering the risk of crossing multiple climatic tipping points. They were computed for three Representative Concentration Pathways, RCP4.5, RCP6 and RCP8.5 representing possible future GHG emission trajectories for the world. The  $MCTP_{endpoint}$  factors are expected to be the largest for the highest emission pathway RCP8.5, because a sharp increase in temperature levels as projected in this path is expected to cause the strongest impacts on terrestrial species biodiversity.

## 2. Methods

### 2.1. Impact pathway mechanisms

The MCTP factor represents the fraction of the remaining capacity that is taken up by a unit emission and is expressed in parts per trillion of remaining capacity per unit emission of a greenhouse gas *i* (ppt<sub>rc</sub>  $\cdot$  kg<sub>i</sub><sup>-1</sup>). As explained in Fabbri et al. (2020), it was modelled by computing radiative forcing increase from the emission, expressed as atmospheric CO<sub>2</sub>-equivalent concentration increase, in relation to remaining atmospheric capacity to absorb the emission without crossing the tipping point. The midpoint MCTP is then linked to temperature increase per fraction of carrying capacity taken up, and, further on in the impact pathway, to the potential loss of species biodiversity resulting from that temperature increase (see Figure 1). Note, that in contrast to damage-oriented GWP CFs, which model impacts attributed to marginal GHG emissions (adding on top of the background emissions), damage modeling in the MCTP approach applies an *average* perspective by assuming that an increase in atmospheric CO<sub>2</sub>-equivalent concentration is part of the anthropogenic background. Furthermore, the crossing of a given tipping point reduces remaining carrying capacity for all subsequent tipping points. This corresponds to an additional temperature increase, which further contributes to loss of species diversity. The resulting potential loss of species is thus a function of the global temperature levels resulting from the background emissions and effects from crossing of

tipping points on temperature increase. The MCTP<sub>endpoint</sub> CF represents the share that the characterized emission has in the total predicted species loss.



**Figure 1**. Impact pathway for climate tipping used for developing the multiple climate tipping points potential based on ecosystem damage.

#### 2.2. Modelling framework

The endpoint MCTP ( $MCTP_{endpoint}$  in PDF·kg<sup>-1</sup>) of a given GHG *i* emitted at year  $T_{emission}$  is derived from the midpoint MCTP by using a 'midpoint-to-endpoint' factor:

$$MCTP_{\text{endpoint},i}(T_{\text{emission}}) = MCTP_i(T_{\text{emission}}) \cdot MEF(T_{\text{emission}})$$
(1)

where  $MCTP_i$  [ppt<sub>re</sub>·kg<sub>i</sub><sup>-1</sup>] is the multiple climate tipping points potential at midpoint of gas *i* emitted at year  $T_{emission}$ , and MEF [PDF·ppt<sub>re</sub><sup>-1</sup>] is the midpoint-to-endpoint factor, translating the impact from contribution to tipping of the emission at  $T_{emission}$  to the potentially disappeared fraction of species [PDF] at either local or global level. Note, that unlike other damage-oriented CFs of climate impacts (including GWP), exposure duration is not included in the unit of our endpoint MCTP. The exposure duration is considered when computing time-integrated increase in  $CO_2$ -equivalent concentration, but it cancels out when the impact is related to the carrying capacity. Implications of this on harmonization of metrics across impact categories will be discussed later.

#### 2.3. Multiple climate tipping potential at midpoint

As in Fabbri et al. (2021), the multiple climate tipping points potential at midpoint, MCTP<sub>*i*</sub>, in [ppt<sub>rc</sub>·kg<sub>*i*</sub><sup>-1</sup>] (parts per trillion of remaining capacity taken up by a unit emission) of gas *i* emitted at year  $T_{\text{emission}}$  is defined as the sum of the ratios between the *impact of the emission* and the corresponding remaining capacity for each of the *m* tipping points occurring after the emission year:

$$MCTP_{i}(T_{\text{emission}}) = \sum_{j=1}^{m} \frac{I_{\text{emission},i,j}(T_{\text{emission}})}{CAP_{j}(T_{\text{emission}})}$$
(2)

where *j* indicates the *j*th tipping point occurring after the emission year (in order of occurrence) and can take any value from 1 to *m*, which is the total number of tipping points that are predicted to be crossed under the assumed background emission pathway (RCP);  $I_{emission,i,j}$  is the *impact of the emission* of gas *i* with respect to the *j*th tipping point, *CAP<sub>j</sub>* is the remaining capacity up to the *j*th tipping point, and the emission year  $T_{emission}$  can be any year from 2021 (or the year when emissions are expected to start taking place) up to the year of the last tipping point.

Details of computing impact and remaining carrying capacity are presented in Fabbri et al. (2021). Briefly, the  $I_{\text{emission},i,j}$  is computed as the radiative forcing of gas *i* 

 $(RF_i)$  integrated over time between the emission and the tipping (referred to as the absolute climate tipping potential, ACTP) [W·m<sup>-2</sup>·yr·kg<sub>i</sub><sup>-1</sup>] divided by the radiative efficiency (RE) of 1 ppm of CO<sub>2</sub> [W·m<sup>-2</sup>·ppm CO<sub>2</sub><sup>-1</sup>]. The *CAP<sub>j</sub>* [ppm CO<sub>2</sub>e·yr] represents the increase in atmospheric CO<sub>2</sub>-equivalent concentration that can still take place before reaching the concentration level (in ppm CO<sub>2</sub>e) that will trigger tipping *j*. This capacity depends on background anthropogenic emissions, and it can be reduced when preceding tipping points are crossed.

#### 2.4. Midpoint to endpoint factor

The midpoint-to-endpoint factor,  $MEF(T_{emission})$  as it depends on the emission year, is given by:

$$MEF(T_{\text{emission}}) = \frac{\Delta TEMP(T_{\text{emission}})}{1 \cdot 10^{12}} \cdot \frac{\Delta PDF(T_{\text{emission}})}{\Delta TEMP(T_{\text{emission}})}$$
(3)

where  $\frac{\Delta TEMP(T_{emission})}{1\cdot 10^{12}}$  [°C·ppt<sub>rc</sub><sup>-1</sup>] is the global atmospheric temperature change ( $\Delta TEMP$ ) resulting from one part per trillion reduction of the remaining capacity [ppt<sub>rc</sub>] (i.e., per unit of the midpoint MCTP ) and  $\frac{\Delta PDF(T_{emission})}{\Delta TEMP(T_{emission})}$  [PDF·°C<sup>-1</sup>] is the rate of potential species loss, at either global or local level (PDF<sub>global</sub> and PDF<sub>local</sub> respectively), per unit change in global average atmospheric temperature. The factor  $1 \cdot 10^{12}$  [ppt<sub>rc</sub><sup>-1</sup>] is needed to re-convert the midpoint *MCTP<sub>i</sub>* into unitless fraction of remaining capacity. Note that both  $\Delta TEMP$  and  $\Delta PDF$  depend on the emission year. The factor  $\frac{\Delta TEMP(T_{emission})}{1\cdot 10^{12}}$  quantifies the link between the fraction of remaining capacity eaten up by the emission occurring at  $T_{emission}$  (calculated by the midpoint MCTP) and the temperature increase associated with taking up that fraction of remaining capacity. To relate these two variables, we consider the overall remaining capacity from the emission year ( $T_{emission}$ ) up to the year when the last possible tipping point is exceeded under the assumed background emission pathway and the average temperature change expected to occur over the same period (eq. 4).

$$\frac{\Delta TEMP(T_{\text{emission}})}{1\cdot 10^{12}} = \frac{TEMP(T_{\text{tipping}j_{\text{last}}}) - TEMP(T_{\text{emission}})}{1\cdot 10^{12}}$$
(4)

where  $TEMP(T_{tipping,j_{last}})$  is the temperature in the year where the last tipping point is exceeded and  $TEMP(T_{emission})$  is the temperature in the emission year.  $\Delta TEMP$  results from the combination of the background evolution of GHG emissions according to the assumed background emission pathway and the effect of crossing tipping points. Note, that in eq. 4 the remaining capacity  $(1 \cdot 10^{12} \text{ ppt}_{rc})$  is independent of the emission year. It represents the total capacity that is left up to the last tipping point at each considered emission year.

The factor 
$$\frac{\Delta PDF(T_{emission})}{\Delta TEMP(T_{emission})}$$
 represents the rate of potential species loss per

unit of temperature increase. The change in potentially disappeared fraction of species  $\Delta PDF(T_{\rm emission})$  is calculated as the difference between the foreseen fraction of species lost ( $F_{\rm lost}$ ) at the highest considered temperature increase, corresponding to that expected

at the last tipping point,  $F_{\text{lost}}(T_{\text{tipping},j_{\text{last}}})$ , and the foreseen fraction of species lost at the emission year,  $F_{\text{lost}}(T_{\text{emission}})$  (eq. 5).

$$\frac{\Delta PDF(T_{\text{emission}})}{\Delta TEMP(T_{\text{emission}})} = \frac{F_{\text{lost}}(T_{\text{tipping},j_{\text{last}}}) - F_{\text{lost}}(T_{\text{emission}})}{TEMP(T_{\text{tipping},j_{\text{last}}}) - TEMP(T_{\text{emission}})}$$
(5)

Studies estimate that this rate is not constant but accelerates as global temperature levels rise (see section below). This acceleration is accounted for by calculating a different rate for each emission year, so that emissions occurring at higher levels of warming are attributed a higher potential fraction of species loss per unit of temperature increase caused by the emission.

Following the approach developed in Fabbri et al. (2021) for calculation of midpoint MCTP, we consider model uncertainties in the exact location of the temperature thresholds that trigger the identified potential tipping points and compute  $MCTP_{endpoint}$  factors as a function of the emission year using Monte Carlo simulation (10000 iterations), simulating possible developments with different timing and sequence of the tipping points. The uncertainties behind each of the 13 considered tipping points and their implementation into the model are presented in Fabbri et al. (2021) and summarized in Table S1 in Supplementary Information-1. Results are given as the geometric mean calculated over the iterations.

#### **2.5.** Determination of temperature change

Future temperature changes are obtained from the global mean temperature projections estimated starting from the Representative Concentration Pathways (RCPs) in (Meinshausen et al., 2011). The choice of pathway, in particular the projected rate of GHGs concentration increase, strongly affects the magnitude and the trend of the midpoint MCTPs over emission time, potentially influencing the climate tipping performance of products (Fabbri et al., 2021). To reflect how this choice affects the damage due to GHG emissions, we consider the three pathways RCP4.5, RCP6 and RCP8.5 (numbers referring to the resulting radiative forcing [W·m<sup>-2</sup>] in 2100). The lower emission path RCP2.6 is excluded as deemed probably unrealistic (Sanford et al., 2014; van Vliet et al., 2009).

In addition, we account for the potential temperature change caused by crossing tipping points, starting from the estimated CO<sub>2</sub>-equivalent concentration increase following tipping that was used for computing the midpoint MCTPs. This is relevant for eight of the thirteen tipping points considered (Fabbri et al., 2021). The resulting global temperature rise is that associated with the corresponding CO<sub>2</sub>-equivalent concentration under the chosen RCP, up until the maximum concentration level predicted in the given RCP pathway. This implies that while the predicted warming based on the baseline RCP projection is anticipated, the maximum expected temperature increase will never exceed that projected by the RCP. Implications of this modeling choice will be discussed.

#### 2.6. Determination of fraction of species lost

The potentially disappeared fraction of species per unit change in global average temperature increase,  $\frac{\Delta PDF(T_{emission})}{\Delta TEMP(T_{emission})}$  is derived from studies that estimate species loss under a given emission pathway. Here we consider both measures of local species loss, when species are lost locally but with possible reintroduction from neighboring regions, and global species loss, when species become globally extinct and there is no possibility for recolonization.

Local species loss due to climate change is obtained from (Newbold, 2018), who calculated a global average of local losses in terrestrial vertebrate biodiversity projected over four RCP pathways. It was chosen as one of the most recent studies focusing on climate change effects on local biodiversity loss, from which it was possible to obtain sufficient data points to derive a curve relating changes in species occurrence to changes in global mean temperature. (Newbold, 2018) included four vertebrate groups (amphibians, birds, reptiles and mammals) and used species distribution models for estimating local losses in response to climate change. These models relate species distribution at known locations all over the world with bioclimatic data typical of those locations, to predict the distribution under future climates (Elith and Leathwick, 2009). The estimated losses are then averaged across all terrestrial areas of the world to obtain a global average of the losses at local level. A species is considered lost from a certain area when that area becomes climatically unsuitable for that species, however, the model accounts for possible offsets due to colonization from new species for which that area has become climatically suitable. By combining the losses predicted based on the future evolution of four climate variables with the temperature change expected in 2070 under a given RCP, the study shows that temperature increases of 2, 3 and 4.3°C relative to 1960 – 1990 would lead, on average across terrestrial areas and assuming intermediate dispersal ability, to 3, 10 and 20% local loss of species, respectively.

Global species loss is taken from a large synthesis of studies predicting extinction risk from climate change carried out in (Urban, 2015). This study was chosen as it provides the most comprehensive and recent estimates of global species loss from climate change and has already been used to develop damage-oriented GWP factors in the ReCiPe 2016 and LC-IMPACT methods (Huijbregts et al., 2017; Verones et al., 2020, 2019). (Urban, 2015) compiled 131 predictions covering seven taxonomic groups, different dispersal abilities and different modeling techniques to derive the global mean extinction rate per unit of future global temperature rise. Besides exceedance of the bioclimatic limits of species, mechanisms explaining global species loss here also include loss of habitats due to the changing climate. Global losses of 3, 5, 8, 16 and 21% are expected for temperature increases of respectively 0.8, 2, 3, 4.3 and 5°C above preindustrial levels.

To integrate the models of Newbold and Urban with our midpoint MCTP factors while enabling Monte Carlo simulations, simplified linear regressions were developed based on predictions from the original models of Newbold and Urban. The regressions predict fraction of species lost (logit-transformed) from temperature change. Details of the regression analyses are presented in the Supplementary Information-1. Figure 2 shows predictions of the regression models. Predictions at local and global scale show high similarity in trend and magnitude, implying that resulting MCTP<sub>endpoint</sub> factors will not be significantly different from each other in terms of numerical values.



**Figure 2**: Fraction of local and global species loss as a function of global temperature change above pre-industrial levels, *TEMP*. 'Data from model' refers to the pairs of values linking a change in species loss with a change in temperature retrieved from (Newbold, 2018) and (Urban, 2015) and found in Table S2. Since both reference studies for local and global species loss do not provide estimates beyond 5°C, computations of the MCTP<sub>endpoint</sub> under RCP8.5, which is the only pathway where temperature projections exceed 5°C, terminate at the year when the temperature level reaches 5°C in each iteration.

#### 2.7. Case study

Application of the MCTP characterization factors is expected to have particular relevance when studying the performance of products that have GHG emissions occurring over extended periods of time, such as slowly degrading plastics (Fabbri et al., 2021). We illustrate the application of the calculated MCTP<sub>endpoint</sub> factors in a case study on the endof-life stage of four types of degradable plastic polymers during incineration or landfilling of 1 kg of each material. Details on the considered polymers, scenarios and assumptions are found in Fabbri et al. (2021), and an overview is provided in Table 1. Under the anaerobic conditions typical of municipal landfills, the polymers degrade at different rates, from fast (90% degradation < 2 years) to very slow (1% degradation <100 years), resulting in different  $CO_2$  and methane (CH<sub>4</sub>) emission profiles derived from the carbon contained in the polymer. In contrast, during incineration only CO<sub>2</sub> emissions are released and all at the same time. These differences in emission timing are expected to influence the performance of the polymers when measured with the MCTP approach. Starting from reported carbon content and degradation rate constants of the polymers, yearly emitted quantities of GHGs are calculated, multiplied by the corresponding yearspecific average MCTP<sub>endpoint</sub> factor per unit emission and summed over the period from the first GHG emission release (here assumed to be 2021) up to the last tipping point  $(T_{\text{tipping}, j_{\text{last}}})$  and over each GHG *i*. The result is the total impact score (IS) in terms of potentially disappeared fraction of species (PDF) from the end-of-life degradation of 1 kg of plastic (eq. 6):

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$$IS = \sum_{i} \sum_{T_{\text{emission}}=2021}^{T_{\text{tipping,}j_{\text{last}}}} m_i(T_{\text{emission}}) \cdot MCTP_{\text{endpoint},i}(T_{\text{emission}})$$
(6)

where  $m_i(T_{\text{emission}})$  is the mass of GHG *i* emitted at year  $T_{\text{emission}}$ . Impacts scores are calculated with the MCTP<sub>endpoint</sub> factors at both local and global level and calculations are done with CFs representing each of the three RCPs. For comparison, we also compute impact scores using the complementary GWP-based metric of damage to terrestrial ecosystems included in the LCIA method ReCiPe 2016, where metric scores are expressed in [species·yr].

Scenario	Polymer	Degradation	Note
		rate constant,	
		k (day <sup>-1</sup> )	
1. Incineration	Generic fossil-based	Not relevant	All carbon contained
			in the polymer,
			which is the same for
			all scenarios, is
			released as CO <sub>2</sub> in
			year 1
Plastic degradation rate			
2. Fast (90% degradation	Polycaprolactone	2.97·10 <sup>-3 (a)</sup>	In total, 71% of the
in 2 years)	(PCL) - fossil-based		carbon is released as
3. Medium (90%	Polybutylene	2.02·10 <sup>-4 (b)</sup>	$CO_2$ and 29% as
degradation in 31	succinate (PBS)		CH <sub>4</sub> , in different
years)	fossil-based		years depending on
4. Slow (90% degradation	Polystyrene (PS)	6.00·10 <sup>-5 (c)</sup>	the degradation rate
in 105 years)	fossil-based		constant <sup>(d)</sup>
5. Very slow (1%	Polylactic acid (PLA)	2.77·10 <sup>-7 (d)</sup>	
degradation in 100	- bio-based		
years)			
Delayed degradation			
6. After 20 years (fast	Polycaprolactone	2.97·10 <sup>-3 (a)</sup>	Degradation in
rate)	(PCL) – fossil-based		landfill of the fast-

**Table 1:** Overview of the seven scenarios considered for the case study. Adapted from (Fabbri et al., 2021)

7. After 50 years (fast rate)	Polycaprolactone (PCL) – fossil-based	2.97·10 <sup>-3 (a)</sup>	degrading plastic (scenario 2) is assumed to be
			delayed by 20 and 50
			years, respectively.

<sup>(a)</sup> (Ishigaki et al., 2004); <sup>(b)</sup> (Cho et al., 2011); <sup>(c)</sup> (Tansel, 2019); <sup>(d)</sup> (Rossi et al., 2015).

# 3. Results

Results for  $CO_2$  are first presented for a sample iteration (i.e. a Monte Carlo simulation representing a possible scenario in which nine different tipping elements cross their tipping point) under the RCP6 pathway. To illustrate the influence of the adopted approach on the final MCTP<sub>endpoint</sub> values, results are shown separately for all the factors underlying the MCTP<sub>endpoint</sub>. Next, results from 10000 Monte Carlo iterations accounting for current uncertainties in tipping occurrence are presented and compared between RCP pathways. Finally, main outcomes from the case study are presented. The MCTP<sub>endpoint</sub> values for  $CO_2$ ,  $CH_4$  and  $N_2O$  can be found in Supplementary Information-2.

#### 3.1. MTCPs for a sample iteration

Figure 3a shows a sample  $MCTP_{endpoint}$  for  $CO_2$  in terms of both local and global fraction of species loss, as depending on emission time. The first observation is that  $MCTP_{endpoint}$ factors are overall proportional to their corresponding midpoint MCTP (Figure 3b) and follow a similar pattern. As already shown in (Jørgensen et al., 2014) and (Fabbri et al., 2021), midpoint MCTPs peak just before the passing of a tipping point, indicating that the contribution of an emission to cross the tipping point increases as the emission pathway approaches the tipping point. Here, the increase in MCTP<sub>endpoint</sub> suggests that an emission occurring before an expected tipping threshold has a higher potential to cause ecosystem damage due to its larger contribution to deplete the remaining capacity and cross the tipping point. On the contrary, emissions after the tipping point have smaller contribution to crossing subsequent tipping points. This is seen as a discontinuity in the MCTP<sub>endpoint</sub> curve.

MCTP<sub>endpoint</sub> values generally increase until ca 2045, but they are almost 2 orders of magnitude lower for emissions occurring toward the end of the century. This decreasing trend is explained by the fact that the temperature change per fraction of remaining capacity taken up by the emission decreases as the emission occurs later in time. Therefore, despite the fact that the potential species loss per unit temperature increase, e.g. in 2070, is expected to be higher than that in 2035 (Figure 3c and Table S3 in Supporting Information-1), the resulting damage from an emission in 2070 is lower than that in 2035 because the corresponding temperature change induced by that emission is also lower (Figure 3d). This observation may seem counterintuitive if one would expect larger impact to be computed for emissions occurring later in time (consistently with Figure 2) but is in line with an average approach to modeling of characterization factors for use in LCA. As argued in Fabbri et al. (2021), the MCTP factors represent average impact as they depend on the background level. Thus, averaging temperature change between emission year and year of the last tipping point (making the resulting  $\Delta TEMP$  decrease with later emission time) is necessary to calculate indicator scores for

emissions occurring at that specific emission year. These emissions cannot be made responsible for the temperature increase and resulting ecosystem damage that happened before the emission year of interest.

Finally, MCTP<sub>endpoint</sub> factors calculated using local species loss estimates show little difference from those obtained using global species loss estimates. Results for local losses are maximum 13% larger and 5% smaller compared to results for global losses, depending on the emission time. However, we stress that their interpretation is not the same. Local losses represent potentially reversible damages through the loss of ecosystem functioning caused by local loss of species, whereas global extinctions represent irreversible losses of biodiversity.



**Figure 3:** (a) Endpoint MCTP (MCTP<sub>endpoint</sub>) for emission of 1 kg of  $CO_2$  expressed as Potentially Disappeared Fraction (PDF) of species at local (dashed line, left axis) and global (solid line, right axis) level in a sample iteration under RCP6. The scale of the right axis was incremented by a factor 10 to facilitate visualization of the two curves that would otherwise overlap. (b) Midpoint

MCTP for emission of 1 kg of CO<sub>2</sub>. (c) Potentially Disappeared Fraction of species (PDF) at local (dashed line, left axis) and global (solid line, right axis) level per degree Celsius increase in global temperature. (d) Temperature change per fraction of remaining capacity. (e) Mid-to-endpoint factor (MEF) for local (dashed line, left axis) and global (solid line, right axis) species loss. (f) Temperature change per kg of CO<sub>2</sub> emitted. Specific results for three different emission times are reported in Table S3 in Supporting Information-1.

#### **3.2.** Uncertainty and sensitivity

When uncertainties about occurrence and timing of tipping points are accounted for with Monte Carlo simulations, average (geometric mean) MCTP<sub>endpoint</sub> factors at both local and global level are somewhat smoothened compared to a single iteration, indicating that uncertainties in the exact location of the tipping point are so large that single tipping events are not clearly distinguishable (Figure 4). Nevertheless, some peaks are visible, indicating periods when the probability of tipping points to occur is the largest. These findings are consistent with observations noted in Fabbri et al. (2021) for the midpoint MCTP. Emissions between 2040 and 2060 have the largest potential to cause species loss as a consequence of crossing tipping points assuming RCP6. After this period, potential damage per unit emission decreases, confirming the trend observed in the sample iteration. Average MCTP<sub>endpoint</sub> factors calculated at the local and global levels are numerically similar. Under RCP6, average (geometric mean) MCTP<sub>endpoint</sub> factors based on local species loss range between  $2.7 \cdot 10^{-17}$  and  $1.1 \cdot 10^{-15}$  PDF per 1 kg of CO<sub>2</sub>,

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depending on the year of emission, with 90% of the iterations oscillating between  $2.2 \cdot 10^{-17}$  and  $2.3 \cdot 10^{-15}$  PDF per unit emission (Figure 4a). The MCTP<sub>endpoint</sub> factors at global level can be up to 5% larger and 13% lower than results for local species loss, depending on the emission year.

The comparison between RCP pathways shows that potential local and global species loss is generally larger under RCP8.5 and lower under RCP4.5. This is consistent with expectations that more species will be lost at higher temperature levels, and it is in contrast to what was found in Fabbri et al. (2021), where midpoint MCTPs for RCP8.5 were lower than those for RCP4.5. This reflects the inability of the midpoint CFs to represent ecosystem damage, unless weighting factors are developed, or damage modelling is done as presented here. MCTP<sub>endpoint</sub> factors at local level can be up to 4 and 87 times larger (depending on emission time) under RCP8.5 compared to RCP6 and RCP4.5, respectively, whereas at global level they are up to 3 and 35 times larger than the other two pathways. Similar trends are observed for CH<sub>4</sub> and N<sub>2</sub>O, and MCTP<sub>endpoint</sub> values for these two gases are on average 83 and 273 times larger, respectively, compared to those of CO<sub>2</sub> (Figure S1).



**Figure 4:** Average (geometric mean) endpoint MCTP (MCTP<sub>endpoint</sub>) of 1 kg of CO<sub>2</sub> based on local (**a**) and global (**b**) species loss (solid lines) and corresponding uncertainty ranges (shaded areas enclosed between the 5<sup>th</sup> and 95<sup>th</sup> percentiles) calculated under RCP4.5, RCP6 and RCP8.5.

#### 3.4. Findings from a case study

Ranking between plastic end-of-life scenarios obtained with the MCTP<sub>endpoint</sub> calculated in this study shows some differences when compared to ranking using the damage GWP (Table 2). For the damage GWP, the lowest impacts are calculated when the plastic material degrades slowly enough so that the amount of GHGs emitted in 100 years is at a minimum, explaining why the very slowly and the fast-degrading plastics are the best and the worst scenarios respectively. This is also the case for our MCTP<sub>endpoint</sub> (at both local and global level) for very slowly degrading plastic, which is seen to have lowest impacts due to the very low amounts of GHGs emitted. However, contrary to the GWP, where impacts are rather insensitive to biodegradation kinetics, climate tipping impacts also depend on emission timing, and are largest when emissions occur at the point in time where their contribution to cross tipping points is the largest (2040-2060). This corresponds to fast biodegradation rate with a lag phase, followed by a scenario with medium biodegradation rate without a lag. Ranking of scenarios from fast to slow degradation rate differs slightly among the three RCP pathways, but the overall trends are the same (scenarios 6 and 3 are seen as the worst). The main difference here between RCP pathways is that MCTP<sub>endpoint</sub> scores calculated under RCP8.5 are always higher than scores under the other two RCP pathways, reflecting potentially larger species loss in a high emissions pathway and, thus, the dependency of the product's performance on the chosen emission path.

**Table 2**: Total impact scores for the considered end-of-life scenarios according to endpoint MCTP (MCTP<sub>endpoint</sub>) at both local and global level and the complementary metric of damage to ecosystems from ReCiPe 2016. Ranking between scenarios (within columns) is indicated using red shading for highest impact scores and green shading for the lowest.

Scenario	MCTP <sub>endpoint</sub> at local level (PDF/kg plastic)		MCTP <sub>endpoint</sub> at global level (PDF/kg plastic)			Damage GWP (ReCiPe 2016) (Species · yr/kg	
	RCP4.5	RCP6	RCP8.5	RCP4.5	RCP6	RCP8.5	plastic)
1. Incineration	4.1E-16	1.2E-15	3.7E-15	5.0E-16	1.2E-15	3.2E-15	5.1E-09
Plastic degradation rate							
2. Fast	3.3E-15	7.8E-15	3.0E-14	4.0E-15	8.2E-15	2.6E-14	2.3E-08
3. Medium	4.2E-15	1.2E-14	4.3E-14	5.0E-15	1.2E-14	3.7E-14	2.3E-08
4. Slow	2.7E-15	1.0E-14	3.0E-14	3.2E-15	1.0E-14	2.5E-14	2.1E-08

5. Very slow	2.0E-17	9.0E-17	2.3E-16	2.3E-17	8.9E-17	1.9E-16	2.2E-10
Delayed degradation							
6. After 20 years (fast rate)	5.6E-15	1.7E-14	5.7E-14	6.5E-15	1.7E-14	4.8E-14	2.3E-08
7. After 50 years (fast rate)	1.2E-15	9.1E-15	2.7E-14	1.5E-15	8.7E-15	2.1E-14	2.3E-08

# 4. Discussion

#### 4.1. Metrics based on ecosystem damage

The MCTP<sub>endpoint</sub> factors calculated here measure the potential loss of species biodiversity from a GHG emission that contributes to passing climate tipping points. We emphasize that this potential species loss should be seen as the translation of the contribution of an emission to tipping (expressed at midpoint level) into the resulting potential loss of species. The focus here is on impacts through contributions to climate tipping and not on assessing the biodiversity loss from GHG emissions through the time-integrated radiative forcing impact pathway (linking radiative forcing change to time-integrated temperature change and to final species loss) that is represented by the GWP-based metric for ecosystem damage.

In our model we have accounted for the acceleration of species loss with increasing temperature levels in line with recent estimates (Newbold, 2018; Urban, 2015). Thus, we could have expected the impact on species to be larger for future emissions (i.e. occurring at higher levels of warming) than for emissions today, returning increasing MCTP<sub>endpoint</sub> results over time. However, we found that this acceleration is counteracted by the simultaneous decline in the contribution of an emission to temperature rise over time. As a unit emission of  $CO_2$  leads to a lower temperature increase when emitted closer to the year of the last tipping point (see Figure 3f), in line with the *average* approach to modelling characterization factors, it follows that the impact on species diversity can be proportionally lower for emissions occurring later, toward the end of century. Therefore, the resulting decrease in MCTP<sub>endpoint</sub> factors should not be interpreted as, e.g., lower sensitivity of the climate to future emissions or other climate related mechanisms.

In contrast to other endpoint metrics (including damage GWP) that assess effects of GHG emissions on biodiversity in LCA, the MCTP<sub>endpoint</sub> introduces a temporal perspective also in the midpoint to endpoint factor. As a consequence, the MCTP<sub>endpoint</sub> for a specific gas depends on the emission year. The results from the case study suggest that use of the new metric gives additional insights about the performance of the compared products, capturing larger potential impacts when emissions from the product occur in periods when probability of tipping points is the largest (between 2040 and 2060), distinguishing it from the damage GWP. This finding is in line with what was found when applying the CFs at the midpoint level (Fabbri et al., 2021). The added value is, however, that interpretation our damage CFs becomes more environmentally relevant.

We find little difference between the  $MCTP_{endpoint}$  factors that express species loss at local and global level. This is due to the similarity of the curves used to

describe local and global species loss as function of temperature rise (Figure 2). This observation seems at odds with the expectation that local losses should be larger than global because a substantial local loss of species is likely to occur before those species start becoming globally extinct. However, the outcome depends on the spatial distribution of species and on which species are lost first. For instance, if the loss involves very narrowly distributed species, then global extinctions could become high without having a large impact on local diversity. Another factor could be the difference in taxonomic groups considered in the studies estimating local and global losses. Indeed, local losses refer to vertebrates only, while a larger number of taxonomic groups is included in global losses estimates. The inclusion of large groups such as invertebrates, which are dominant contributors to Earth's terrestrial biodiversity (Collen et al., 2012), might lead to higher estimates of local species loss compared to the global figures. Therefore, we emphasize that the provided MCTP<sub>endpoint</sub> factors at local level are limited to vertebrates. An additional reason could be that the estimates of global losses from the study of (Urban, 2015), which were extrapolated from local and regional studies, are, in reality, more representative for losses at local level, explaining the similarity with figures from (Newbold, 2018).

#### 4.2. Applicability in life cycle assessment

Emission year-specific MCTP<sub>endpoint</sub> factors for the three gases (CO<sub>2</sub>, CH<sub>4</sub> and N<sub>2</sub>O) provided here (Supporting Information-2) are directly applicable in LCA studies to assess

the potential species loss stemming from the life cycle of products or services. As for the midpoint MCTP, use of MCTP<sub>endpoint</sub> is relevant when a time-differentiated inventory is available for the assessed products. However, since temporarily disaggregated inventories are not yet easy to implement into dominant LCA software, calculation of MCTP<sub>endpoint</sub> impact scores (through eq. 6) has to be conducted offline. For situations where temporal disaggregation of the inventories is not deemed relevant, we recommend using MCTP<sub>endpoint</sub> factors calculated for single year (e.g. 2021) to match with aggregated emissions for the same year.

Advancing the midpoint MCTP to endpoint level should ideally allow for comparison with the damage caused by other environmental impacts, such as eutrophication or ecotoxicity but also other climate-related impact categories. For instance, comparison of our MCTP<sub>endpoint</sub> at global level with the damage GWPs from ReCiPe 2016 could be possible as the species loss considered in both MCTP and GWP-based methods are based on global extinction risks of (Urban, 2015). However, for direct comparisons harmonization of units is required. This requires two steps. In the first step, conversion of the potentially disappeared fraction of species (used in MCTP<sub>endpoint</sub>) to absolute number of species used (used in methods such as ReCiPe 2016) is needed. This can be done by multiplying the final MCTP<sub>endpoint</sub> impact score of the assessed product (calculated through eq. 6) with the total number of terrestrial species on the planet. This value is estimated to be approximately 6.5 million (Mora et al., 2011), of which 1.6 million are the species that have been classified (Goedkoop et al., 2009). Even though the

former value would be recommended as it gives a more realistic measure of species diversity, the latter should be used when the purpose is to compare with ReCiPe 2016 (as this is the value adopted in ReCiPe). Moreover, we stress that the conversion to absolute number of species using estimates of the total terrestrial species is applicable only to the MCTP<sub>endpoint</sub> at global level, as for the model at local level this would not lead to a meaningful approximation. The second step addresses the time (exposure duration), which is not explicit in the MCTP<sub>endpoint</sub> unit. Other damage-oriented CFs include a time dimension when expressing impacts on biodiversity, e.g., species yr (ReCiPe 2016) or PDF·yr (LC-IMPACT), which may represent the duration (in years) of the period of exposure to the pressure (e.g. the residence time of the emission in the environment). To harmonize the units of the MCTP<sub>endpoint</sub> with other damage-oriented metrics, an idea could be to multiply the MCTP<sub>endpoint</sub> impact scores (in either PDF or species) by the total number of years from the first emission up to the last expected tipping point in each RCP pathway. This number corresponds to 70, 97 and 85 years for RCP4.5, RCP6 and RCP8.5, respectively, for emissions starting in year 2021. The resulting MCTP<sub>endpoint</sub> impact scores for the case study therefore become 2-3 orders magnitude higher when compared to scores obtained using damage GWPs.

#### 4.3. Limitations

One limitation in the midpoint to endpoint factor is that the uncertainties related to estimation of species loss with temperature change were not considered. (Newbold, 2018) reports that temperature increases between 2.5 and 4.8°C (relative to pre-industrial)

would lead to approximately a maximum 9% gain and 39% loss of species at local level (overall figures across all used RCP scenarios and species distribution models). At global level, uncertainties documented by (Urban, 2015) for similar temperature increases (2 - 4.3°C relative to pre-industrial) are proportionally lower as estimated species loss range from about 4 to 20%.

Second, given the dependency of the damage MCTP factors on the number of considered climate tipping points, a limitation is our lack of knowledge about all potential present and future tipping points. Our framework uses the current knowledge about tipping points, but it can be readily updated when additional potential tipping points are discovered.

A third limitation is the inability of the damage MCTP factors to capture direct impacts from climate tipping. The way in which species could respond to, e.g. a recurring sea ice-free summer in the Arctic or a gradual but irreversible dieback of the Amazon forest is difficult to predict (Post et al., 2009). Several models assessing the impacts of future climate change on biodiversity have been developed (see e.g. Pearson and Dawson, 2003; Thuiller et al., 2013), but estimates of the consequences of specific tipping events are lacking or incomplete. For this, direct impacts such as those derived from loss or degradation of the natural habitat of species, e.g., biodiversity loss from forest dieback or intensified droughts, were not considered.

Fourth, there is a limitation in the way in which the temperature rise following a tipping event was determined. This measure depends on several uncertain factors, such as the potential consequences on the climate from tipping, the rate at which the consequences unfold and the response of the climate to these changes. We used available estimates of carbon emissions and relative radiative forcing change caused by tipping, but no uncertainty estimates were included as they are rarely available. In addition, the approach adopted to calculate the temperature increase following carbon emissions, which in practice assumes that temperature increases faster but never exceeding the projection of each RCP pathway, is an oversimplification of the climate mechanisms involved. A more appropriate measure would require the use of climate models simulating the climate-carbon-cycle system, such as Earth system models (ESMs) (Millar et al., 2017). The main implication of these model limitations is to underestimate the potential temperature increase induced by passing tipping points, which could actually rise above RCP projections, and, consequently, indicate an underestimation of the resulting loss of species. This may affect the magnitude of MCTP<sub>endpoint</sub> factors to some extent, but it is not expected to change the observed overall trends.

#### 4.4. Priorities for further developments

As every biodiversity loss metric focusing only on the loss of species diversity, our metric assigns an equal weight to all species without considering e.g. the functional role that species play in the ecosystem, assuming that the damage to biodiversity is independent of which species are lost. However, in terms of consequences for the natural ecosystems, it is not given that all species should be weighed equally, and furthermore it is not given that species which remain in the future should have the same weight as

species living today. For example, losing species in the future, when many others have already disappeared, may compromise the ecosystems' functions more severely than when species diversity is still (relatively) high, as of today. Further, the loss keystone species, playing a critical role in the ecosystem, may weight more than a larger decline of species performing less crucial functions. Complex interactions exist between species in ecological communities and, for this, the loss of certain critical species from a community could cause a cascade of secondary extinctions of many other species (Brodie et al., 2014; Dunne and Williams, 2009). Ideally these dynamics could be included in our metric by introducing a *severity* factor in in eq. 1, providing a measure of severity of damage. As our ability to predict these mechanisms is rather limited, however, calculation of such a severity factor is not straightforward.

# 5. Conclusions

Our work is the first attempt to link midpoint multiple climate tipping points metrics of GHG emissions to loss of terrestrial species biodiversity at local and global scales. The resulting metric complements existing damage-level metrics used in LCIA and we therefore recommend including it as new damage category. For consistency with other impacts, we recommend using MCTP<sub>endpoint</sub> values predicting global species loss. Differences in how time is treated in MCTP<sub>endpoint</sub>, however, when compared to other damage metrics used in LCA warrant further harmonization efforts. In the broader LCA

context, our MCTP<sub>endpoint</sub> penalizes emissions occurring closer to tipping points, particularly those occurring between 2040 and 2060. Their use thus aims to discourage emissions attributed to product life cycles that will occur when they matter most and result in largest damage, offering the possibility to postpone the tipping, e.g. through carbon storage in products, thus buying time for the implementation of climate change mitigation and/or adaptation solutions (Jørgensen et al., 2015).

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# **Supplementary information**

Supplementary methods and results (Supplementary Information-1) Emission-year specific MCTP<sub>endpoint</sub> values (Supplementary Information-2)

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# Supplementary Information-1

# Development of metrics for climate tipping in life cycle assessment based on damage to ecosystems

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- S2. Determination of fraction of species lost
- S3. Additional results

# S1. Overview of selected tipping elements

**Table S1:** Summary of considered tipping elements, uncertainty range of tipping thresholds andoccurrence of tipping points under RCP4.5, RCP6 and RCP8.5 (taken from Fabbri et al., 2021).

Selected tipping element	Tipping mechanism	Temperature threshold range	Occurrence			
		(global mean temperature above pre-industrial level in °C)	RCP4.5	RCP6	RCP8.5	
Arctic summer sea ice loss (AS)	Melting of sea exposes larger areas of ocean surface to solar radiation, decreasing the albedo and increasing heat absorption by the ocean, thus amplify the warming. This loss of sea ice could lead to ice cap melting beyond certain size/thickness at which complete melting is likely to occur every summer.	1.5 – 2.6	Expected	Expected	Expected	
Greenland ice sheet melt (GI)	Increased air temperatures cause surface ice melting, which lowers ice altitude and increases surface temperature (due to higher temperatures at lower elevation) causing further warming and melting (melt- elevation feedback) to a point beyond which there is net mass loss and GI shrinks radically (Good et al., 2018).	1.6 - 3.5	Potential	Expected	Expected	
West Antarctic ice sheet collapse (AI)	The collapse is due to the combination of (i) surface melting (see GI) and (ii) the retreat of the submerged grounding line caused by the intrusion of warmer ocean water, which increases the ice flux and induces further retreat (Lenton, 2012) (Good et al., 2018).	1.9 - 4.8	Potential	Potential	Expected	
Amazon rainforest dieback (AF)	Warmer temperatures cause reduction in precipitations, lengthening of the dry season and directly affect vegetation productivity, leading to forest dieback, which in turn further reduces precipitations (Jones et al., 2009).	2.8 - 5.0	Potential	Potential	Expected	
Boreal forest dieback (BF)	Increased water stress, peak summer heat stress, vulnerability to disease and fire frequency due to higher temperatures cause boreal forest dieback and transition to open woodlands or	3.4 - 5.4	Not expected	Potential	Expected	

	grasslands, which in turn would amplify summer heat stress, drying and fire frequency (Lenton 2012)				
El Niño- Southern Oscillation change in amplitude (EN)	Increased heat uptake in the equatorial Pacific could lead to a permanent deepening of the thermocline, which could result in more persistent El Niño-like conditions. However, it is not excluded that stronger warming of the west Equatorial Pacific than the east could lead to more persistent La Niña-like conditions (Lenton et al., 2008). Complex and uncertain mechanism.	3.4 - 5.9	Not expected	Potential	Expected
Permafrost loss (P)	Thawing of permafrost (highly rich in organic carbon) in the northeastern Siberia (Yedoma) triggers biochemical decomposition of the organic matter, which generates heat that further increases warming and melting.	$5 - 8.5^{\ddagger}$	Not expected	Not expected	Expected
Arctic winter sea ice loss (AW)	Besides ice-albedo feedback (see Arctic summer sea ice) also reduced ice thickness creates a positive feedback that leads to complete ice loss.	4.8 - 8.2 <sup>§</sup>	Not expected	Not expected	Expected
Atlantic thermohaline circulation shutoff (TC)	Addition of freshwater in the North Atlantic (due to sea ice and Greenland ice sheet melting, river inputs and ocean precipitation) may reduce the density-driven sinking of North Atlantic waters until the Atlantic thermohaline circulation is significantly slowed down or even stopped (US CCCEF, 2009).	3.1 - 4.6	Not expected	Potential	Expected
North Atlantic subpolar gyre convection collapse (SG)	Warming and freshening of the North Atlantic subpolar gyre (an area of cyclonic ocean circulation in the Northwest Atlantic) leads to stratification (as consequence of lower surface density), that weakens the local deep convection, which in turn amplifies the stratification (because of reduced inflow of saltier water from the surroundings), eventually leading to permanent convection collapse. This collapse involves only the subpolar gyre (which is	1.2 - 3.8	Potential	Expected	Expected

	part of the TC) and not the whole				
	North Atlantic TC.	20.44			
Sahara/Sahel and	Warming of sea surface	2.9 – 4.4	Potential	Potential	Expected
west Alfican	direction of the West African				
monsoon sniit	direction of the west African				
(Alvi)	roinfall in the Sahara/Sahal				
	ragion. It is uncertain whether				
	WAS will shift porthward				
	(leading to increased rainfall) or				
	southward (leading to further				
	drying of the Sahel)(Lenton				
	2012).				
Alpine glaciers	Increased temperatures cause	1.2 - 3.0	Expected	Expected	Expected
loss (AG)	reduction in snow and ice cover,		1	1	r
. ,	originating a positive ice-albedo				
	feedback, and prolongation of				
	the melting season, which				
	destabilizes the glacier mass				
	balance towards glacier thinning				
	and disintegration (Levermann et				
	al., 2012)				
Coral reefs	Increased sea temperature due to	1.2 - 2.5	Expected	Expected	Expected
deterioration	global warming results in coral				
(CR)	bleaching (breakdown of				
	symbiosis between corals and the				
	algae that live inside their				
	tissues) and mortality. Moreover,				
	increased atmospheric $CO_2$				
	vertaka hu accora whom CO				
	reacts to form carbonic acid				
	which reduces the availability of				
	carbonate ions and the rate of				
	calcification of corals ultimately				
	favoring erosion. Both processes				
	trigger multiple ecological				
	feedback loops that eventually				
	drive reefs to a non-coral				
	dominated state (Hoegh-				
	Guldberg et al., 2007).				

\* Selected as potential tipping element as in done in Fabbri et al. (2021), but not considered in the calculation of endpoint

 $MCTP_{endpoint}$  because tipping thresholds are expected only at global temperatures above 5°C, which are not modelled due to lack of species loss estimates at these temperature levels.

<sup>§</sup> Considered only when potential tipping thresholds fall between 4.8 and 5°C.

## S2. Determination of fraction of species lost

For local species loss, five pairs of data linking a change in species loss with a change in global mean temperature based on (Newbold, 2018) are fitted to a linear regression model to obtain a continuous curve for species loss as a function of temperature change. Four of these data pairs were derived by combining the predicted losses due to the future evolution of four climate variables (minimum temperature of the coldest month, total annual precipitation, growing degree days and water balance) with the temperature change expected in 2070 for each of the four RCP (Representative Concentration Pathway) scenarios considered in the study (RCP2.6, RCP4.5, RCP6 and RCP8.5). This was done through separate runs of the model in (Newbold, 2018) and by excluding any weighting (by cell area and by total natural vertebrate species richness) performed in the study that would otherwise introduce a bias in our calculations. The fifth data pair was set to be (0,0), so that no change in temperature corresponds to no change in species loss. The regression model was fitted to the logit-transformed species loss estimates and keeping the original reference period, 1960 - 1990, for the temperature change data. The obtained curve was then converted to a pre-industrial reference (as in Figure 2 of the main article) by shifting the curve by  $0.5^{\circ}$ C on the x-axis, corresponding to the additional warming since pre-industrial to 1980 - 1999 period (Meinshausen et al., 2011), and by 0.0069 on the y-axis, corresponding to the additional fraction of species lost since preindustrial extrapolated from the initial curve fit (i.e. obtained by substituting x = 0.5°C in the fitted curve equation). Using the value  $(0.5^{\circ}C)$  for additional warming since preindustrial to 1980 - 1999 period, rather than up to period 1960 - 1990, could introduce a slight bias, however no closer estimate was found.

For global species loss, a total of 6 pairs of data was used: four were taken directly from the text in (Urban, 2015), one was derived graphically from Figure 2 in (Urban, 2015) using the online tool WebPlotDigitizer and, similarly to the above, one was set to be (0,0) as no species loss is assumed without temperature changes. The regression model was fitted to the logit-transformed species loss estimates without the need for additional transformations, as the study uses temperature changes that are already referenced to the pre-industrial period.

**Table S2**: Linear models fitted to the logit-transformed predictions of local and global fraction of species lost ( $\Delta F_{loss}$ ) as a function of global temperature change, and goodness-of-fit statistics. SSE: sum of squares due to error, RMSE: Root mean squared error.

	Local species loss Global species loss			loss
Data from model ((Newbold, 2018) for local and (Urban, 2015) for global model)	Temperature change relative to 1960 – 1990 (°C)	$\Delta F_{ m loss}$	Temperature change relative to pre-industrial (°C)	$\Delta F_{\rm loss}$
	0	0	0	0
	1.96	0.029	0.8	0.028
	2.88	0.096	2	0.052
	2.92	0.095	3	0.085
	4.32	0.20	4.3	0.16
			5	0.21 <sup>a</sup>
Fitted curve equation	y=a*x+b		y=a*x+b	
a (95% confidence bounds)	0.785 (0.601, 0.969)		0.600 (0.384, 0.815)	
b (95% confidence bounds)	-4.574 (-5.090, -4.059)		-4.116 (-4.780, -3.452)	
SSE	0.102		0.460	

R-square	0.984	0.937
Adjusted R-square	0.979	0.922
RMSE	0.184	0.339

<sup>a</sup> Retrieved graphically from Figure 2 in (Urban, 2015).

# **S3.** Additional results

**Table S3:** Factors used in the calculation of endpoint MCTP of 1 kg  $CO_2$  (*MCTP*<sub>endpoint,CO<sub>2</sub></sub>) for three different emission years (2020, 2050 and 2100) in the sample iteration illustrated in Figure 3 of the main article. Factors are as described in equations 1 - 5. Shaded background indicates ranking between emission years, with darker color for higher values.

	Emission year ( $T_{\text{emission}}$ )		n)
	2020	2050	2100
$MCTP_{CO_2}(T_{emission})$ - midpoint MCTP [pptrc/kg]	7.22E-03	8.16E-03	9.60E-03
$T_{\text{tipping},j_{\text{last}}}$ - Year of the last tipping point [year]	2103		
$TEMP(T_{tipping, j_{last}})$ - Temperature at last tipping point [°C]	3.64		
$TEMP(T_{emission})$ - Temperature at emission year [°C]	1.10	1.92	3.52
$\Delta TEMP(T_{\text{emission}}) - [^{\circ}C]$	2.54	1.72	0.12
$\frac{\Delta TEMP(T_{emission})}{1 \cdot 10^{12}} - [°C/ppt_{rc}]$	2.53E-12	1.71E-12	1.16E-13
$F_{\text{lost}}(T_{\text{tipping},j_{\text{last}}})$ - Fraction of species lost at $T_{\text{tipping},j_{\text{last}}}$ [unitless]	0.13		
$F_{lost}(T_{emission})$ - Fraction of species lost at $T_{emission}$ [unitless]	0.03	0.05	0.12
$\Delta PDF(T_{\text{emission}})$ - [unitless]	0.1	0.08	0.01
$\frac{\Delta PDF(T_{emission})}{\Delta TEMP(T_{emission})} - [PDF/^{\circ}C]$	0.04	0.05	0.08
$MEF(T_{emission})$ - Mid-to-endpoint factor [PDF/ppt <sub>rc</sub> ]	9.56E-14	7.71E-14	7.46E-15
$MCTP_{\text{endpoint},CO_2}(T_{\text{emission}})$ - endpoint MCTP [PDF/kg]	6.90E-16	6.29E-16	7.16E-17



**Figure S1**: Average (geometric mean) endpoint climate tipping potential (MCTP<sub>endpoint</sub>) of 10 kg of CO<sub>2</sub> (cyan), 1 kg of CH<sub>4</sub> (black) and 1 kg of N<sub>2</sub>O (red) under RCP6 pathway, expressing potentially disappeared fraction of species at global level at different emission times.

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# Supplementary Information-2

# Development of metrics for climate tipping in life cycle assessment based on damage to ecosystems

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Supporting information 2 is an Excel file providing multiple climate tipping point potential (MCTP) values at endpoint for 1 kg CO<sub>2</sub>, CH<sub>4</sub>, N<sub>2</sub>O and for three Representative concentration pathways (RCP). Values are divided into potential species loss at local and global levels.

# **Article III**

Implications of accounting for multiple climate tipping impacts in life cycle assessment: examination of two case studies

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# Implications of accounting for multiple climate tipping impacts in life cycle assessment: examination of two case studies

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## Abstract

Multiple climate tipping is a new impact category suggested for use in life cycle assessment (LCA) of products and services. It is complementary to traditional greenhouse gas (GHG) accounting using global warming potentials (GWP) as emission metric, as it captures the contribution of greenhouse gas (GHG) emissions to crossing several climatic tipping points, including Arctic summer sea ice loss, West Antarctic ice sheet collapse, or El Niño-Southern Oscillation change in amplitude. We examined two agricultural LCA case studies on chars made from biomass with different stabilities in soils (i.e., biochar and hydrochar) to test the new emission metric, the multiple climate tipping points potential (MCTP), in a comparative LCA context. We found that hydrochar with low stability performed best in relation to multiple climate tipping, which is in contrast to assessments using GWP metrics. Ranking of biochar with different stabilities was, however, the same for both impact categories (and it was the biochar with the high stability in soil, which consistently performed best). The magnitude of MCTP impact scores was found to depend on both the total amount of carbon evolved as GHG over the time frames for which MCTPs are relevant, and on the stability of a given char in the soil. This shows that inclusion of multiple climate tipping as impact category is particularly relevant in LCA of those chars, which degrade and release GHGs within next one to two centuries.

## **1. Introduction**

Climate tipping is as a life cycle impact category which addresses potential contribution of greenhouse gas (GHG) emissions to crossing climate tipping points, like Arctic summer sea ice loss, West Antarctic ice sheet collapse, or El Niño-Southern Oscillation change in amplitude [1–3]. In this approach, the impact caused by a GHG emission is compared to the remaining capacity of the atmosphere to absorb that impact without exceeding climatic tipping points. The resulting emission metric, the multiple climate tipping points potential (MCTP), is therefore expressed as a fraction of the remaining carrying capacity taken up by the emission (here, in parts per trillion of the remaining capacity). The MCTP values are sensitive to emission timing, and on the projected time of the tipping points, as they depend on global temperature levels that trigger tipping and evolution of background anthropogenic GHG emissions. The MCTP factors represent a separate impact category and should be seen as complementary to the existing global warming potential (GWP) and global temperature change potential (GTP) metrics [3–5].

Temperature thresholds triggering tipping points are uncertain. For example, the West Antarctic ice sheet collapse tipping point is projected to occur at temperature increases between 1 to 5.7 °C [6]. Accounting for these uncertainties shows that the probability of different climate tipping points to occur is highest between year 2040 and 2060 for the background GHG concentrations following RCP6 pathway (Representative Concentration Pathway stabilizing the climate to 6 Wm<sup>-2</sup> after 2100) [3]. MCTP values are nearly twice higher for emissions in 2050 when compared to emissions occurring in 2021. This was found important for climate tipping impacts from degradation of plastic polymers. For example, significantly higher impact scores were computed for stable, but still biodegradable, polymers (like those with mineralization kinetics corresponding to 90% degradation in 105 years) when compared to more readily biodegradable ones (with kinetics corresponding to 90% degradation in 2 years) [3]. This is because a significantly higher portion of emissions from more stable polymers was released in the period when probability of tipping points to occur was the largest.

Biochar and hydrochar are examples of carbonaceous products for which climate tipping impacts can be relevant [7–10]. Both chars are made from biomass residues and

can be used in agriculture for increasing crop yields, while providing additional benefits from carbon sequestration and (temporary) storage [7,8,11–13]. Biochar stability in soils can vary by up to three orders of magnitude, depending on the type of feedstock and pyrolysis conditions [14,15]. Hydrochar, however, degrades faster due to the simpler chemical structure and larger content of labile carbon [12]. Alternative applications of the chars include their use as bioenergy source, e.g. for household cooking [16,17]. Environmental performance of biochar and hydrochar systems has been assessed in several LCA studies published so far [18–24]. Climate tipping impacts of hydrochar have previously been studied in Owsianiak et al. [2] using the climate tipping potential metric of Jørgensen et al. [1], which considers one tipping point (Arctic Summer sea ice loss). Potential impacts of chars on crossing multiple climate tipping points have not been quantified until now.

The aim of our paper is to assess the performance of biochars and hydrochars from a multiple climate tipping perspective. For this purpose, we revisited two earlier LCA studies. The first study assessed and compared life cycle impacts of biochar production and agricultural use in Indonesia [20]. The second study evaluated the environmental performance of hydrochar production and agricultural use in Spain [2]. Degradation of chars in soils was assumed to follow bi-exponential decay kinetics, and comparisons were made between chars representing a relatively wide range of mineralization rate constants [14,25]. In addition, we modelled impacts for a new scenario where biochar is used as a source of energy for household cooking. Resulting

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inventories of GHG emissions were used as direct input to quantification of multiple climate tipping impacts using MCTPs factors of Fabbri et al. [3]. Comparisons were made with GWP100 as complementary emission metric.

#### 2. Methods

#### 2.1 Examined case studies

The goal and the functional units of the examined case studies are the same as in the underlying studies. The reader should note that the functional units do not allow for direct comparisons between biochar and hydrochar systems to be made. Thus, both cases should be interpreted separately from each other. Details of the examined case studies are presented in Table 1.

#### 2.1.1 Biochar

The biochar case is based on Owsianiak et al. [20], who conducted an LCA on biochar production and its agricultural use in Indonesia. The study included the complete life cycle of biochar from the collection of biowaste for biochar production to application and mineralization of biochar on agricultural soil. Four biochar scenarios were analyzed (Table 1). Three of them consider variations in the mineralization rate of biochar when applied to soil according to measured kinetic parameters, representing scenarios for low, average, and fast mineralization kinetics, respectively, for both labile and recalcitrant fractions of biochar. In the fourth scenario, biochar is used as energy source in replacement of wood for household cooking. This additional scenario was not included in Owsianiak et al. [20], and was modeled here to represent a case in which the carbon stored in the material is immediately released to the atmosphere during use, without any temporally differentiated process involved in the life cycle. System boundaries for this case include production and disposal of the cooking stove, avoided cooking using wood (mainly avoided emissions to air), and emissions to air from biochar burning (Figure S1 in Supplementary Material).

#### 2.1.2 Hydrochar

For the hydrochar system, we considered three scenarios from the case study in Owsianiak et al. [2], studying the full plant scale production of hydrochar from green waste for soil conditioning application in barley cultivation. System boundaries include a full life cycle starting from collection of green waste, production of hydrochar at the hydrothermal carbonization (HTC) plant, transport and application to agricultural soil. Similarly to biochar, hydrochar can have different stabilities in the soil, thus also in this case the three compared scenarios represent slow, average and fast mineralization rates scenarios of hydrochar, for both labile and recalcitrant pools. Mineralization of hydrochar in the soil is the only relevant time-differentiated process in the life cycle that was modeled. Composting of green waste (included as replaced waste treatment by the hydrochar system) could be the other process where carbon emissions from the green waste are distributed over time. However, it was not considered because the

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mineralization kinetic constants found for different composting substrates suggest that degradation occurs in relatively rapid periods (typically within one year), making it not relevant to model dynamic emissions from composting (see Section S1.2 in

Supplementary Material).

**Table 1.** Overview of scenarios considered in this study taken from the biochar and hydrochar

 case studies examined in [2,20]. Default values were assumed for parameters that were perturbed

 in the original studies (Table 2 in [2] and Table 3 in [20]), except for mineralization rate constants.

 Potential emissions of methane, nitrous oxide, and ammonia from hydrochar application to soil

 examined in the original study were not considered, as they were not included in the baseline

 scenarios of the underlying studies.

Details of the case study	Biochar				Hydrocha	r			
Goal of the underlying study	"to assess and compare life cycle impacts of biochar systems in Indonesia in order to support decision making related to the implementation of biochar as a waste management strategy in four Indonesian island communities "			"to evaluate the application of hydrochar to agricultural soils as a potential technology for carbon sequestration and temporary storage"					
Functional unit (f.u)	"Treatment of 1 kg of biogenic carbon from biomass residues in rural areas in Indonesia"			"Average application and storage of 1 kg of biogenic HTC carbon to a temperate agricultural soil"					
Scenario a,b	B1	B2	B3	B4	H1	H2	H3		
Char application	Soil cond	oil conditioner Energy Soil conditioner source							
Geographic location	Indonesia			•	Spain				
Biowaste type	Biomass 1	ass residues Green waste							
Production technique	low-cost pyrolysis technology based on "Kon Tiki" flame curtain kiln			Hydrothermal carbonization installation operating at full commercial scale		ation full			
Production capacity	~30 kg/da	y (dry weig	ght)		~30,000 kg	g/day (dry we	eight)		
Replaced waste management system	None (not required by the functional unit) Composting								
Avoided crop production	Maize			Not relevant	Barley	Barley			

Avoided fertilizer	NPK and urea			Not	NPK			
				relevant				
Avoided heat	Not releva	Not relevant			Not relevant			
generation process				using				
				wood				
Negative priming	Considere	ed		Not	Not consid	Not considered		
effect				relevant				
Mineralization rate	Slow	Average	Fast	Not	Slow	Average	Fast	
constant of labile	(1.67E-	(7.18E-	(1.75E-	relevant	(1.20E-	(8.10E-	(1.40E-	
carbon pool (day-1)	03)	03)	02)	(immediate	02)	02)	01)	
				release)				
Mineralization rate	Slow	Average	Fast	Not	Slow	Average	Fast	
constant of	(2.52E-	(2.35E-	(1.67E-	relevant	(1.40E-	(3.00E-	(1.40E-	
recalcitrant carbon	08)	06)	05)	(immediate	04)	04)	03)	
pool (day <sup>-1</sup> )				release)				
Time differentiated	Mineralization in soil		None	Mineralization in soil				
life cycle process								

<sup>a</sup> Scenarios B1, B2, and B3 represent scenarios 1 in Owsianiak et al. [20], with default (B1), and perturbed mineralization rate constants (minimum for B2 and maximum for B3). Scenario H4 was not included in ref [20] and is modelled separately in this study

<sup>b</sup> Scenarios H1, H2, and H3 represent scenario 1 default in Owsianiak et al. [2], with default (H1), and perturbed mineralization rate constants (low for H2 and high for H3)

#### 2.2 Impact assessment

Multiple climate tipping impact scores were calculated using the MCTP metric using data on life cycle GHG emissions inventories reported in the underlying studies [2,20]. The total MCTP impact score ( $IS_{MCTP}$ ) was calculated by summing indicator scores calculated for the time-differentiated processes with the indicators scores calculated for those processes that are not temporally distributed [3]. Application of biochar and hydrochar to soil was assumed to take place in year 2021, and evolution of CO<sub>2</sub> through mineralization of the chars applied to soil was the only time-differentiated process in our scenarios. Thus, the annual masses of CO<sub>2</sub> evolved from the soil from the application year 2021 until the year when MCTP factors are available (i.e., the year of last tipping point) were multiplied by emission-year specific MCTPs, and the resulting indicator scores added (eq.1 given for generic GHG *i*). The same was done for those emissions, which were not temporarily differentiated. These emissions were characterized using MCTP factors for year 2021.

$$IS_{\text{MCTP}} = \sum_{i} \sum_{T_{\text{emission}}=2021}^{T_{\text{tipping}, j_{\text{last}}}} m_i(T_{\text{emission}}) \cdot MCTP_i(T_{\text{emission}})$$
(1)

where  $T_{\text{emission}}$  is the year of emission,  $T_{\text{tipping},j_{\text{last}}}$  is the last year for which MCTP factors are available,  $m_i(T_{\text{emission}})$  is the mass of GHG *i* emitted in a given year  $T_{\text{emission}}$  and  $MCTP_i(T_{\text{emission}})$  is the MCTP of GHG *i* for year  $T_{\text{emission}}$ . Given that MCTP factors vary according to the assumed background GHG concentrations scenario, we calculated three sets of MCTP impact scores using MCTP factors for RCP4.5, RCP6 and RCP8.5 pathways, as provided in Fabbri et al. [3]. Based on this,  $T_{\text{tipping},j_{\text{last}}}$ corresponds to year 2093, 2117 and 2212 for the three pathways, respectively. MCTP scores were expressed in parts per trillion of remaining capacity, ppt<sub>rc</sub>, expressing the total fraction of remaining capacity depleted by the assessed functional unit.

Ranking of biochar and hydrochar scenarios according to their multiple climate tipping impact scores was compared with the ranking obtained using GWP100 as emission metrics. Climate change (GWP100) impact scores were calculated following the ILCD's recommended method (ILCD 2011 Midpoint+, version 1.09 as implemented in SimaPro, version 9.1.0.11, PRé Consultants bv, the Netherlands) which gives credits for the (temporary) storage of carbon due to delayed emissions [26].

#### 3. Results and discussion

#### 3.1. Multiple climate tipping impacts for biochars

Figure 1 shows multiple climate tipping impact scores for the four biochar scenarios calculated with the MCTP factors, and climate change impact scores calculated with the GWP100 factors. The following observations can be made. First, multiple climate tipping impact scores are all positive (indicating no contribution to climate change mitigation), except for the bioenergy scenario where negative impact scores are calculated. This observation for the multiple climate tipping impact category remains unaffected by the RCP pathway considered. Second, all four biochar systems, including the bioenergy system, are expected to bring environmental benefits in terms of climate change (GWP100) impacts. The third observation is that ranking biochar systems remains unaffected by the type of metric used. Increasing biochar stability in soils improves environmental performance of biochar, and the bioenergy scenario is always better than agricultural use.



**Figure 1**. Characterized MCTP (in ppt<sub>rc</sub>) (**a**) and GWP100 (in kg CO<sub>2</sub> eq.) (**b**) impact scores for the four biochar scenarios (presented in Table 1) with functional unit 'treatment of 1 kg of biogenic carbon from biomass residues in rural areas in Indonesia'. For each scenario, three MCTP scores are presented based on MCTP factors for RCP4.5, RCP6 and RCP8.5, respectively. Impact scores are reported in Table S2 of Supplementary Material.

Figure 2 shows that multiple climate tipping impacts of the biochar systems are mainly driven by emissions of  $CO_2$  during the production stage of biochar. Contribution from mineralization of the biochar is important for the least stable biochar only (up to 30% contribution to total tipping impact). For the bioenergy scenario, emissions from biochar burning are also important, but combined emissions from biochar burning and production modelled in this scenario become outweighed by credits from replaced cooking using wood.

Somewhat different pattern is observed for the GWP100 approach, where biochar production is seen to bring environmental benefits, rather than burdens. This is because impacts from CO<sub>2</sub> emissions in the GWP100 approach are outweighed by benefits stemming from carbon fixation when biomass is grown and becomes feedstock for pyrolysis, which were considered in the underlying biochar study. Biomass used for biochar production originates from annual cropping systems, and CO<sub>2</sub> released from biochar mineralization is assumed to be re-captured quickly due to fast  $CO_2$  uptake by crop re-growth. Thus,  $CO_2$  sequestered from air into crop biomass was assigned a GWP equal to -1 kg CO<sub>2</sub> eq., consistently with recommendations of IPCC [27]. The MCTP metrics does not account for this carbon sequestration mechanism. Yet, ranking of biochar systems with MCTP was not influenced by this methodological difference, which can be explained by the fact that differences between biochar systems depended solely on the amounts of  $CO_2$  evolved from the soil over time (rather than emission timing). Biochar is relatively recalcitrant and the total amount of carbon that is re-emitted to the atmosphere (over relevant time frames) differed significantly between the three scenarios. For instance, 46% was released over 100 years for the least stable biochar (fast mineralization) when compared to 9 and 1% released for the two more stable chars. This, ranking between biochar depended mainly on differences in total re-emitted carbon, rather than timing of  $CO_2$  emissions. For the scenario where biochar is used as energy source, both metrics attribute most of the benefits to avoided emissions from cooking using wood.

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**Figure 2**. Contribution of life cycle processes to total MCTP (left) and GWP100 (right) impacts scores for the biochar scenarios, scaled to 100% of the total impact. Note that 'mineralization' is the only possible process that can vary among the scenarios for slow (B1), average (B2) and fast (B3) biochar mineralization rates, however full contribution analysis is shown to highlight differences between the two metrics.

#### 3.2. Multiple climate tipping impacts for hydrochars

Characterized results for the hydrochar scenarios are presented in Figure 3. First, it shows that multiple climate tipping impact scores are generally negative (indicating contribution to climate change mitigation), except for the scenario with slow mineralization kinetics. This is mainly due to benefits from the avoided waste management system for the green waste (not considered in the biochar system as it was not required by the functional unit). Second, as for biochar, all systems are expected to bring benefits in terms of climate change (GWP100) impacts. The third observation is that ranking of hydrochar systems is somewhat affected by the metric chosen. More stable hydrochar performed better when GWP100 is used as emission metric, but the opposite is found for the MCTP metrics

(where more stable hydrochars perform worse). This finding is in contrast to the biochar cases, where the choice of metric did not influence the identification of the type of biochar that performed best. In addition, the choice of RCP pathway is slightly more influential for hydrochar, when compared to biochar. The choice of scenario was particularly relevant for the stable hydrochar, where burdens are expected assuming RCP4.5 and RCP6 pathways, but not the RCP8.5 pathway. Despite this sensitivity to the RCP pathway, there was no influence on which hydrochar performed best in terms of multiple climate tipping.



**Figure 3**. Characterized MCTP (in  $ppt_{rc}$ ) (**a**) and GWP100 (in kg CO<sub>2</sub> eq.) (**b**) impact scores for "average application and storage of 1 kg of biogenic HTC carbon to a temperate agricultural soil'. GWP100 results showed in (b) are taken from ref. [2]. For each scenario, three MCTP scores are presented based on MCTP factors for RCP4.5, RCP6 and RCP8.5, respectively. Impact scores are reported in Table S2 of Supplementary Material.

The contribution analysis for hydrochar shows that total impact scores are determined by emissions from mineralization of hydrochar, combined with replaced biowaste treatment (composting) (Figure 4). The multiple climate tipping impacts from the carbon re-emitted during mineralization increase with increasing stability of the hydrochar due to differences in emission timing and corresponding magnitude of MCTP factors (which were largest for emissions from most stable hydrochar). As total CO<sub>2</sub> emissions released over the time frames considered by MCTP factors (i.e. 73, 97 and 192 years for MCTP based on RCP4.5, RCP6 and RCP8.5, respectively) were similar, timing of emissions and, in particular, their proximity to climate tipping points become very important. The least stable hydrochar, which degrades by 99.5% in 10 years, is associated with lower impacts because most emissions occur within the first 10 years and will not contribute to trigger tipping points that are expected after this time. By contrast, the most stable hydrochar, also releasing 99.5% of its carbon but in 100 years, performs worst because emissions are distributed over a longer period and have higher chance to occur in periods with higher risk of crossing tipping points (where MCTP factors are the largest). This is different from the GWP100, where the impact of emissions from mineralization increases with decreasing stability of the hydrochar due to increasing benefits from temporary carbon storage.

Analogous results for hydrochar were found in ref. [2], where the same scenarios were assessed with the climate tipping potential (CTP) of Jørgensen et al. [1] which considers just one tipping point (Arctic Summer sea ice loss). CTP scores also increase as

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hydrochar stability increases, but our MCTP scores are higher because the time frame for which MCTP factors are available is longer (indeed, CTP factors of Jørgensen et al. are available only until 2032), and furthermore because in the original CTP approach the carbon sequestered from the atmosphere and later stored is given credits when stored sufficiently long beyond the tipping time (50 years). In the current MCTP approach, emissions occurring after 50 years of storage contribute to crossing other tipping elements.



**Figure 4**. Contribution of life cycle processes to total MCTP (left) and GWP100 (right) impacts scores for the hydrochar scenarios, scaled to 100% of the total impact. GWP100 results are taken from ref. [2].

#### 3.3 Does MCTP add value in LCA?

We showed that the added value from including multiple climate tipping as an impact category in LCA of chars products depended on the type of char. The magnitude of MCTP impacts depends both on the stability of a given char in the soil (and associated temporal evolution of GHG emissions), and on the total amount of carbon mineralized and evolved as GHG over the relevant time frame (i.e., time frame for which MCTPs are relevant and available). Relatively high stability of biochar when compared to hydrochar means that only a small part of total biochar-carbon evolves as GHG within this time frame. Thus, differences in biochar mineralization kinetics have large influence on total GHG emissions, increasing or decreasing MCTP scores in concert. Timing of GHG emissions becomes in those cases not important. For hydrochars, however, nearly all hydrochar-carbon becomes mineralized over the relevant time frame, and it is then the timing of emissions, rather that total emitted mass, that determines magnitude of MCTP impact scores. These scores are higher for more stable hydrochar, because for these hydrochars the largest portion hydrochar-carbon is emitted in close proximity to climate tipping points (in years ca. 2040-2060). Thus, in the comparative LCA context, additional insights (when compared to the GWP100 metrics) were only gained for hydrochars. It can be expected that inclusion of multiple climate tipping as an impact category can influence LCA results and ranking of products made from materials which degrade gradually over time, reaching at least 95% degradation in around 70 years. This includes not only hydrochars, but also a range of biodegradable plastics [28].

## 4. Conclusions

We evaluated the relevance of considering multiple climate tipping as an impact category in LCA of two carbonaceous materials (biochar and hydrochar). In the comparative LCA context, we showed that MCTP does brings additional insights mainly in the case of hydrochar, and not so much for hydrochar. We therefore recommend including multiple climate tipping in LCA, particularly for those materials which release most of their carbon as GHGs over next two centuries. As the choice of underlying RCP scenario for the MCTP factors had some influence on identification of which hydrochar performed best, we also recommend testing sensitivity of comparative LCA results to RCP pathways. Future improvement of the MCTP metrics should address carbon sequestration and accounting for temporary storage of carbon in bio-based materials. For MCTP, which considers multiple tipping points beyond Arctic sea ice and for which a carbon emission will always contribute to trigger some tipping point no matter when it is re-emitted, assigning credits to temporary storage is, however, not so straightforward.

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### **Supplementary Material**

Supplementary methods and results
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# Supplementary material for

# Implications of accounting for multiple climate tipping impacts in life cycle assessment: examination of two case studies

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S1. Supplementary methods

- S1.1 System boundaries for biochar system energy source application
- S1.2 Mineralization kinetics during composting
- S2. Supplementary results

# S1. Supplementary methods





**Figure S1**: System boundaries for management of 1 kg of biogenic carbon from biowaste with energy recovery (scenario B4 in Table 1 in the main article).

#### S1.2 Mineralization kinetics during composting

First order kinetics is often used assuming either one or two or even three carbon fractions with different stabilities [1,2]. The mineralization kinetic constants of found for different composting substrates suggest that degradation is quite fast and typically most of the carbon is re-emitted within one year (Table S1). No data was found for composting of green waste only; however it is assumed that the material is likely to be mixed with other biowaste types in a real compost facility, resulting in similar kinetics.

**Table S1**: Mineralization rate constants during composting for different biowaste types. k1 refers either to the mineralization rate of the faster carbon fraction when used in a bi- exponential decay model or the rate of the whole carbon fraction used in single exponential models. k2 is the mineralization rate of the slower carbon fraction in bi-exponential models.

Biowaste type	k1 (day <sup>-1</sup> ) <sup>a</sup>	k2 (day-1) <sup>b</sup>	Source
Different blends of wheat straw, cotton	0.4	0.06	[3]
cardings, meat bone meal, hydrolyzed leather,	0.5	0.07	
blood meal and horn and hoof meal	0.9	0.04	
Municipal solid waste (organic fraction)	0.053		[4]
	0.180		
	0.095		
	0.10		
	0.17		
	0.048		
	0.12		
	0.13		
	0.17		
	0.26		
	0.26		
	0.33		
Different blends of olive mill waste, winery	0.040		[2]
waste, sewage sludge and reeds	0.049		
	0.070		
	0.085		
	0.035		
	0.025		
	0.134		
	0.079		
	0.022		
	0.031		
	0.070		
	0.086		
	0.057	0.0025	
	0.067	0.0052	
	0.103	0.0052	
	0.125	0.0079	
	0.054	0.0038	
	0.068	0.0010	
	0.137	0.0135	
	0.135	0.0074	1
	0.046	0.0003	
	0.049	0.0014	

0.108	0.0060	
0.110	0.0081	

# **S2.** Supplementary results

**Table S2**: Characterized MCTP and GWP impact scores per functional unit (f.u.) for the examined biochar and hydrochar scenarios. 'Slow', 'Average' and 'Fast' correspond to the mineralization rates during application to soil.

	MCTP for	MCTP for	MCTP for	GWP100		
	RCP4.5	RCP6	RCP8.5	(kg CO <sub>2</sub> eq.		
	(pptrc/f.u.)	(pptrc/f.u.)	(pptrc/f.u.)	/ <b>f.u.</b> )		
Biochar (Functional unit: "Treatment of 1 kg of biogenic carbon from biomass residues in						
rural areas in Ind	onesia")					
B1 - Slow	1.45E-02	1.15E-02	1.41E-02	-1.01E+00		
B2 - Average	1.58E-02	1.27E-02	1.50E-02	-9.61E-01		
B3 - Fast	2.24E-02	1.80E-02	1.87E-02	-7.06E-01		
B4 - Biochar as	-2.73E-03	-3.21E-03	-2.53E-03	-2.69E+00		
energy source						
Hydrochar (Functional unit: "Average application and storage of 1 kg of biogenic HTC						
carbon to a temperate agricultural soil")						
H1 - Slow	3.56E-03	2.81E-03	-6.99E-03	-1.19E+00		
H2 - Average	-2.41E-03	-7.82E-05	-5.57E-03	-8.57E-01		
H3 - Fast	-1.10E-02	-5.40E-03	-1.14E-02	-6.14E-01		

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# **Article IV**

# Environmental performance of polyhydroxyalkanoate (PHA)-based plastics with improved barrier properties.

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# Environmental performance of polyhydroxyalkanoate (PHA)-based plastics with improved barrier properties

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# Abstract

There is an increasing interest in lowering permeability of bioplastics materials toward oxygen, water vapor and aromas, to make them suitable for contact with food. Barrier properties of polyhydroxyalkanoate (PHA)-based plastics can be improved by combining PHA with layers of poly(lactic acid) (PLA), aluminum, or aluminum oxides. However, nothing is known about environmental performance of improved PHA plastics when the whole value chain is considered. We employed life cycle assessment (LCA) to quantify environmental impacts of the value chain, discover sensitivities and determine decisive factors. To provide additional insights into environmental performance, we included a new impact category relevant for LCA of biodegradable materials, the multiple climate tipping. Results suggest that: (1) sugar beet molasses used as feedstock is an environmental hot spot, contributing significantly to a wide range of environmental problems; (2) increasing PHA production scale from pilot to full commercial scale increases environmental impacts, mainly due to differences in PHA yield; (3) PHA films

with high biodegradability perform best in relation to climate tipping, but are not necessarily the best in relation to radiative forcing increase or global temperature change; and (4) further process optimization is necessary for the PHA-based plastics to become attractive alternatives to fossil-based plastics.

**Keywords:** bioplastic, circular economy, climate tipping points, sustainability, waste management

# **TOC/Abstract Graphic**



# **Synopsis**

Life cycle assessment of improved PHA-based bioplastics highlights the need to consider *multiple climate tipping* as a new impact category.

# **1. Introduction**

Bioplastics are a diverse group of materials which have been in the focus of research as alternative to conventional plastics (Spierling et al. 2018, García et al. 2019, Kookos et al. 2019, Pavan et al. 2019, Rameshkumar et al. 2020). Bioplastics consist of three subcategories and can either be (1) "fossil-based and biodegradable", (2) "bio-based and biodegradable" or (3) "bio-based and non-biodegradable". The last two categories can also be combined with the term bio-based plastics (Endres *et al.* 2011). The market share of bioplastics is predicted to continue to grow within the next years to 2.8 Mio. tonnes in

2025, an increase of 35 % compared to the production capacities in 2020 (European Bioplastics 2020b).

This study focuses on polyhydroxyalkanoate (PHA), a bio-based and biodegradable polyester which can be produced by bacterial fermentation (Chen et al. 2020, Moretto et al. 2020). The PHAs are produced as intracellular high-molecular inclusion bodies, which have a role as carbon- and energy storage compounds within the bacteria. The selection of different microbial production strains as well as adaptions of the bioprocess allows the composition of different PHA types (homo-, co-, ter-, and quadpolyesters), resulting in up to 150 different PHA structures which have been identified so far. Based on their carbon atoms used for the monomeric unit PHAs can be differentiated in two main groups: (1) short-chain-length PHAs with 3-5 carbon atoms and mediumchain-length PHAs with 6-14 carbon atoms. The most well-known and common PHA type is poly- $\beta$ -hydroxybutyrate (PHB) (Koller 2017, Kourmentza *et al.* 2017, Troschl *et* al. 2018). Additionally, for the production of PHA a wide range of feedstocks can be utilized, ranging from e.g. renewable materials like sugar, to industrial waste and byproduct streams as well as  $CO_2$ , which can be utilized by cyanobacteria types (Koller 2017, Kookos et al. 2019, Moretto et al. 2020, Wongsirichot et al. 2020). This makes PHA a versatile plastic type within the bioplastics and bio-based plastics.

Molasses, a co-product of sugar beet, is often considered as feedstock for PHA production (Baei *et al.* 2009, Keunun *et al.* 2018, Kiran Purama *et al.* 2018, Remor Dalsasso *et al.* 2019). Molasses contains about 50% of the disaccharide sucrose and is commonly used as an energy supplement to livestock feed. PHA exhibits physical and mechanical properties similar to those of conventional plastics, such as polyethylene (PE) and polypropylene (PP) (Kookos et al. 2019). A number of international patents about plastic materials based on PHA have been obtained (Elvers *et al.* 2016 and references therein). Yet, global production of PHA is relatively low (25,320 tons in year 2019), accounting for only 1.2% of the bioplastics market (Rameshkumar et al. 2020). The latest

market data for PHA predicts an increase to 11.5 % of the bioplastics market till 2025 (European Bioplastics 2020a). Currently PHA is manufactured worldwide at both pilot and industrial scale. Manufacturers are based in Canada, Germany, Italy, China, USA, Japan as well as Malaysia. On these scales mainly first-generation feedstock like sugar (e.g. from sugar beet) as well as vegetable oil (e.g. canola oil or palm oil) is dominant (Kourmentza *et al.* 2017). The reason for the low market share of PHAs is mainly due to high production costs (García et al. 2019, Kookos et al. 2019, Pavan et al. 2019), that are estimated to be 5–10 times higher than the cost of traditional polymers (Kookos *et al.* 2019).

One potential application of PHA is as food packaging material (Khosravi-Darani *et al.* 2015). For example, bioplastic is considered for packaging of high quality bakery products, replacing fossil based polypropylene. Yet, high permeability toward water, oxygen and aromas makes PHA a rather poor packaging material (Kassavetis et al. 2012). It is thus necessary to improve the barrier properties to lower permeability if PHA is to be used in contact with food (Struller et al. 2014). This can be done by lamination with (poly)lactic acid (PLA) or metallization with aluminium (Al) or aluminum oxides (AlOx) (Kassavetis et al. 2012). Until now, nothing was known about sustainability implications of lamination or metallization of PHA, which improve barrier properties but may impair biodegradability in their end-of-life. Environmental assessments of PHA production from molasses generally focused on the fermentation and PHA recovery steps, without considering other important process in the PHA-based plastic film life cycle like post-treatment and end-of-life (Leong et al. 2017, Kookos et al. 2019).

The purpose of this paper was to assess the environmental performance of the whole value chain of PHA-based plastics with improved barrier properties. We considered lamination using PLA or metallization using Al or AlOx as two viable surface treatment options. The environmental performance was assessed using life cycle assessment (LCA) conducted in accordance with the requirements of the ISO 14044

standard and the guidelines of the EU Commission's ILCD Handbook (ISO 2006, EC-JRC 2010). To provide additional insights, we present the inclusion of a new, relevant impact category for bioplastics LCA, the multiple climate tipping (Fabbri *et al.* 2021). The new multiple climate tipping points potential (MCTP) metric was used in concert with the two other recommended metrics of climate change (the global warming potential, GWP<sub>100</sub>, and the global temperature change potential, GTP<sub>100</sub>), and next to seventeen other categories of environmental impacts commonly covered in LCA.

# 2. Methods

#### 2.1 Scenarios

Molasses (containing the carbohydrate sucrose) was chosen as a feedstock and the Gramnegative bacterium *Ralstonia eutropha* as fermenting microbe because they were found promising for full scale applications (Baei *et al.* 2009, BioBarr 2019, Remor Dalsasso *et al.* 2019). Both pilot and large scale were modelled and compared. They differ in means of how feedstock is collected, pre-treated, fermented, recovered and purified. In addition to testing the influence of plant scale, we considered differences in (i) geographic location of the PHA plant, (ii) conventional use of molasses, (iii) composition of PHAbased films and other packaging materials, (iv) yield of PHA in the fermentation process, (v) thickness of the PHA layer, and (vi) fate of the improved bioplastic in its end-of-life. Production of poly-β-hydroxybutyrate (PHB) was modelled.

Italy and Germany were chosen as two representatives of countries where production of PHA is currently conducted. Differences in electricity grid mixes and waste management systems between the countries were considered. The waste management systems were modelled according to country-specific rates for recycling, incineration and landfilling of plastic packaging (Eurostat 2017). Bioplastic packaging is currently not recyclable. Thus, it was assumed that the remaining fraction was treated proportionally to the treatment of non-recovered plastic waste (that is, 50% landfilled and 50% incinerated in Italy and 100% incinerated in Germany). The conventional use of molasses is as animal feed, however, it can be also used for ethanol production (Takriti et al. 2017) and these two scenarios were also explored. We investigated optimization potentials for PHAbased plastics made from molasses, which lie in selection of the material for lowering permeability of the PHA (either PLA or Al or AlOx), optimizing PHA production yield and reducing thickness of the plastic layers. The PHA-based plastics were compared with fossil-based alternatives, namely PP and PE. Comparisons were also made with PLA. Merits of temporary carbon storage are often debated for bioplastics, and the end-of-life stage of the plastics life cycle is the only stage where temporal carbon storage can occur. PHA is generally considered as readily biodegradable (the actual duration of degradation depends on product dimensions as well as environmental parameters like temperature), but it is currently unknown how improving barrier properties influences biodegradability during landfilling (Emadian et al. 2017, Meereboer et al. 2020). Thus, fast degradation was assumed in the baseline scenario. Delayed biodegradation may be caused by differences in availability of water and oxygen during landfilling (Meereboer et al. 2020). Moreover, combining PHA with PLA has shown to reduce biodegradability of PHA (Meereboer et al. 2020). To explore sensitivities toward mineralization rates, different biodegradation rates and extents of lag phases were explored for the landfilling scenarios. We conservatively assumed that no PHA plastic is lost to the environment owing to generally sound management of plastic waste in Europe (Ryberg et al. 2019). In total, 53 scenarios were considered (refer to Table S3, Section S2 of SI for an overview of all scenarios).

#### 2.2 Literature review

Parameters and installations for fermentation, recovery and purification of PHA at pilot and large scales were modelled based on parameters retrieved from scientific literature, identified through a systematic literature review (See Section S1 of the SI for further details). The review encompassed studies focusing on both technical and environmental aspects of PHA production. It was carried out using Scopus in March 2020, applying a set of keyword strings. We retrieved those studies, which: (i) report parameters relevant for the PHA production (feedstock type and its water content, producing microorganism, plant scale and capacity), (ii) are either at pilot (as defined by the study itself or between 10-1000 L fermenter volume) or large (above 1000 L) scales, and (iii) either report PHA yield (kg<sub>PHA</sub>/kg<sub>feedstock</sub>), or sufficient data to estimate the yield. In total, 25 studies were retrieved. We found four studies which use disaccharides, and report data on resource consumptions (e.g. electricity, water and chemicals) (see Table S2 in Section S1). These four studies were used for extraction of parameters and bills of materials needed to model PHA production installations in our LCA.

#### 2.3 Overview of PHA installations

The pilot and large scale systems differ in how feedstock collection, pre-treatment and fermentation, recovery and purification are carried out (see Section S2 of the SI, Figure S1 for an overview of their installations). The remaining steps are the same and represent large-scale systems. The feedstock is transported by truck at pilot scale, whereas at large scale the feedstock is transported using pipes. At both scales, the feedstock is sterilized by steam and the sterilized feedstock is cooled down using a heat exchanger. At pilot scale, the sterilized feedstock is fermented in one 10-m<sup>3</sup> reactor for 80 hours. At large scale, three 102-m<sup>3</sup> reactors for 54 hours are used. Electricity input for aeration and agitation are different for the two scales. Fermentation yield is higher at pilot than at large scale (0.360 and 0.268 kg<sub>PHA</sub>/kg<sub>substrate</sub>, respectively). At both scales, PHA is extracted from fermenting cells and purified in a sequence of steps, involving centrifugation and spray drying, but electricity inputs are higher and consumption of materials generally lower at the pilot scale. Hydrochloride is used for extraction at pilot scale, while hydrogen peroxide and enzymes are used at large scale. The obtained PHA powder is compounded and blended with additives (plasticize, nucleating agent, stabilizer and

reinforcing filler) before extruding it into PHA pellets. These pellets are subsequently extruded into a PHA film. This film is either laminated with a layer of PLA, or metallized using aluminum. The aluminum layer can be optionally oxidized to aluminum oxide (AlOx) to make the resulting film transparent. Details of the parameters underlying LCA model are presented in the SI, Section S2.

#### 2.4 Life cycle assessment

#### 2.4.1 Functional unit and reference flow

The primary function of the PHA-based bioplastic in the context of this study is to protect dry food against environment during transport and storage. We choose a croissant as an exemplar of dry food product. The functional unit was therefore defined as "Protection of one average croissant (ca. 40 g) against migration of oxygen, water and aromas (according to global and specific migration standards BS EN 1186 and UNE-EN 13130 for migration of aromatic primary amines, pthalic acid, crotonic acid, acrylic acid and the elements Al, B, Ba, Cu, Co, Fe, Li, Mn, Ni and Zn) during transport and storage for 30 days". This functional unit was chosen as it allows a consistent comparison with alternative plastics used as packaging materials. The reference flow is equal to 0.06384 m<sup>2</sup> of PHA-based plastic film with improved barrier properties, and the same reference flows apply to other plastics fulfilling this functional unit. Yet, differences in thicknesses of the PHA based plastic films and other plastics result in different reference flows when expressed on a mass basis.

#### 2.4.2 Modeling framework and system boundaries

Production of PHA-based bioplastic with improved barrier properties and its use in food supply is a relatively new technology and its implementation is not expected to cause large scale market consequences (for example the need to install new power plants). Therefore, consistent with ILCD's recommendations, the current LCA is considered a microlevel decision support situation (type A) (EC-JRC 2010). This implies that: (i) system expansion is the preferred way to solve multifunctionality, and (ii) average processes are to be used to model the background system of the study. The consequential version of the ecoinvent v3.5 database was employed to model the background system because it prioritizes system expansion rather than allocation (Bjørn *et al.* 2017). However, this consequential database systematically uses marginal processes rather than average ones. Therefore, to make the database more consistent with the attributional approach, some processes were adapted to be based on average rather than marginal mixes. Details on these adaptations are presented in SI, Section S2 (Table S9). For example, as in (Bohnes 2020), the marginal electricity grid mix originally included in the consequential database was adapted to represent the average mix of 2018. The use of marginal data was considered negligible for other processes in the bioplastic life cycle and their adaptation was not deemed necessary. The product systems were modelled in SimaPro, version 8.3.0.0 (PRé Consultants B.V., the Netherlands).

An overview of system boundaries, specifying processes included in the LCA, is presented in Figure 1. Background processes include (avoided) conventional use of the feedstock, production of energy and chemicals, construction and disposal of equipment, and treatment of biological waste. The use stage includes transport from production site to the customer. The end-of-life stage comprises waste management processes according to the waste management of system in the country of interest. The foreground system comprises all processes, as presented in Figure S1 of the SI.



Figure 1. System boundaries of the PHA-based plastics with improved barrier properties.

#### 2.4.3 Life cycle impact assessment

Environmental impact scores were mainly calculated using ReCiPe 2016 as LCIA methodology, applying midpoint indicators and hierarchist perspective. Impact scores were calculated for all ReCiPe impact categories, except climate change which was replaced by the approach of ILCD (2011) combined with updated GWP100 values from IPCC AR5 (IPCC 2014). The ILCD (2011) approach was preferred as it gives credits to delayed emissions of greenhouse gases (GHGs), which are particularly relevant for the end-of-life stage of the PHA-based plastics. In addition to the GWP100, which is the default metric in LCA and addresses short/medium term climate impacts, we employed the global temperature change potential (GTP100) and the multiple climate tipping points potentials (MCTPs) as characterization factors (CFs). The GTP100 is recommended for use in LCA, next to the GWP100, as it focuses on long-term impacts, representing global average temperature increase of the atmosphere at 100 years that results from the emission (Shine et al. 2005, Levasseur et al. 2016). The MCTP is a recently developed metric for climate tipping impacts (Fabbri et al. 2021), building on earlier work of Jørgensen et al. (2013). It specifically addresses the potential contribution of GHG emissions to trigger multiple climate tipping points in the earth system (like loss of Arctic summer sea ice or the El Niño-southern oscillation intensification), considering in total 13 tipping elements that could pass a tipping point with increasing warming. The

contribution to tipping is measured as the share of remaining carrying capacity up to each tipping point that is consumed by the emissions, using eq. 1 (Fabbri *et al.* 2021), and is expressed as fraction of depleted remaining capacity in parts per trillion, ppt<sub>rc</sub>, per kg GHG emission:

$$MCTP_{i}(T_{\text{emission}}) = \sum_{j=1}^{m} \frac{I_{\text{emission},i,j}(T_{\text{emission}})}{CAP_{j}(T_{\text{emission}})}$$
(1)

Where  $MCTP_i(T_{emission})$  is the characterization factor for GHG *i* emitted at time  $T_{emission}$ , *j* is the *j*th out of *m* potentially exceeded tipping points,  $I_{emission,i,j}$  is the increase in CO<sub>2</sub>-equivalent concentration caused by the emission with respect to tipping point *j*, and  $CAP_j$  is the remaining capacity of the atmosphere to absorb this concentration increase without triggering tipping point *j* (Fabbri *et al.* 2021). Given that the MCTP is sensitive to the timing of emissions, the metric is particularly relevant for the end-of-life of PHA-based plastics, as emissions are distributed over time and could contribute to crossing tipping points (Fabbri *et al.* 2021). The three climate-related sets of indicators are complementary to each other and represent three different impact categories. Details of calculation of impact scores using these three approaches are presented in Section S3 of the SI.

#### 2.5 Sensitivity and uncertainty analyses

Sensitivities of the LCA results to discrete parameters were evaluated in a scenario analysis (see Section 2.1). Sensitivities to PHA yield, which is a continuous parameter, was also considered for selected scenarios from Table S3, Section S2 of SI. Quantification of inventory uncertainties is currently not possible to carry out with the consequential version of the ecoinvent database as attached to SimaPro. To compensate for this limitation, we conducted a qualitative uncertainty analysis discussing limitations of the study considering the specificity of the inventory data.

# 3. Results and discussion

In the following sections, we present an overview of life cycle impact assessment results for selected scenarios, identify factors which determine overall environmental performance of the PHA plastics, and identify optimization potentials.

#### 3.1 Environmental hot-spots in the PHA value chain

To identify processes with the largest contribution to this burden, process contribution analysis was carried out on PHA laminated with PLA at pilot and large scale systems in Italy (Figure 2). Refer to Table S13, Section S4 of the SI for tabulated impact scores for the two scenarios. Irrespective of the plant scale, incumbent management of feedstock had the highest contribution to environmental burden for most, but not all, impact categories (up to 94% of total impact, depending on the impact category). Molasses is a residual product from production of sugar and therefore no burdens are attributed to its production. However, environmental burdens occur when the molasses waste stream is diverted for production of PHA, rather than its conventional use as animal feed. Consistently with system expansion being prioritized over allocation when handling multifunctional processes, this animal feed has to be produced from other sources, like barley grains. Thus, relatively high contribution of incumbent management of feedstock is explained by burdens associated with production of animal feed from barley grains. Negative impact scores (indicating environmental benefits) are observed for the climate change impact category. They are a result of fixation of CO<sub>2</sub> during cultivation of barley grains. These environmental benefits are, however, outweighed by the burden stemming from the fermentation itself which uses energy and emits  $CO_2$ , treatment of wastewater, and incineration of plastic waste in the end-of-life treatment.

The fermentation had relatively small contribution (up to 8% of total impact), except the three climate-related impact categories where its contribution ranged from 21 to 64% of the total impact. The post-treatment processes (recovery, purification, compounding and pelletizing), however, altogether contributed up to 60% of the total impact, depending on the impact category. Previous studies on PHA production from sucrose (including collection, pre-treatment, fermentation and PHA recovery), reported global warming impacts which were higher (1.96 kg  $CO_2$  eq/kg PHA<sub>recovered</sub> in Harding *et al.* (2007)) and lower (-2.58 kg  $CO_2$  eq/kg PHA<sub>recovered</sub> in Kookos *et al.* (2019) owing to energy recovery from bagasse), compared to 0.76 CO<sub>2</sub> eq/kg PHA<sub>recovered</sub> in the large scale system of this study. As in Kookos *et al.* (2019), direct emissions of CO<sub>2</sub> during fermentation were important contribution to climate change burdens in our study. Harding *et al.* (2007), on the other hand highlighted steam and electricity use as the most contribution to global warming impacts (in our LCA modelled as non-ionic surfactant), neither Harding *et al.* (2007) nor Kookos *et al.* (2019) found that the surfactant was the hot spot. Compared to the former study, the consumption of surfactant in our study was 16 times higher, while Kookos *et al.* (2019) applied a negative GHG emission factor for surfactant based on data from Akiyama *et al.* (2003).

Relatively high contribution of recovery and purification was mainly caused by the use of steam for spray drying in the pilot system and surfactant in the large scale system. Surfactant contributed to 55, 24 and 15% of total freshwater ecotoxicity, fossil resource scarcity and climate change impacts. Negative contributions to total impact scores on freshwater eutrophication observed in our study for recovery and purification and filmmaking and functionalization are unexpected, but can be explained by system expansion mechanisms occurring in non-ionic surfactant applied during recovery and purification and ink applied in filmmaking and functionalization processes.

Electricity consumption for processing of the recovered PHA into PHA pellets explains 23 and 19% of total impact for climate change and human carcinogenic toxicity. Negative impact scores for waste management systems for several other impact categories, indicating environmental benefits, were due to incineration with energy



recovery (61% of the packaging is incinerated in Italy), substituting production of energy (in this case, electricity and heat for reuse in municipal waste incineration).

Figure 2. Contribution of life cycle processes to total impacts from PHA-based packaging at pilot and large scale. The scores for each impact category are scaled to 100%.

#### 3.2 Effects of upscaling

The large scale system has slightly higher impact scores than the pilot scale one consistently for all impact categories, except climate change and freshwater eutrophication (Table S13, Section S4). The largest differences were observed for freshwater ecotoxicity followed by, water consumption, land use and marine eutrophication, where large scale production shows impacts from ~1.5 to ~2.5 times higher than at pilot scale, respectively. This finding was unexpected, because upscaling of technologies is often associated with decreasing environmental impacts perf unit of

output (although generalization across different technologies cannot be made) (Gavankar et al. 2015, Owsianiak et al. 2016). The different result in our case can be explained by differences in environmental performance of; (i) recovery and purification steps (all impact categories, except climate change and stratospheric ozone depletion), (ii) fermentation (all impact categories), (iii) collection of feedstock fermentation (all impact categories) and (iv) incumbent use of molasses (all impact categories, except climate change). Increased impacts for recovery and purification were due to higher consumption of surfactant in the large scale system, particularly so for freshwater ecotoxicity where the large scale systems shows 7.7 times higher impact. This increase outweighed benefits from a lower electricity and steam consumption in the large scale. Increasing impacts from fermentation were mainly due to a higher electricity consumption for aeration. Furthermore, slightly lower yield in the large scale system resulted in higher consumption and collection of molasses per unit of PHA output, increasing impacts. Similar, the lower yield at large scale increased incumbent use of molasses and impacts for all categories except climate change where increased amount of CO<sub>2</sub> fixated reduced impact scores. By contrast, reduced impacts from pre-treatment were due to lower consumption of steam, but these reductions were generally insufficient make the large-scale system perform better.

#### 3.3 Influence of geographic location and incumbent use of feedstock

Impact scores decreased for 12 out of 20 impact categories when (large-scale) PHA production and functionalization took place in Germany instead of in Italy (see Section S4 of the SI, Figure S2). The largest differences were for the climate change and multiple climate tipping impact categories (decrease by 32 and 20%, respectively) followed by fine particulate matter formation and terrestrial acidification (decrease by 17 and 16%, respectively). For climate change, the reductions were due differences in waste management systems between the two countries (the majority of plastics is incinerated in Germany, while landfilling is the dominant treatment option in Italy). Incineration is seen

beneficial over landfilling because it does not result in emission of potent GHG, methane (71% of carbon is assumed to be released as methane during landfilling (Rossi *et al.* 2015)). For fine particulate matter and terrestrial acidification, lower impacts in Germany can be explained by a lower portion of oil in the electricity grid mix in Germany (3.7% and 0.9% in Italy and Germany, respectively), which has a high contribution to these impact categories.

Impact scores increased for 13 out of 20 impact categories when molasses was used as feedstock for ethanol production (scenario 5) rather than for animal feed (scenario 2) in Italy. The largest increase was observed for impacts related to mineral resources, human non-carcinogenic toxicity, terrestrial ecotoxicity and global temperature change (increase by 64, 36, 31 and 28%, respectively) (see Section S4 of the SI, Figure S3). This was due to generally higher environmental impacts from production of ethanol than production of animal feed (per unit of molasses). Substantial reductions in impact scores were seen for freshwater eutrophication, land use and marine eutrophication (decrease by 365, 138 and 94%, respectively), with negative impact scores for the first two categories ( $-1.6 \times 10^{-5}$  kg P eq and  $-4.0 \times 10^{-2}$  m<sup>2</sup>a crop eq, respectively) and low impacts for marine eutrophication ( $1.1 \times 10^{-5}$  kg N eq) in scenario 5. These negative scores were due to handling a waste product from ethanol production from maize by system expansion, replacing soybean meal. Similar observations were made for Germany, where both increases and decreases in impact scores were observed when the incumbent treatment of molasses was as feedstock for ethanol production.

#### 3.4 Influence of PHA stability

Impact scores of the PHA value chain for the three climate-related impact categories are influenced by mineralization kinetics and extent of the mineralization lag phase in landfilling (Table 1). For all three indicators, lowest impact scores were consistently identified for the very slow degradation scenario (scenario 51). This was mainly due to

incomplete degradation over 100 year time (GWP and GTP) and over 94 years (MCTP), where only 1% of initial plastic degraded in this scenario, resulting in lower impact scores. Plastics with fast and medium mineralization kinetics generally performed worse according to GWP as credits given for temporary carbon storage are lower compared to more stable plastics. By contrast, climate tipping impact scores increased with decreasing mineralization rates, because the probability that a significant portion of emissions is released in proximity to tipping points, where MCTP values are the largest, was higher for the more stable plastics. This was even more pronounced for cases where a mineralization lag phase of 20 and 40 years was assumed (scenarios 52 and 53 in Table 1). In those cases, a larger share of the emissions was released close to the year 2050, where MCTPs are the highest. Mineralization kinetics was not found to matter for the GTP metric, because this approach disregards any benefits from temporary carbon storage and does not account for when GHG emissions occur in the life cycle.

Table 1. Impact scores per functional unit (f.u.) of the PHA value chain as depending on stability of the PHA plastics in landfilling conditions (mineralization rate constant and extent of mineralization lag phase) and the climate-related impact category. Increasing share of red shade indicates increasing impact (per impact category). The scenarios tested for stability and degradation are; fast kinetics: 90% degradation in 2 years (100% degraded in 100 years), medium kinetics: 90% degradation in 31 years (99.9% degraded in 100 years), slow kinetics: 90% degradation in 105 years (89 % degraded in 100 years), very slow kinetics: 90% degraded in 22798 years (1% degraded in 100 years), delayed (20): degradation delayed by 20 years, fast kinetics, delayed (40): degradation delayed by 40 years, fast kinetics (see a full overview of scenarios in Table S3, Section S2)

	GWP <sub>100</sub> (kg CO <sub>2</sub> eq/f.u.)	MCTP <sub>RCP6</sub> (ppt <sub>rc</sub> /f.u.)	GTP <sub>100</sub> (kg CO <sub>2</sub> eq/f.u.)
Fast (scenario 2)	5.25E-02	1.22E-03	1.04E-01
Medium (scenario 49)	4.53E-02	1.40E-03	1.04E-01
Slow (scenario 50)	3.57E-02	1.45E-03	1.03E-01
Very slow (scenario 51)	2.81E-02	9.40E-04	9.31E-02
Fast with 20-yr lag phase (scenario 52)	4.17E-02	4.95E-03	1.04E-01
Fast with 40-yr lag phase (scenario 53)	3.08E-02	4.93E-03	1.04E-01

#### 3.5 Making PHA-based plastics more sustainable

PHA-based plastics can be made more sustainable by optimizing PHA yield, thickness of the PHA layer, and choice of material for ensuring barrier properties. Figure 3 shows the effects of these parameters on environmental performance for selected impact categories. Comparisons were also made with pure PLA or pure fossil-based PE, and pure fossil-based PP. Increasing PHA yield generally improves environmental performance of the PHA-based packaging. For MCTP, fossil resource scarcity and land use, impacts decreased from 87 to 28% if yield increases from the minimum to the maximum values reported in the literature for PHA made from molasses (i.e. from 0.083 to 0.245 kg PHA<sub>raw</sub>/kg<sub>molasses</sub>; scenarios 3-18 in Table S3, Section S2). However, only a small increase was observed for climate change (by 2%).This relatively small increase was due to the fact that the decreasing fixation of CO<sub>2</sub> (hence increasing impacts with increasing yield), was outweighed by decreased emissions of CO<sub>2</sub> from fermentation and reduced amount of carbon-containing wastewater to be treated (per unit of PHA output).

The results also showed that PHA combined with either Al or AlOx (scenarios 7 and 8) were more sustainable than the PHA combined with PLA (scenario 2). Impact scores were consistently reduced for all impact categories, except for ionizing radiation (Figure 3 and Table S14 in the SI, Section S4). The reduction was, however, modest (up to 11% for fossil resource scarcity). Despite relatively large differences in environmental

impacts per kg of each alternative material (e.g. higher impacts for Al when compared to PLA), significantly less Al or AlOx (10-nm layer) than PLA (20-µm) is needed to fulfill the functional unit, explaining small differences between PLA and Al (or AlOx).

PHA-based plastics can also be made more sustainable if thickness of underlying materials is reduced (while still allowing the packaging to fulfill the function). However, the extent of required improvements is relatively large. For example, thickness of the PHA layer in the PHA/PLA alternative needs to be reduced to ca. 20 µm for this alternative to be able to compete with pure PLA of 91µm (in terms of climate change and multiple climate tipping). If PHA yield increases, these PHA-based films would be able to compete with PLA of 50µm thickness (again, assuming that their functional performance parameters are the same). Irrespective of yield and assumed PHA thickness, however, packaging made of PHA generally does not perform as good as PP- and PE-based packaging does (scenarios 11 and 12 in Table S3) (Figure 3). The differences were by factor of 2 to 5, depending on the impact category, even if high yield and low thickness of PHA were assumed.



Figure 3. Impact scores for climate change, multiple climate tipping, fossil resource scarcity and land use as influenced by PHA yield, and type and thickness underlying materials (scenarios 7-48 in Table S3, Section S2 of SI). Yields are based on literature data, where the minimum yield is from Kookos et al. (2019) and the maximum yield is estimated from a theoretical yield from Yamane (1993) and assuming that 95% of the accumulated biomass is PHA.

# 4. Limitations and data gaps

This study presents full life cycle inventory and impact assessment results for PHA-based plastics with improved barrier properties. The main limitations of the study relate to: (1) variability and uncertainty in parameters used for modelling life cycle inventories, (2) the choice of LCI database for modelling background system, and (3) deficiencies in impact assessment method.

First, we modelled pilot and large scale PHA production systems basing on data retrieved from the literature, but several parameters are known to be variable or uncertain. This may influence comparisons between scales. For example, PHA yield varies, but is an important parameter which determines performance of the PHA vale chain, and the large scale system would generally perform better than the pilot scale if the PHA yield was in higher range of possible values (0.245 kgPHA<sub>raw</sub>/kg<sub>molasses</sub>) (data not shown).

Second, biodegradation kinetics of the PHA-based plastics in the environment is highly uncertain (Emadian *et al.* 2017, Meereboer *et al.* 2020), and furthermore it is unknown how surface treatment may influence biodegradation kinetics in landfilling conditions. Our sensitivity analyzes show that this parameter is important not only for the end-of-life, but for the performance of the whole PHA value chain (in terms of climate change and multiple climate tipping impacts).

Third, the surfactant in the current study was modelled as a generic non-ionic surfactants, which consists of ethylene oxide (66%) and fatty acid (33%) derivatives. Impacts of surfactants vary considerably (Schowanek *et al.* (2018). For example, if the fatty acid derivate was used, freshwater eutrophication and ecotoxicity impacts would decrease by 114% and 45%, respectively (data not shown). It is therefore important to address this data gap in future studies on PHA.

Fourth, the consequential background database was consistently applied for background processes, with the exception of electricity processes, which were adapted to average grid mixes rather than marginal mixes. The sensitivity of this was tested for incumbent use of molasses and found to have a high influence on the overall results. Although contribution from other processes of the background system is expected to be smaller when compared to energy and avoided incumbent use of molasses, there is some uncertainty as average mixes (rather than marginal mixes) should ideally be used consistently for all processes in the background system.

Finally, owing to the limitations of the ecoinvent database indirect land use changes (ILUC) were not considered in the PLA value chain (PLA is made from maize). If they were considered, impacts of those PHA-based plastics which include PLA would increase. This would further favor those alternatives which use either Al or AlOx as barrier materials.

# 5. Implications for PHA value chain

We showed that PHA-based plastics with improved barrier properties have higher environmental impacts than alternative packaging made from PE, PP and potentially even PLA. These results are not surprising given that PHA production is still relatively immature when compared to the aforementioned alternatives. The largest optimization potentials (which are also challenges to PHA technology developers), are: 1) reduction of PHA thickness while maintaining functional properties of the PHA plastic, 2) increase PHA production yield, 3) increase the energy efficiency during compounding and pelletizing, 4) decrease amount and change type of surfactant used in recovery and purification processes, 5) consider feedstock other than molasses, that do not have a highly beneficial alternative treatment and use. Industrial wastewater could be considered as feedstock, as it avoids incumbent management of the wastewater (Heimersson *et al.* 2014). Furthermore CO<sub>2</sub> could be a promising alternative feedstock for PHA production (Troschl *et al.* 2018), but separate LCA would be needed to evaluate performance of PHA made from other feedstock. 6) consider alternative end-of-life options. Although the biodegradability of PHA offers aerobic and anaerobic end-of-life pathways in comparison to conventional plastics, recent research results for PLA show that also recycling (e.g. mechanical recycling) is a potential option which can offer additional benefit from an LCA as well as circular economy perspective (Maga *et al.* 2019, Spierling *et al.* 2020). Our study may suggest that that Al (or AlOx) is the preferred material to ensure barrier properties. However, unknown influence of the Al layers on biodegradability of PHA in the environment warrants further studies.

# **Supporting Information**

Details of literature review, data underlying LCA model, details of life cycle impact assessment, additional results (Section S1-S5), Simpro model processes (Section S6)

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# Environmental performance of polyhydroxyalkanoate (PHA)-based plastic film with improved barrier properties

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### S1. Details of literature review

Recall, that a literature review was conducted specifying type of feedstock, microorganism used in the fermentation, scale of production, capacity of production and polymer yield, to support collection of data relevant for the LCA. Studies were identified in the search engine Scopus in March 2020 in two steps:

- Limiting the search to review articles published after 2017 (assuming that these recently published review articles refer to relevant, older studies) and applying key words related to PHA and its synonyms and plant scale (pha OR polyhydroxyalkanoate\* OR \*polyhydroxybutyrate\* OR phb OR hbv AND "large scale" OR "industrial plant" OR pilot OR "large-scale" OR "large scale" OR "scale-up")
- 2. Applying key words related to PHA and to LCA to identify studies related to environmental assessment of PHA production were identified (lca AND pha OR polyhydroxyalkanoate\* OR \*polyhydroxybutyrate\* OR phb OR phbvv). An additional search for studies producing PHA by fermenting molasses by R. eutropha (i.e. not limited to review articles) was conducted to ensure that recent studies similar to the large scale plant, not captured in the reviews, were identified (key words: pha OR polyhydroxyalkanoate\* OR \*polyhydroxybutyrate\* OR phb OR phbvv AND molasses AND ralstonia OR necator OR "R.eutropha" AND fermentation).

Cited and citing studies that were found to contain relevant data were consulted to complement the search, and this process was iterated until no new study was found. In total, 25 studies were included in the review (see Table S1 for an overview).

Study	Type of study	Feedstock (substrate)	Microorganism	Production scale <sup>a</sup>	Capacity	Polymer yield	
(Valappil et al., 2007)	Fermentation technology	Sterilized glucose and soybean dialysate	Bacillus cereus SPV	Pilot*	20 L	0.114 g/g substrate	
(Koller et al., 2015)	Fermentation technology	Glucose	Haloferax mediterranei DSM 1411	Pilot*	10 L	0.23 g/g substrate	
(Koller et al., 2007a)	Fermentation technology	Hydrolyzed whey permeate	Haloferax mediterranei DSM 1411	Pilot*	42 L	0.29 g/g substrate	
(Koller et al., 2007b)*	Fermentation technology	Hydrolyzed whey permeate	Haloferax mediterranei DSM 1411	Pilot*	10 L	0.2 g/g substrate	
(Bengsston et al., 2017; Werker et al. 2018)	Fermentation technology	Wastewater from candy factory (Volatile fatty acids (VFA))	Mixed microbial cultures	Pilot	1200 L	0.4 g/g substrate	
(Larriba et al., 2020)	Fermentation technology	Wastewater sludge (VFA)	Nitrite oxidizing bacteria	Pilot	2500 L	0.05 g/g COD	
(Moretto et al., 2020)	Fermentation technology	from AD of biowaste (VFA)	Mixed microbial cultures	Pilot	100-380 L	3.86 g/L OFMSW	
(Ntaikou et al., 2014)	Fermentation technology	Olive-mill wastewater (VFA)	Enriched culture of <i>Pseudomonas sp</i>	Pilot	50 L	$7.58 \pm 0.06 \text{ g/L}$	
(Tamis et al., 2014)	Fermentation technology	Waste water from Mars candy bar factory (VFA)	P. acidivorans	Pilot	200 L	0.37 g/g substrate	
(Amulya et al., 2015)	Fermentation technology	Waste water from acidogenic fermentation of municipal solid waste (VFA)	Anaerobic consortia (mixed culture) procured	Pilot	34 L	0.17 g/g substrate	
(Morgan- Sagastume et al., 2015)	Fermentation technology	Activated wastewater sludge (VFA)	Mixed culture: active sludge	Pilot	400 L	0.38 g/g substrate	
(Jia et al., 2014)	Fermentation technology	Activated wastewater sludge (VFA)	Mixed culture: active sludge	Pilot	70 L	0.17 g/g substrate	

Table S1. Overview of studies identified in the literature analysis conducted to support the inventory data collection.

(Valentino	Fermentation	Organic fraction of MSW	Mixed microbial culture	Pilot	140 L	0.39-0.47 g/g VSS
et al., 2018)	technology	(VFA)				
(Elbahloul	Fermentation	Octanoate	<i>P. putida</i> GPo1	Pilot*	650 L	0.41 g/g substrate
and	technology					
Steinbüchel,						
2009)						
(Kshirsagar	Fermentation	Maltose	Halomonas campisalis	Pilot*	14 L	0.09 g/g substrate
et al., 2013)	technology					
(Wang and	Fermentation	Glucose	Recombinant Escherichia	Pilot*	50 L	0.27-0.28 g/g
Lee, 1997)	technology		coli (A. eutrophus PHA			substrate
			biosynthesis genes)			
(Mohammad	Fermentation	Glycerol	Zorbellella denitrifican	Pilot*	42 L	0.25 g/g substrate
and	technology					
Steinbüchel,						
2009)						
(Kellerhals	Fermentation	Octanoic acid	P. putida KT2442	Pilot*	30 L	0.22 g/g substrate
et al., 2000)	technology		_			
(Kellerhals	Fermentation	Oleic acid	P. putida KT2442	Pilot*	30 L	0.56 g/g substrate
et al., 2000)	technology		_			
(Nath et al.,	Fermentation	Cheese whey (lactose)	Methylobacterium sp.	Pilot*	30 L	0.315 g/g substrate
2008)	technology	• • • •	ZP24			
(Harding et	LCA	Sugar cane (sucrose)	Cupriavidus necator	Pilot (upscaled)	1 L	0.36 g/g substrate
al., 2007)			*			00
(Leong et	Environmental	Glycerol	Cupriavidus necator	Large scale	9000 t	0.36 g/g substrate
al., 2017)	and economic	5	*	(simulated)	polymer/year	00
. ,	assessment			· · · · ·		
(Kookos et	LCA	Seed oil and sucrose	Ralstonia eutropha	Large (upscaled)	10000 t	0.17 g/g substrate
al., 2019)			*		polymer/year	00
(Pavan et	Economic	Citric molasses	Cupriavidus necator	Large (upscaled)	2000 t	0.28 g/g substrate
al., 2019)	analysis		*		polymer/year	
(Koller et	Environmental	Whey	Haloferax mediterranei	Pilot	300 L	0.188 g/g substrate
al., 2013)	assessment		DSM 1411			

<sup>a</sup> Scale as defined by the study itself or between 10-1000L (indicated with "\*")

Table S2. Overview of studies used as data sources in this LCA study for parameters related to fermentation, recovery and purification installations at pilot and large scale.

Study	Details	Scale	Parameters used in LCA modelling
(Harding et al.	LCA study on a PHA pilot production facility (1 t PHA/year)	Pilot	Steam for sterilization and spray drying, yield of
2007)	fermenting sucrose from sugar cane by R. eutropha. The data are		fermented PHA, wastewater, consumptions of water,
	obtained combining data scaled up from lab-scale study and process		surfactant, enzyme and hydrogen peroxide and bill of
	flowsheet from a pilot plant.		materials.
(Leong <i>et al</i> .	Economic and environmental assessment on a PHA large scale	Large	Yield of fermented and recovered PHA, waste and
2017)	facility (9000 t PHA/year) fermenting glycerol by R. eutropha. The	scale	wastewater, consumption of water and surfactant and
	large scale facility is simulated based on heuristics and experience.		NaOCl and bill of materials.
(Kookos et al.	LCA study on a PHA large scale facility (10000 t PHA/year)	Large	Steam for sterilization and spray drying, yield of
2019)	fermenting sucrose by R. eutropha. The large scale facility is	scale	fermented and recovered PHA, consumptions of
	simulated based on lab-scale PHA production study.		electricity, ammonia and surfactant and NaOCl, CO <sub>2</sub>
			emissions.
(Pavan <i>et al</i> .	Economic analysis of a PHA large scale facility (2000 t PHA/year)	Large	Yield of fermented PHA and consumptions of ammonia.
2019)	fermenting sucrose from citric molasses by R. eutropha. The large	scale	
	scale facility is simulated based on lab-scale PHA production study.		

#### S2. Data underlying LCA model

Figure S4. Process set-up for PHA-film packaging production at two scales s (where s=P and s=L for pilot and large scale, respectively). The numbers in italics in parenthesis indicate the number of installations. Collection of feedstock, pre-treatment, fermentation, and recovery and extraction are modelled differently at pilot and large scale, the following parameters are distinct: steam applied for sterilizing feedstock during pre-treatment (M<sub>st.pt.s</sub> in kWh/kg<sub>feedstock</sub>), electricity used for agitation and aeriation during fermentation (E<sub>ag.s</sub> and E<sub>aer.s</sub> in kWh/kg<sub>PHA</sub>), mass of equipment applied during pre-treatment and fermentation (M<sub>eq.ptf.s</sub> in kg material/kg<sub>PHA</sub>), yield of raw PHA (Y<sub>s</sub> in kg<sub>PHA</sub>/kg<sub>substrate</sub>), mass of CO<sub>2</sub> emitted during fermentation (M<sub>CO2,s</sub> in kg/kg<sub>PHA</sub>), volume of wastewater during fermentation (V<sub>ww,f.s</sub> in m<sup>3</sup>/kg<sub>PHA</sub>), mass of equipment applied during recovery and purification M<sub>eq.rec.s</sub> in kg material/kg<sub>PHA</sub>), electricity used for centrifugation, mixing, spray drying and cell disruption during recovery and purification (E<sub>centri,s</sub>, E<sub>mix,s</sub>, E<sub>dry,s</sub> and E<sub>dis.s</sub> in kg/kg<sub>PHA,recovered</sub>), water and steam consumed during recovery (M<sub>water,s</sub> and M<sub>steam,rec,s</sub> in kg/kg<sub>PHA,recovered</sub>), mass of enzyme and chemicals applied for recovery and purification (M<sub>enzyme,s</sub> M<sub>H2O2,s</sub>, M<sub>NaOCL,s</sub> and M<sub>sufact,s</sub>, in kg/kg<sub>PHA,recovered</sub>) and volume and mass of wastewater and waste effluent recovery (V<sub>ww,rec,s</sub> in m<sup>3</sup>/kg<sub>PHA</sub> and M<sub>waste,s</sub> in kg/kg<sub>PHA,recovered</sub>).



Table S3. Overview of scenarios for sensitivity analysis and perturbed parameter values assessed for PHA-based plastic value chain. All scenarios apply to the PHA-based bioplastic, except scenarios 9-12 which apply to PLA, PP and PE only.

# scenario	Sensitivity parameter	Plant scale <sup>a</sup>	Geographic location <sup>b</sup>	Conventional use of molasses	Material and surface treatment	Thickness of layers (µm) <sup>c</sup>	Yield (kg PHA <sub>raw</sub> /kg molasses) <sup>d</sup>	Landfilling degradation kinetics <sup>e</sup>
1	Baseline	Pilot	IT	Used as animal feed	PHA+PLA	76.5+20	0.176	Fast
2	Plant scale	Large scale	IT	Used as animal feed	PHA+PLA	76.5+20	0.131	Fast
3-4	Geographic location	Pilot, Large scale	DE	Used as animal feed	PHA+PLA	76.5+20	0.131	Fast
5-6	Avoided treatment of molasses	Large scale	IT, DE	Used for ethanol production	PHA+PLA	76.5+20	0.131	Fast
7-12	Material and surface treatment	Large scale	IT	Used as animal feed	PHA+Al, PHA+AlOx, PLA(91), PLA(50), PP, PE	76.5+0.01, 76.5+0.01, 91, 50, 31, 31	0.131	Fast
13-18	Yield	Large scale	Π	Used as animal feed	PHA+PLA	76.5+20	0.083, 0.110, 0.150, 0.176, 0.210, 0.245	Fast
19-48	Thickness of PHA film	Large scale	IT	Used as animal feed	PHA+PLA	15.5+15.5, 20+20, 40+20, 60+20, 100+20	0.083, 0.110, 0.150, 0.176, 0.210, 0.245	Fast
49-53	End of life degradation	Large scale	IT	Used as animal feed	PHA+PLA	76.5+20	0.131	Medium, Slow, Very slow, Delayed (20), Delayed (40)

<sup>a</sup>details on the difference between pilot and large scales are presented in Section 2.3

<sup>b</sup>IT: Italy, DE: Germany. The following parameters are updated according to the geographic location: electricity grid mix and conventional waste management technologies.

<sup>c</sup>Thicknesses are within range of relisting values and were chosen based on ongoing experimental trials (BioBarr 2019) for the PHA-based plastics with improved barrier properties, or based on current practice for the PLA, PP and PE.

<sup>d</sup>Yields for baseline pilot and large scale plants are based on literature data (see details in Table S4). Yields for scenarios 13-18 are based on minimum PHA fermentation from molasses yield in literature (Kookos *et al.* 2019) and an estimated maximum theoretical yield (based on a theoretical yield from Yamane (1993) and assuming that 95% of the accumulated biomass is PHA) and yields in between this range.

<sup>e</sup>Fast kinetics: 90% degradation in 2 years (100% degraded in 100 years), medium kinetics: 90% degradation in 31 years (99.9% degraded in 100 years), slow kinetics: 90% degraded in 105 years (89 % degraded in 100 years), very slow kinetics: 90% degraded in 22798 years (1% degraded in 100 years), delayed (20): degradation delayed by 20 years, fast kinetics, delayed (40): degradation delayed by 40 years, fast kinetics

Parameter	Pilot scale Average	Large scale	Unit	Note	Main data source
	(min-max)	Average			
	77 /•	(min-max)			
Feedstock and c	collection				
Electricity (pumping)	Not relevant	50	kWh/t <sub>feedstock</sub> , dw	<ul> <li>Electricity use for pumping of feedstock into the reactor.</li> <li><i>Pilot scale:</i> The feedstock is transported to the plant by truck. Hence, electricity for pumping is not relevant.</li> <li><i>Large scale:</i> Electricity consumed to pump the feedstock is assumed similar to the electricity reported in Owsianiak <i>et al.</i> (2016) for pumping of wet biowaste at full scale.</li> </ul>	L: Assumed based on Owsianiak <i>et al.</i> (2016)
Transportation distance	50	Not relevant	km	<ul> <li>Transportation distance from biomass collect point to the fermentation plant</li> <li><i>Pilot scale:</i> The feedstock is transported to the plant by lorry (Ecoinvent process; "Transport, freight, lorry 16-32 metric ton, EURO4 {RoW}  transport, freight, lorry 16-32 metric ton, EURO4 [Conseq, U"). It is assumed that its transportation distance is 50 km.</li> <li><i>Large scale:</i> The feedstock is transported in pipeline system from a neighboring provider (sugar production plant). Hence, transportation by truck is not relevant.</li> </ul>	P: Assumed L: not relevant
Substrate content	49 (46-52)	49 (46-52)	% ww	<ul> <li>Content of substrate (sucrose) in sugar beet molasses.</li> <li><i>Pilot scale:</i> The sucrose content is calculated based on 8 data points from literature (ÇALIK et al., 1939; El-Geddawy et al., 2012; Šarić et al., 2016)</li> <li><i>Large scale:</i> Assumed the same as for the pilot scale</li> </ul>	P and L: (ÇALIK et al., 1939; El- Geddawy et al., 2012; Šarić et al., 2016)
Water content	18 (16-25)	18 (16-25)	% ww	<ul> <li>Content of water in sugar beet molasses.</li> <li><i>Pilot scale:</i> The water content is calculated based on 8 data points from literature (ÇALIK et al., 1939; El-Geddawy et al., 2012; Šarić et al., 2016)</li> <li><i>Large scale</i>: Assumed the same as for the pilot scale</li> </ul>	P and L: (ÇALIK et al., 1939; El- Geddawy et al., 2012; Šarić et al., 2016)
Stoom	0 15	0.04	ka /ka	Steam use for starilizing the feedsteak by steam	D: (Harding at al
(sterilization)	0.15	0.04	Kgsteam/Kgfeedstock	<ul> <li><i>Pilot scale:</i> The steam consumed is assumed same as Harding <i>et al.</i> (2007) (converted from 1.06 kg/ kg<sub>PHA,recovered</sub>) considering yield of raw PHA and recovered PHA). The electricity consumed to heat the stream is 0.1016 kWh/kg feedstock (as the Ecoinvent process</li> </ul>	<ul> <li>2007)</li> <li>L: Kookos et al.</li> <li>(2019)</li> </ul>

Table S4. Overview of parameters and data sources for feedstock collection, pre-treatment, fermentation and PHA recovery at pilot and large scales.

				<ul> <li>"Steam, in chemical industry {RER}  market for steam, in chemical industry   Conseq, U").</li> <li><i>Large scale:</i> The steam consumed is assumed same as in Kookos et al. (2019) (converted from 0.347 kg/ kg<sub>PHA,recovered</sub>) considering yield of raw PHA and recovered PHA). The electricity consumed to heat the stream is 0.1016 kWh/kg feedstock (as the Ecoinvent process "Steam, in chemical industry {RER}  market for steam, in chemical industry   Conseq, U").</li> </ul>	
Ammonia (NH <sub>3</sub> )	0.27 (0.13 - 0.41)	0.27 (0.13 - 0.41)	kg/kg <sub>PHA,raw</sub>	<ul> <li>Ammonia is added as source of nitrogen for fermenting bacteria.</li> <li><i>Pilot scale:</i> Nitrogen consumed is assumed to be the same as in the large scale facility.</li> <li><i>Large scale:</i> Minimum and maximum mass of ammonia added is based on Kookos et al., (2019) and Pavan et al., (2019), respectively.</li> </ul>	P: Assumed L: (Kookos et al., 2019; Pavan et al., 2019)
Fermentation	•	•	·		
Yield (raw PHA)	0.360	0.268 (0.170 – 0.360)	kgpHA,raw/kgsubstrate	<ul> <li>Mass of raw PHA produced per mass of substrate in feedstock. Raw PHA refers to the PHA product effluent fermentation that has not yet undergone a recovery and extraction process.</li> <li><i>Pilot scale:</i> The yield of raw PHA per mass of substrate is equal to the one reported in Harding et al., (2007). The yield per mass of molasses feedstock is 0.176 considering a substrate content of 49% in molasses.</li> <li><i>Large scale:</i> The average, minimum and maximum yield is based on the yield of (Kookos et al., 2019; Leong et al., 2017; Pavan et al., 2019). The yield per mass of molasses feedstock is 0.131 (0.083 – 0.176), considering a substrate content of 49% in molasses.</li> </ul>	P: (Harding et al., 2007) L: (Kookos et al., 2019; Leong et al., 2017; Pavan et al., 2019)
Electricity (agitation)	0.31	0.25	kWh/kg <sub>PHA,raw</sub>	<ul> <li>During the fermentation process, electricity is needed to agitate the feedstock in the fermenter.</li> <li><i>Pilot scale:</i> Assumed equal to the electricity for agitation as of Harding et al. (2007) (converted from 1.36 MJ/kg<sub>PHA,recovered</sub> considering the recovery yield of 0.81 kgPHA<sub>recovered</sub>/kg PHA<sub>raw</sub>).</li> <li><i>Large scale:</i> Electricity consumed for agitation is assumed equal to the one of Kookos et al. (2019).</li> </ul>	P: (Harding et al., 2007) L: (Kookos et al., 2019)
Electricity (aeration)	0.12	0.5	kWh/kg <sub>PHA,raw</sub>	<ul> <li>During fermentation, electricity is needed for aeration, which is necessary to supply oxygen and to remove carbon dioxide from microbial cells suspended in the culture broth.</li> <li><i>Pilot scale:</i> Assumed similar to the electricity for aeration as of Harding et al. (2007) (converted from 0.512 MJ/kg<sub>PHA,recovered</sub>/kg PHA<sub>raw</sub>).</li> </ul>	P: (Harding et al., 2007) L: (Kookos et al., 2019)

				• <i>Large scale</i> : Electricity consumed for aeration is assumed equal to the one of Kookos et al. (2019)	
Carbon emitted as CO <sub>2</sub>	0.37	0.37	Kg <sub>carbon</sub> /kg <sub>carbon,feed</sub>	<ul> <li>Carbon emitted as CO<sub>2</sub> during fermentation as a portion of incoming carbon in feedstock.</li> <li><i>Pilot scale:</i> Calculated as for to large scale facility</li> <li><i>Large scale:</i> Mass of CO<sub>2</sub> emissions is calculated assuming that the same portion of carbon present in the feedstock is emitted as CO<sub>2</sub> as in Kookos et al., (2019) (0.884 kg CO<sub>2</sub>/kg sucrose). This is calculated based on the total CO<sub>2</sub> emissions (6.5 kg CO<sub>2</sub>/kg PHA<sub>recovered</sub>), recovery yield (0.8 kg PHA<sub>recovered</sub>/kg, and PHA yield (0.17 kg PHA<sub>raw</sub>/kg sucrose). Combined with carbon content of sucrose (0.42kg C/kg sucrose, calculated considering sucrose's chemical structure), the amount of carbon emitted as CO<sub>2</sub> is calculated.</li> <li>Even though this parameter is equal for the pilot and large scale system, overall, more CO<sub>2</sub> is emitted in the large scale system, as this system has a higher amount of feedstock).</li> </ul>	P and L: Calculated and assumed based on Kookos et al., (2019)
Wastewater	0.0006	0.0006	m <sup>3</sup> /kg <sub>feedstock</sub>	<ul> <li>Liquid waste from fermentation</li> <li><i>Pilot scale:</i> Volume of wastewater is calculated considering water content of feedstock and the part of the feedstock that is not turned into PHA-biomass is considered (calculated based on yield of raw PHA).</li> <li><i>Large scale:</i> Calculated as for the pilot scale facility.</li> <li>Even though this parameter is equal for the pilot and large scale system, overall, more wastewater is emitted in the large scale system, as this system has a lower yield hence a higher consumption of feedstock.</li> </ul>	P and L: Calculated
PHA recovery a	und purificatio	)n			1
Yield (recovered PHA)	0.81 (0.80	0.81 (0.80	kgPHA <sub>recovered</sub> /kg PHA <sub>raw</sub>	<ul> <li>The proportion of raw PHA recovered as PHA powder after the recovery and extraction process.</li> <li><i>Pilot scale:</i> Assumed same as large scale</li> <li><i>Large scale:</i> Minimum and maximum values from Leong et al., (2017) and Kookos et al., (2019), respectively.</li> </ul>	P and L: (Kookos et al., 2019; Leong et al., 2017)
Electricity (centrifuges)	0.073	0.062	kWh/kgpHA,recovered	<ul> <li>Electricity consumed by centrifuges.</li> <li><i>Pilot scale:</i> Electricity consumption is assumed equal to as reported in Harding et al. (2007).</li> <li><i>Large scale:</i> Electricity consumption is assumed equal to as reported in Kookos et al. (2019).</li> </ul>	P: (Harding et al., 2007) L: (Kookos et al., 2019)

Flootricity	0.010	0.016	kWh/kg	Electricity peeded to egitate the formented broth and mix it with water	D: (Harding at al
(agitation and	0.010	0.010	K W II/ KgpHA, recovered	during the recovery process and electricity consumed by contributes	1. (flatung et al., 2007)
(agitation and				auting the recovery process and electricity consumed by centringes.	2007) L: (Kookos et al
mixing)				• Pliot scale: Electricity consumption is assumed equal to as reported in Harding et al. (2007)	$\frac{1}{2010}$
				In Flatting et al. $(2007)$ .	2019)
				• Large scale: Electricity consumption is assumed equal to as	
El stat de	0.500	0.260	1 XX71. /1	Fiberti i te man la la face de la constante de	D. (II. all'a surf al
Electricity	0.590	0.260	KWN/KgPHA, recovered	Electricity needed to for spray drying.	P: (Harding et al.,
(spray dryer)				• <i>Pilot scale:</i> Electricity consumption is assumed equal to as reported	$\frac{2007}{100}$
				in Harding et al. (2007).	L: (Kookos et al., $2010$ )
				• <i>Large scale</i> : Electricity consumption is assumed equal to as	2019)
				reported in Kookos et al. (2019).	
Electricity	0.502	Not	kWh/kg <sub>PHA,recovered</sub>	Biomass cells are disrupted in a high pressure homogenizer at pilot scale.	P: (Harding et al.,
(cell		relevant		• <i>Pilot scale:</i> Electricity consumption is assumed equal to as reported	2007)
disruption)				in Harding et al. (2007)	L: not relevant
				Large scale: No high pressure homogenizer is applied at large scale	
Tap water	65.2	8.81	$kg/kg_{PHA,recovered}$	Process water used for blending and washing during extraction and	P and L: Leong et
				purification	al. (2017
				• <i>Pilot scale:</i> Water consumption is assumed equal to as reported in	
				Harding et al. (2007).	
				• <i>Large scale</i> : Water consumption is assumed equal to as reported in	
				Leong et al., (2017).	
Steam	3.819	0.603	kg/kg <sub>PHA,recovered</sub>	Steam fed to the spray drier.	P: (Harding et al.,
				• <i>Pilot scale:</i> Steam consumption is assumed equal to as reported in	2007)
				Harding et al. (2007).	L: (Kookos et al.,
				• <i>Large scale</i> : Electricity consumption is assumed equal to as	2019)
				reported in Kookos et al. (2019).	
Surfactant	0.034	0.535	kg/kg <sub>PHA,recovered</sub>	Surfactant added to lower the surface tension during PHA recovery. It is	P: (Harding et al.,
		(0.247-		assumed that type of surfactant used is a non-ionic surfactant in both the	2007)
		0.822)		pilot and large-scale model.	L: (Kookos et al.,
				• <i>Pilot scale:</i> Amount of surfactant applied is assumed equal to as	2019; Leong et al.,
				reported in Harding et al. (2007) (converted from 0.000033 m <sup>3</sup> /kg	2017)
				conisdering a density of 1.02 kg/L for Synperonic, which is the	
				sufactant applied in Harding et al. (2007)).	
				• <i>Large scale</i> : Surfactant consumption is assumed equal to minimum	
				and maximum values Kookos et al., (2019) and Leong et al.,	
				(2017), respectively.	
NaOCl	Not	0.19 (0.17	kg/kg <sub>PHA,recovered</sub>	NaOCl added to extract PHA from biomass at large scale.	P: not relevant
	relevant	-0.22)		• <i>Pilot scale:</i> NaOCl is not applied in pilot scale system	

				• <i>Large scale</i> : Minimum and maximum values from Leong et al., (2017) and Kookos et al., (2019), respectively.	L: (Kookos et al., 2019; Leong et al., 2017)
H <sub>2</sub> O <sub>2</sub>	0.053	Not relevant	kg/kg <sub>PHA,recovered</sub>	<ul> <li>Hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) is added for purification at pilot scale.</li> <li><i>Pilot scale:</i> The amount applied is assumed equal to as reported in Harding et al. (2007).</li> <li><i>Large scale:</i> Hydrogen peroxide is not applied in large scale system</li> </ul>	P: (Harding et al., 2007) L: not relevant
Enzyme	0.0024	Not relevant	kg/kg <sub>PHA,recovered</sub>	<ul> <li>Enzyme applied during recovery and extraction at pilot scale.</li> <li><i>Pilot scale:</i> It is assumed that enzyme (optimase) is applied during recovery and extraction at pilot scale as reported in Harding <i>et al.</i> (2007)</li> <li><i>Large scale:</i> Enzyme is not applied in large scale system</li> </ul>	P: (Harding et al., 2007) L: not relevant
Wastewater	65.2	8.81	kg/kg <sub>PHA,recovered</sub>	<ul> <li>Wastewater from recovery and extraction.</li> <li><i>Pilot scale:</i> Amount of wastewater is assumed equal to as reported in Harding et al. (2007). The major part of the wastwater is from washing reactors between batches.</li> <li><i>Large scale:</i> Amount of wastewater is assumed equal to Leong et al., (2017)</li> </ul>	P: (Harding et al., 2007) L: (Leong et al., 2017)
Waste	0.24	1.23	kg/kg <sub>PHA,recovered</sub>	<ul> <li>Solid biowaste from recovery and extraction.</li> <li><i>Pilot scale:</i> Amount of biowaste is assumed equal to as reported in Harding et al. (2007).</li> <li><i>Large scale:</i> Amount of biowaste is assumed equal to Leong et al., (2017)</li> </ul>	P: (Harding et al., 2007) L: (Leong et al., 2017)
Equipment					
Capacity (PHA output)	99	9000	t <sub>PHA,recovered</sub> /year	<ul> <li>Capacity in mass of recovered PHA produced per year.</li> <li><i>Pilot scale:</i> The capacity is calculated based on capacity of each batch (1 t<sub>PHA,recovered</sub>/batch), time of fermentation (80 h/batch) as of Harding et al. (2007) and assuming same yearly operating hours as at large scale (7920 h/year) (Leong et al., (2017).</li> <li><i>Large scale:</i> The capacity is assumed to be equal as for the PHA production plant of Leong et al., (2017) with time of fermentation of 54 hours (including turnaround time required for cleaning and recharging).</li> </ul>	P: Calculated L: (Leong et al., 2017)
Life time of equipment	20	20	Year	Life time of fermenter and other equipment is assumed the same for pilot and large scale	P: Assumed L: Assumed
Number of pumps	Not relevant	1	piece	<ul> <li>Pump for pumping of feedstock into the reactor.</li> <li><i>Pilot scale:</i> The feedstock is transported to the plant by truck. Hence, pump is not relevant.</li> </ul>	P: not relevant L: Assumed

				• <i>Large scale:</i> It is assumed that one pump is used to pump the feedstock into the reactor. The material for the pump is assumed same as in the the Ecoinvent process "Pump station {RoW}  construction   Conseq, U" with a capacity of 644546 m <sup>3</sup> and a lifetime of 70 years.	
Mass, steel	7025	111659	kg	<ul> <li>Mass of steel in the equipment applied during pre-treatment, fermentation, and recovery and extraction. It is assumed that the steel type is chromium steel.</li> <li><i>Pilot scale:</i> The mass is calculated based on the process set-up by Harding et al., (2007). See Table S3 for details. Considering a life time of the equipment of 20 years and yearly capacity, the mass of steel per mass of recovered PHA is 3.5E-03 kg/kgPHA,recovered.</li> <li><i>Large scale:</i> The mass is calculated based on the process set-up by Leong <i>et al.</i> (2017). See Table S4 for details. Considering a life time of the equipment of 20 years and yearly capacity, the mass of steel per mass of recovered PHA is 6.2E-04 kg/kgPHA,recovered.</li> </ul>	P: Calculated based on Harding et al., (2007) L: Calculated based on Leong <i>et al.</i> (2017)
Mass, plastic	54	811	kg	<ul> <li>Mass of plastic in the equipment applied during pre-treatment, fermentation, and recovery and extraction. It is assumed that the plastic type is polypropylene.</li> <li><i>Pilot scale:</i> The mass is calculated based on the process set-up by Harding et al., (2007). See Table S3 for details. Considering a life time of the equipment of 20 years and yearly capacity, the mass of plastic per mass of recovered PHA is 2.7E-05 kg/kg<sub>PHA,recovered</sub>.</li> <li><i>Large scale:</i> The mass is calculated based on the process set-up by Leong <i>et al.</i> (2017). See Table S4 for details Considering a life time of the equipment of 20 years and yearly capacity, the mass of plastic per mass of recovered PHA is 6.2E-04 kg/kg<sub>PHA,recovered</sub>.</li> </ul>	P: Calculated based on Harding et al., (2007) L: Calculated based on Leong <i>et al.</i> (2017)

Table S5. Bill of materials for equipment used during pre-treatment, fermentation, and recovery and extraction at pilot scale based on installations described in Harding et al., (2007). It is assumed that the steel type is chromium steel and plastic type is polypropylene.

Equipment	Mass, steel (kg)	Mass, plastic (kg)	Note
Pre-treatment and ferm	entation	(145)	
Heat sterilizer (pre- treatment)	218	1	The number of sterilizers (1) is assumed equal as in Harding et al., (2007). The weight is estimated by matching it to a pilot scale heat sterilizer from a commercial supplier with the volume of 0.55 m <sup>3</sup> and assuming a cylindrical shape for this equipment with a height of 2 m, a wall thickness of 0.005 m (Chandrashekhar and Rao, 2010) and that it consists of 100% steel with a density of 7850 kg/m <sup>3</sup> . Moreover, additional parts are considered (e.g. motors, control panels etc.), by assuming that the additional parts add 33% to the total weight (as in (Alfalava, n.d.). It is assumed that these additional parts consist of 98% steel and 2% plastic.
Fermenter reactor	1323	7	The volume (10 m <sup>3</sup> ) and number reactors (1) is assumed equal as in Harding et al., (2007). The weight is calculated assuming a cylindrical shape for this equipment with a height of 2 m, a wall thickness of 0.005 m and that it consists of 100% steel with a density of 7850 kg/m <sup>3</sup> . Moreover, additional parts are considered (e.g. motors, control panels etc.), by assuming that the additional parts add 33% to the total weight (as in (Alfalava, n.d.). It is assumed that these additional parts consist of 98% steel and 2% plastic.
<b>Recovery and purificati</b>	ion	<u>.</u>	
High pressure homogenizer	218	1	The number homogenizer (1) is assumed equal as in Harding et al., (2007) and the weight is assumed same as the heat sterilizer.
Centrifuges	1147	23	The number of centrifuges (3) is assumed equal as in Harding et al., (2007). The weight per centrifuge is assumed to be equal to the small centrifuge from Flottweg, (n.d.) (390 kg/centrifuge) and assumed to consist of 100% steel and 2% plastic.
Reactor tanks	2645	13	The number of reactor tanks (2) is assumed equal as in Harding et al., (2007). The weight is assumed the same as the fermenter reactor.
Mixing tanks	1395	7	The number of reactor tanks (3) is assumed equal as in Harding et al., (2007). The volume of each tank is assumed to be half the volume of fermenter reactor (5 m <sup>3</sup> ). The weight is calculated assuming a cylindrical shape for this equipment with a height of 2 m, a wall thickness of 0.005 m and that it consists of 100% steel with a density of 7850 kg/m <sup>3</sup> . Moreover, additional parts are considered (e.g. motors, control panels etc.), by assuming that the additional parts add 33% to the total weight (as in (Alfalava, n.d.). It is assumed that these additional parts consist of 98% steel and 2% plastic.
Spray dryer	78	2	The number of spray dryer (1) was assumed equal as in Harding et al., (2007). The weight is assumed to be equal the gross weight of the small spray dryer from commercial supplier (Yamato, 2017) (80kg/spray dryer) and assumed to consist of 98% steel and 2% plastic.

Table S6. Bill of materials for equipment used during pre-treatment, fermentation, and recovery and extraction at large scale based on installations described in Leong et al. (2017). It is assumed that the steel type is chromium steel and plastic type is polypropylene.

Equipment	Mass,	Mass,	Notes
	steel (kg)	plastic	
		(kg)	
Pre-treatment and ferme	entation		
Blending tank (Tank 1 in Figure 2)	7163	36	The volume (76.6 m <sup>3</sup> ) and number tanks (1) is assumed equal as in Leong <i>et al.</i> (2017). The weight was calculated assuming a cylindrical shape for this equipment with a height of 5 m, a wall thickness of 0.007 m (Chandrashekhar and Rao, 2010) and that it consists of 100% steel with a density of 7850 kg/m <sup>3</sup> . Moreover, additional parts are considered (e.g. motors, control panels etc.), by assuming that the additional parts add 33% to the total weight (as in (Alfalava, n.d.). It is assumed that these additional parts consist of 98% steel and 2% plastic.
Heat sterilizer (pre- treatment)	1814	9	The dimensions (diameter=0.8m and length=15.6 m) and number of sterilizers (1) is assumed equal as in Leong <i>et al.</i> (2017). The weight was calculated assuming a cylindrical shape for this equipment with a height of 5 m, a wall thickness of 0.007 m (Chandrashekhar and Rao, 2010) and that it consists of 100% steel with a density of 7850 kg/m <sup>3</sup> . Moreover, additional parts are considered (e.g. motors, control panels etc.), by assuming that the additional parts add 33% to the total weight (as in (Alfalava, n.d.). It is assumed that these additional parts consist of 98% steel and 2% plastic.
Fermenter reactor	25928	131	The volume (102 m <sup>3</sup> ) and number reactors (3) is assumed equal as in Leong <i>et al.</i> (2017). The weight is calculated assuming a cylindrical shape for this equipment with a height of 5 m, a wall thickness of 0.007 m (Chandrashekhar and Rao, 2010) and that it consists of 100% steel with a density of 7850 kg/m <sup>3</sup> . Moreover, additional parts are considered (e.g. motors, control panels etc.), by assuming that the additional parts add 33% to the total weight (as in (Alfalava, n.d.). It is assumed that these additional parts consist of 98% steel and 2% plastic.
Piping	12750	-	The length of the piping (300) is assumed and its weight was estimated by matching it to commercial pipes (The process piping, n.d.), assuming an inner diameter of 200 mm and a standard wall thickness (8.2 mm).
<b>Recovery and purification</b>	on		
Flat-bottom tank (Tank 2 in Figure 2)	9189	47	The volume (112 m3) and number tanks (1) is assumed equal as in Leong et al. (2017). The weight is calculated assuming a cylindrical shape for this equipment with a height of 5 m, a wall thickness of 0.007 m (Chandrashekhar and Rao, 2010) and that it consists of 100% steel with a density of 7850 kg/m3. Moreover, additional parts were considered (e.g. motors, control panels etc.), by assuming that the additional parts add 33% to the total weight (as in (Alfalava, n.d.). It is assumed that these additional parts consist of 98% steel and 2% plastic.
Disk-stack centrifuges (Centrifuge 1 in Figure 2)	12627	258	The number of centrifuges (6) is assumed equal as in Leong et al. (2017). The weight per centrifuge is assumed to be the average gross weight of industrial scale centrifuges from Flottweg, (n.d.) (2148 kg/centrifuge) and assumed to consist of 100% steel and 2% plastic.
Blending rank (Tank 3 in Figure 2)	16707	85	The volume (8.17 m3) and number tanks (9) is assumed equal as in Leong et al. (2017). The weight is calculated by assuming a cylindrical shape for this equipment with a height of 5 m, a wall thickness of 0.007 m (Chandrashekhar and Rao, 2010) and that it consists of 100% steel with a density of 7850 kg/m3. Moreover,

			additional parts are considered (e.g. motors, control panels etc.), by assuming that the additional parts add 33% to the total weight (as in (Alfalava, n.d.). It is assumed that these additional parts consist of 98% steel and 2% plastic.
Disk-stack centrifuge (Centrifuge 2 in Figure 2)	10523	215	The number of centrifuges (5) was assumed equal as in Leong et al. (2017). The weight per centrifuge is assumed to be the average gross weight of industrial scale centrifuges from Flottweg, (n.d.) (2148 kg /centrifuge) and assumed to consist of 100% steel and 2% plastic.
Disk-stack centrifuge (Centrifuge 3 in Figure 2)	4209	86	The number of centrifuges (2) was assumed equal as in Leong et al. (2017). The weight per centrifuge is assumed to be the average gross weight of industrial scale centrifuges from Flottweg, (n.d.) (2148 kg /centrifuge) and assumed to consist of 100% steel and 2% plastic.
Blending tank (Tank 4 in Figure 2)	6362	32	The volume (38.8 m3) and number tanks (1) was assumed equal as in Leong et al. (2017). The weight is calculated by assuming a cylindrical shape for this equipment with a height of 5 m, a wall thickness of 0.007 m (Chandrashekhar and Rao, 2010) and that it consists of 100% steel with a density of 7850 kg/m3. Moreover, additional parts are considered (e.g. motors, control panels etc.), by assuming that the additional parts add 33% to the total weight (as in (Alfalava, n.d.). It is assumed that these additional parts consist of 98% steel and 2% plastic.
Disk-stack centrifuge (Centrifuge 4 in Figure 2)	4209	86	The number of centrifuges (2) was assumed equal as in Leong et al. (2017). The weight per centrifuge is assumed to be the average gross weight of industrial scale centrifuges from Flottweg, (n.d.) (2148 kg /centrifuge) and assumed to consist of 100% steel and 2% plastic.
Spray dryer	176	4	The number of spray dryer (1) was assumed equal as in Leong et al. (2017). The weight is assumed to be equal the gross weight of industrial scale spray dryer from (Yamato Scientific, 2017) (180kg/spray dryer) and assumed to consist of 100% steel and 2% plastic.

Table S7. Overview of parameters and data sources for production on PHA biofilm, lamination and coating, printing, use and disposal of packing. Parameters are for large scale production, and assumed applicable at pilot scale.

Parameter	Large scale	Unit	Note	Main data
	Average			source
	(min-max)			
Compounding and p	elletizing			
Pellets yield	0.826 (0.785 -	kg	Mass of recovered PHA pellets converted from PHA powder (measured). Perturbation	Assumed
	0.867)	powder/kg <sub>pellet</sub>	values are assumed 5% increase/decrease.	
Amount of additive	0.174 (0.154 –	kg/kg <sub>pellets</sub>	Additives such as plasticizer, nucleating agents, stabilizers are needed to tune	Assumed
	0.170)	-	properties of the material (such as barrier and mechanical properties). The applied	
			additives are selected considering preservation of the intrinsic biodegradability of	
			PHA. It is assumed that the additive used is a plasticizer based on sulfonated	
			melamine formaldehyde and the amount is assumed to be in a realistic range of	
			values. Additives such as reinforcing fillers are added to biopolymers as a nucleating	
			agent to enhance the crystallization and as a thermal barrier, improving the thermal	

			stability of the biopolymer (Bugnicourt et al., 2014). It is assumed that acrylic filler is used as filler in this study and the amount is assumed to be in a realistic range of values. Perturbation values as assumed 5% increase/decrease.	
Electricity for extrusion	4.27 (3.50 – 5.00)	kWh/kg <sub>pellets</sub>	Electricity used for corotating twin screw extruder to melt the compound and for cooling, drying, pelletizing, dehumidifying (assumed to be in a realistic range of values).	Assumed
Tap water	0.040 (0.038 – 0.042)	l/ kg <sub>pellets</sub>	Cooling water for the extrusion. The volume of water applied is assumed to be in realistic range of values.	Assumed
Number of extruders	1	piece	Material for equipment (one extruder) is assumed equal to the equipment in the Ecoinvent process for plastic sheet extrusion ("Extrusion, co-extrusion {FR}] of plastic sheets   Conseq, U").	Assumed based on Ecoinvent
PHA filmmaking				
Yield of biofilm	0.925	$kg_{biofilm}\!/kg_{pellets}$	Mass of biofilm produced per mass of PHA pellet (measured by Tampere University of Technology (TUT), Finland).	Measured
Amount of biowaste	0.075	$kg_{biofilm}/kg_{pellets}$	Mass of biowaste generated during the production of PHA film calculated considering the biofilm yield (1 – biofilm yield).	Calculated
Electricity use	0.1	kWh/kg <sub>pellets</sub>	Electricity consumed for heating, melting, and pumping (measured by TUT).	Measured
Amount of auxiliaries and water	See Ecoinvent process	-	Auxiliaries (detergents and solvents) and water consumed for PHA filmmaking is assumed equal to what is used in the Ecoinvent process for plastic sheet extrusion ("Extrusion, co-extrusion {FR}] of plastic sheets   Conseq, U").	Assumed based on Ecoinvent
Number of extruders	4	piece	The extrusion of biofilm is done at a plant with four extruders with different outputs with the possibility for (co)extrusion coating and lamination, casting, dispersion coating and various surface treatments (including corona, flame, plasma, UV, IR, LFS). Bill of material for each extruder is assumed equal to the material in the Ecoinvent process "Extrusion, co-extrusion {FR}  of plastic sheets   Conseq, U".	Assumed based on Ecoinvent
Ink (varnish and pig	ment)			
Content of acrylic resin	0.224	kg/kg <sub>ink</sub>	Acrylic resin used as solvent for the varnish (measured by KAO Chimigraf).	Measured
Content of silicone defoamer	0.0056	kg/kg <sub>ink</sub>	Silicone used as defoamer (measured by KAO Chimigraf).	Measured
Content of wetting agent (ethoxylate alcohol)	0.012	kg/kg <sub>ink</sub>	Ethoxylate alcohol used as wetting agent in the ink mix (measured by KAO Chimigraf).	Measured
Content of biocide	0.0017	kg/kg <sub>ink</sub>	It is assumed that the biocide used is Benzimidazole-compound (BIT) (measured by KAO Chimigraf).	Measured
Content of wax (polyethylene)	0.003	kg/kg <sub>ink</sub>	Polyethylene applied as wax (measured by KAO Chimigraf).	Measured

Content of retardant accelerator solvent	0.03	kg/kg <sub>ink</sub>	Glycerin used as solvent in the ink mix (measured by KAO Chimigraf).	Measured
Content of water	0.5637	kg/kg <sub>ink</sub>	Water mixed in the ink (measured by KAO Chimigraf).	Measured
Content of pigment (carbon)	0.16	kg/kg <sub>ink</sub>	It is assumed that carbon is used as organic pigment (measured by KAO Chimigraf).	Measured
Use of electricity	0.11	kWh/kg <sub>ink</sub>	Electricity consumed to produce the ink (measured by KAO Chimigraf).	Measured
PHA packaging prod	luction (PHA filn	n functionalizatio	n and printing)	
Weight of PHA layer	88	$g/m^2_{packaging}$	Weight of PHA biofilm measured by Icimendue. This corresponds to a thickness of 76.5 micro m when applying a density of 1.15 g/cm <sup>3</sup> (BioBarr, 2019).	Measured
Weight of PLA layer	24.8	g/m <sup>2</sup> packaging	Weight of the PLA layer laminated with the PHA biofilm (measured). This corresponds to a thickness of 20 micro m when applying a density of 1.24 g/cm <sup>3</sup> (Sousa et al., 2019).	Measured
Yield of PLA biofilm	0.925	$kg_{biofilm}/kg_{pellets}$	Mass of biofilm produced per mass of PLA pellet assumed equal to as for the PHA biofilm.	Assuned
Weight of Aluminum fiber coil	0.027	g/m <sup>2</sup> packaging	Weight of the aluminum consumed as surface treatment of the PHA biofilm (i.e. metallization). The treatment is based on deposition under vacuum of a thin aluminum layer on the biofilm. The weight is calculated based on aluminum layer thickness of 10 nm (measured by Icimendue) and a density of 2.710 g/cm <sup>3</sup> for aluminum. It is assumed that aluminum ingot is representative as aluminum fiber coil, as the majority of the energy consumed during production of both aluminum ingot and coil is for melting the aluminum. Hence, the production step from aluminum ingot to coil is not considered.	Measured and calculated
Weight of AlOx	0.039	g/m <sup>2</sup> packaging	Weight of AlOx layer as surface treatment of the PHA biofilm. As for the aluminum layer, the AlOx treatment is a based on the deposition under vacuum of a thin aluminum layer on the biofilm. In addition, in the case of AlOx treatment, oxygen is introduced in the vacuum chamber oxidizing the aluminum before deposition. The AlOx layer therefore appears transparent. The weight is calculated based on AlOx layer thickness of 10 nm (measured by Icimendue) and a density of $3.95 \text{ g/cm}^3$ for AlOx. Al <sub>2</sub> O <sub>3</sub> constitutes of 47 % O <sub>2</sub> and 53 % Al (weight based).	Measured and calculated
Amount of adhesive	2.2	g/m <sup>2</sup> packaging	Amount of adhesive applied to glue to PHA film with a PLA layer (only relevant in the scenarios where PLA is used for surface functionalization). Measured by Icimendue.	Measured
Amount of ink	19	$cm^3/m^2_{packaging}$	Amount of ink printed on the packaging. Measured by Icimendue.	
Use of electricity, lamination and printing	0.208	kWh/kg <sub>packaging</sub>	Electricity consumed when laminating the PHA + PLA film layer and printing (only relevant in the scenarios where PLA is used for surface functionalization). Assumed to be the same as the electricity consumed for printing and laminating without corona treatment measured by Icimendue.	Measured and assumed

Use of electricity, surface treatment and printing	0.432	kWh/kg <sub>packaging</sub>	Electricity consumed to vaporize the aluminum coil and AlOx during metallization surface treatment and printing (relevant for scenario 7 and 8). Assumed to be the same as the electricity consumed for printing and laminating with corona treatment measured by Icimendue	Assumed based on measurements
Use				
Transport	442	Km	Transport distance from the food manufacturer where the packaging is enwrapped the croissants (at Corsini biscotti, Via delle Cellane, 9, 58033 Castel del Piano GR, Italy) to where the croissant are sold for consumption (Milan). The transport distance is assumed the same in the scenario where Germany is the geographic location.	Calculated
Packaging use and d	lisposal			
Rates for recycling, incineration and landfill	See Table S9	See Table S9	See Table S9	See Table S9
Waste treatment processes	See Table S7	See Table S7	Based on an existing Ecoinvent processes. See Table S6.	See Table S7

# Table S8. Overview of parameters and data sources for packaging based on polypropylene, polyethylene and PLA

Parameter	Large scale Average	Unit	Note	Main data source
	(min-max)			
Polypropylene, weight	29.6	$g/m^2_{packaging}$	Mass of polypropylene film with properties similar to the one for the PHA- based packaging film, which corresponds to a thickness of 31 micro m. Currently used by Corsini biscotti.	Measured by Corsini biscotti
Polyethylene, weight	29.6	g/m <sup>2</sup> <sub>packaging</sub>	Mass of polyethylene film with properties similar to the one for the PHA- based packaging film, which corresponds to a thickness of 31 micro m. Currently used by Corsini biscotti.	Measured by Corsini biscotti
PLA, weight	112.8 and 62	g/m <sup>2</sup> packaging	Mass of polypropylene film with properties similar to the one for the PHA- based packaging. Two scenarios for PLA weight were tested; 1) weight of PLA film was assumed to be equal to the weight of PHA + PLA in the PHA- based packaging film (112.8 g/m <sup>2</sup> ) corresponding to a thickness of 91 micro m (applying a density 1.24 g/cm <sup>3</sup> ) and 2) weight corresponds to 50 micro m thickness assumed by Icimendue.	Assumed
Amount of ink	19	cm <sup>3</sup> /m <sup>2</sup> <sub>packaging</sub>	Amount of ink printed on the packaging. Assumed to be equal to the amount of ink applied for PHA packaging (Table S5).	Assumed

Electricity for printing	0.0208	kWh/kg <sub>packaging</sub>	Electricity consumed for printing on the polypropylene, polyethylene and PLA packaging. Assumed to be 10% of the electricity consumed for printing and laminating as of the PHA packaging (Table S5).	Assumed
Transportation	442	km	Transport distance from manufacturer to the location where the product is sold, is assumed equal to the amount of ink applied for PHA packaging (Table S5).	Calculated
Rates for recycling, incineration and landfill and waste treatment processes	See Table S11	See Table S11	The waste management rates of PLA, PP and PHA packaging is assumed equal as for PHA packaging (Table S5). Landfill and incineration processes for PLA is modelled equal as to PHA. Landfill and incineration processes for PP and PE are modelled according to existing Ecoinvent processes ("plastic, mixture {CH}  treatment of, sanitary landfill   Conseq, U", "Waste polyethylene {CH}  treatment of, municipal incineration with fly ash extraction   Conseq, U", "Waste polypropylene {CH}  treatment of, municipal incineration with fly ash extraction   Conseq, U"), however, updating the substituted electricity and heat processes to processes representing Italy as geographical location.	See Table S11

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Existing	New process	Modifications
Electricity, high voltage {IT}  market for   Conseq, U	Electricity, high voltage {IT}  market for   Average mix, U_2018_EBV	Modified according to average Italian electricity grid mix considering electricity generation by source (2018) from IEA World Energy Balances 2019 and proportion of imported energy based on "Electricity, high voltage {IT}  market for   APOS, U". See Table S8 for details. The electricity grid mix of countries from which Italy import more than 1% from was also updated (France and Switzerland). This update was done by using the APOS electricity process, representing the 2017 grid mix (e.g. "Electricity, high voltage {FR}  market for   APOS, U"), and substituting the individual electricity production processes with consequential versions (to handle multifunctionality with system expansion instead of allocation). See Table S8 for an overview of the resulting average electricity grid mix process.
Electricity, high voltage {DE}  market for   Conseq, U	Electricity, high voltage {DE}  market for   Average mix, U_2018_EBV	Modified according to average German electricity grid mix considering electricity generation by source (2018) from IEA World Energy Balances 2019 and proportion of imported energy based on "Electricity, high voltage {DE}  market for   APOS, U". See Table S8 for details. The electricity grid mix of countries from which Germany import more than 1% from was also updated (France). This update was done by using the APOS electricity process, representing the 2017 grid mix (e.g. "Electricity, high voltage {FR}  market for   APOS, U"), and substituting the individual electricity production processes with consequential versions (to handle multifunctionality with system expansion instead of allocation).
Electricity, low voltage {IT}  market for   Conseq, U	Electricity, low voltage {IT}  market for   Average mix, U_2018_EBV	Links from the market for low voltage electricity were updated to the average mix for high voltage electricity through transformation processes and medium voltage (Electricity, low voltage {IT}  electricity voltage transformation from medium to low voltage   Average mix, U_2018_EBV, Electricity, medium voltage {IT}  market for   Average mix, U_2018_EBV, Electricity, medium voltage {IT}  electricity voltage transformation from high to medium voltage   Average mix U_2018_EBV).
Electricity, low voltage {DE}  market for   Conseq, U	Electricity, low voltage {DE}  market for   Average mix, U_2018_EBV	Links from the market for low voltage electricity were updated to the average mix for high voltage electricity through transformation processes and medium voltage (Electricity, low voltage {DE}  electricity voltage transformation from medium to low voltage   Average mix, U_2018_EBV, Electricity, medium voltage {DE}  market for   Average mix, U_2018_EBV, and Electricity, medium voltage {DE}  electricity voltage transformation from high to medium voltage   Average mix U_2018_EBV).
Electricity, high voltage {IT}  heat and power co-generation, biogas, gas engine   Conseq, U	Electricity, high voltage {IT or DE}  heat and power co- generation, biogas, gas engine   Conseq, U_EBV	Biogas input to the heat and power co-generation was updated from marginal biogas mix for the rest of the world region ("Biogas {RoW}] market for biogas   Conseq, U") (100% biogas from manure) to average biogas mix, according to the APOS process (representing average biogas mix in the rest of the world region) ("Biogas {IT or DE}  market for biogas   Average mix, U"). The average mix consist of 33% biogas from manure, 30% from biowaste, 37% from sewage sludge and 0.31% from vegetable cooking oil by anaerobic digestion. APOS processes were substituted with Conseq, where applicable (for the biogas production from the waste materials, there is not consequential version). Furthermore, biogas from manure was updated from "Biogas {CH}  anaerobic digestion of manure   Conseq, U" to "Biogas {IT or DE}  anaerobic digestion of manure   Conseq, U" by updating the geography of the electricity

		consumed during the anaerobic digestion of manure and substituted when incinerating the digester sludge to Italy or Germany.
Biowaste {CH}  treatment of, municipal incineration with fly ash extraction   Conseq, U	Biowaste {IT or DE}  treatment of, municipal incineration with fly ash extraction   Conseq, U_EBV	It was assumed that metals are not present in the biowaste derived from PHA production. Emissions of metals (aluminium, arsenic, cadmium, chromium, cobalt, copper, iron, lead, mercury, nickel, tin, zinc) to air and water were therefore removed. Waste treatment of "Spent activated carbon with mercury {GLO}  market for   Conseq, U" was removed. Heat and electricity for reuse in municipal waste incineration processes was updated to represent those for Italy or Germany.
Biowaste {CH}  treatment of biowaste, industrial composting   Conseq, U	Biowaste {IT or DE}  treatment of biowaste, industrial composting   Conseq, U_EBV	Electricity and waste treatments was updated to represent electricity grid mix of Italy or Germany.
Biowaste {CH}  treatment of biowaste by anaerobic digestion   Conseq, U	Biowaste {IT or DE}  treatment of biowaste by anaerobic digestion   Conseq, U_EBV	Electricity was updated to represent electricity grid mix of Italy Germany and tap water and wastewater treatment to Europe without Switzerland.
Waste plastic, mixture {CH}  treatment of, municipal incineration with fly ash extraction   Conseq, U	Bioplastic {IT or DE}  treatment of, municipal incineration with fly ash extraction   Conseq, U_EBV	It was assumed that metals are not present in the bioplastic packaging, except aluminum. Emissions of metals (aluminium, arsenic, cadmium, chromium, cobalt, copper, iron, lead, mercury, nickel, tin, zinc) to air and water were therefore removed. Waste treatment of "Spent activated carbon with mercury {GLO}  market for   Conseq, U" was removed. Geography of electricity and heat for reuse in municipal waste incineration processes was updated to Italy or Germany. Emission of fossil CO <sub>2</sub> was replaced by biogenic CO <sub>2</sub> and the mass of CO <sub>2</sub> emitted from incineration is calculated, considering the initial content of C in the packaging and assuming that 100% is emitted as CO <sub>2</sub> (Rossi et al., 2015). Hence, emissions of CH <sub>4</sub> were also removed.
Wastewater, average {Europe without Switzerland}  treatment of wastewater, average, capacity 1E9l/year   Conseq, U	Wastewater, average {Europe without Switzerland}  treatment of wastewater, average, capacity 1E9l/year   Conseq, U_EBV	Carbon-related emissions adapted to carbon content of PHA-fermentation effluent wastewater (parameterized considering yield of raw PHA and associated mass of feedstock). Metal-related emissions are removed, except aluminum, chromium, iron and titanium, as it is assumed that these are related to the input chemicals of the wastewater treatment.
Waste plastic, mixture {CH}  treatment of, sanitary landfill   Conseq, U	Bioplastic, mixture {IT or DE}  treatment of, sanitary landfill   Conseq, U_EBV	It was assumed that metals are not present in the bioplastic packaging, except aluminum. Emissions of metals (aluminium, arsenic, cadmium, chromium, cobalt, copper, iron, lead, mercury, nickel, tin, zinc) to air and water were therefore removed. Geography of heat and electricity consumption was updated. Emission of fossil CO <sub>2</sub> was replaced by biogenic CO <sub>2</sub> and the mass of CO <sub>2</sub> emitted from incineration is calculated considering the initial content of C in the packaging, a degradation fraction (i.e. how much is degraded after 100 years, depending on the degradation scenarios) and assuming that 29% is emitted as CO <sub>2</sub> and 71% as CH <sub>4</sub> (Rossi et al., 2015).

Extrusion, co-	Extrusion, co-	Paper for labelling sheets considered in the original process are not
extrusion {FR}	extrusion {IT or	relevant and were removed. Geography of electricity was update to Italian
of plastic sheets	DE}  of PHA	or German average grid mix and mass as measured in project. Plastic
Conseq, U	plastic sheets	waste was removed, as waste from the PHA bioplastic film extrusion is
	Conseq,	already considered (see Table S4). Material for equipment was removed as
	U_EBV	this was considered separately in the modelling.
Packaging film,	Packaging film,	Electricity applied for extrusion is updated to represent the electricity grid
low density	low density	mix of Italy.
polypropylene	polypropylene	
{RER}	{IT}  production	
production	Conseq,	
Conseq, U	U_EBV	
Packaging film,	Packaging film,	Electricity applied for extrusion is updated to represent the electricity grid
low density	low density	mix of Italy.
polyethylene	polyethylene	
{RER}	{IT}  production	
production	Conseq,	
Conseq, U	U_EBV	

Table S10. Electricity generation by source in Italy and Germany, 2018 (IEA, 2018).

Source	Italy (GWh)	Italy (fraction)	Germany (GWh)	Germany (fraction)
Coal	30542	0.125	241479	0.421
Natural gas	129743	0.530	85043	0.148
Hydro	5925	0.024	1548	0.003
Wind	17492	0.071	111590	0.195
Biofuels	16858	0.069	45101	0.079
Waste	4806	0.020	13244	0.023
Solar	22653	0.093	46164	0.080
Oil	10762	0.044	5231	0.009
Nuclear	0	-	24170	0.042
Geothermal	6080	0.025	0	0

Table S11. Rates of recycling, incineration, and landfilling in Italy and Germany for the major materials in the PHA production plant

Waste	Landfill	ing (%)	Incine (%)	eration	Incineration with energy recovery		Recovery than ener recovery	y other rgy (%)	Source
	Italy	Germany	Italy	Germany	Italy	Germany	Italy	Germany	
Metal waste, ferrous	0.05%	0.26%	0%	0%	0%	0.89%	99.95%	98.85%	Eurostat (2016 data)
Plastic waste	35%	0%	0%	0%	35%	62%	30%	38%	(Plastics Europe, 2019)
Biowaste	2.6%	0.7%	2.5%	1.9%	8.3%	44.9%	86.6% <sup>a</sup>	52.5% <sup>a</sup>	Eurostat (2017 data)

Plastic	18.17%	0.21%	0%	0%	40.01%	50.06%	41.82% <sup>b</sup>	49.73% <sup>b</sup>	Eurostat
packaging									(2017 data)
waste									

<sup>a</sup>In Italy, 52% of the recovered biowaste is treated by composting and 48% by anaerobic digestion (AD) (ENC,

2019) (2017 data), and in Germany, 36% by composting and 64% by AD (Bundesgütegemeinschaft, 2014) (2013 data).

<sup>b</sup>It is assumed that the bioplastic packaging waste that is "recovered other than energy recovery", cannot be recycled, but it treated proportionally to the treatment of non-recovered plastic waste (50% and 0% landfilled and 50% and 100% incinerated with energy recovery for Italy and Germany respectively).

# S3. Details of life cycle impact assessment

	Impact score calculation	Symbols
GWP100 <sub>ILCD</sub> [kg CO <sub>2</sub> eq/functional unit]	$IS_{\text{GWP100}_{\text{ILCD}}} = \sum_{i} M_{i} \cdot GWP100_{i} - Credit_{i}$ $Credit_{i} = \sum_{T=2}^{100} m_{i}(T) \cdot T \cdot EQ_{i}$	$M_i$ = total mass of gas <i>i</i> emitted in 100 years [kg]; <i>GWP100<sub>i</sub></i> = GWP100 of gas <i>i</i> [kg CO <sub>2</sub> eq · kg <sup><i>i</i></sup> ] <sup>a</sup> ; <i>Credit</i> <sub><i>i</i></sub> = ILCD credit for carbon storage; $m_i(T)$ = mass of gas <i>i</i> emitted at (relative) time <i>T</i> ; $EQ_i$ = equivalency factor for gas <i>i</i> (0.01 and 0.34 [kg CO <sub>2</sub> eq · kg <sup><i>i</i></sup> ]. yr <sup>-1</sup> ] for CO <sub>2</sub> and CH <sub>4</sub> respectively(EC-JRC, 2010)
MCTP [ppt <sub>rc</sub> /functional unit]	$IS_{\text{MCTP}} = \sum_{i} \sum_{T_{\text{emission}}=2021}^{T_{\text{tipping},j_{\text{last}}}} m_i(T_{\text{emission}}) \cdot MCTP_i(T_{\text{emission}})$	$T_{\text{tipping}, j_{\text{last}}} = \text{year of last tipping}$ point; $m_i(T_{\text{emission}}) = \text{mass of gas}$ $i \text{ emitted at year } T_{\text{emission}} \text{ [kg];}$ $MCTP_i(T_{\text{emission}}) = \text{MCTP for gas}$ $i \text{ and emission year } T_{\text{emission}} \text{ [pptrc}$ $\cdot \text{ kg}^{-1}$ ]
GTP100 [kg CO2eq/functional unit]	$IS_{\rm GTP100} = \sum_{i} M_i \cdot GTP100_i$	$M_i$ = total mass of gas <i>i</i> emitted over 100 years [kg]; $GTP100_i$ = GTP100 of gas <i>i</i> [kg CO <sub>2</sub> eq · kg <sup>-1</sup> ]

Table S12. Overview of equations used for calculation of impact scores (*IS*) with the three-climate-related metrics.

<sup>a</sup> GWP100 for biogenic and fossil methane used are 34 and 36 kg CO<sub>2</sub>eq/kg CH<sub>4</sub>, respectively from IPCC (2014)

# **S4.** Additional results

Table S13. Characterized impacts, expressed in category-specific units per functional unit for the pilot scale (scenario 1) and large scale PHA value chains (scenario 2). Results for all scenarios are documented in Table SI4.

		Impa	act score
Impact category	Unit	Scenario 1 (Pilot)	Scenario 2 (Large)
Climate change (GWP100)	kg CO2 eq	5.5E-02	5.2E-02
Global temperature change (GTP100)	kg CO2 eq	8.5E-02	1.0E-01
Multiple climate tipping (MCTP <sub>RCP6, 2020</sub> )	ppt <sub>rc</sub>	1.0E-03	1.2E-03
Stratospheric ozone depletion	kg CFC11 eq	5.2E-07	6.8E-07
Ionizing radiation	kBq Co-60 eq	2.3E-04	2.7E-04
Ozone formation, Human health	kg NOx eq	1.5E-04	2.0E-04
Fine particulate matter formation	kg PM2.5 eq	6.6E-05	8.9E-05
Ozone formation, Terrestrial ecosystems	kg NOx eq	1.6E-04	2.1E-04
Terrestrial acidification	kg SO2 eq	2.1E-04	2.6E-04
Freshwater eutrophication	kg P eq	5.0E-06	4.4E-06
Marine eutrophication	kg N eq	1.1E-04	1.6E-04
Terrestrial ecotoxicity	kg 1,4-DCB	2.9E-01	3.7E-01
Freshwater ecotoxicity	kg 1,4-DCB	1.7E-04	4.0E-04
Marine ecotoxicity	kg 1,4-DCB	3.1E-04	4.1E-04
Human carcinogenic toxicity	kg 1,4-DCB	4.6E-04	5.3E-04
Human non-carcinogenic toxicity	kg 1,4-DCB	2.1E-02	2.8E-02
Land use	m2a crop eq	7.7E-02	1.1E-01
Mineral resource scarcity	kg Cu eq	3.3E-04	4.5E-04
Fossil resource scarcity	kg oil eq	1.8E-02	2.2E-02
Water consumption	m3	7.4E-03	1.0E-02

	Unit	S3	<b>S4</b>	S5	<b>S</b> 6	S7	S8	<b>S9</b>	S10	S11	S12	S13	S14
Climate change	kg CO2 eq	3.6E-02	3.5E-02	4.7E-02	3.1E-02	4.9E-02	4.9E-02	4.4E-02	2.5E-02	5.9E-03	6.4E-03	5.2E-02	5.2E-02
Stratospheric ozone depletion	kg CFC11 eq	5.3E-07	7.1E-07	7.4E-07	7.7E-07	6.5E-07	6.5E-07	1.3E-07	7.3E-08	2.2E-09	2.4E-09	1.1E-06	8.1E-07
Ionizing radiation	kBq Co-60 eq	2.2E-04	2.7E-04	2.3E-04	2.3E-04	2.8E-04	2.8E-04	-4.6E-05	-2.6E-05	7.0E-06	1.2E-05	3.2E-04	2.9E-04
Ozone formation, Human health	kg NOx eq	1.4E-04	1.9E-04	2.2E-04	2.2E-04	1.9E-04	1.9E-04	5.0E-05	2.8E-05	5.3E-06	7.0E-06	2.7E-04	2.2E-04
Fine particulate matter formation	kg PM2.5 eq	5.4E-05	7.6E-05	9.9E-05	8.6E-05	8.6E-05	8.6E-05	1.7E-05	9.8E-06	1.5E-06	3.0E-06	1.2E-04	9.8E-05
Ozone formation, Terrestrial ecosystems	kg NOx eq	1.5E-04	2.0E-04	2.3E-04	2.3E-04	1.9E-04	1.9E-04	5.3E-05	3.0E-05	6.1E-06	8.4E-06	2.8E-04	2.3E-04
Terrestrial acidification	kg SO2 eq	1.7E-04	2.3E-04	2.9E-04	2.5E-04	2.6E-04	2.6E-04	4.4E-05	2.6E-05	2.5E-06	1.3E-06	3.7E-04	3.0E-04
Freshwater eutrophication	kg P eq	4.9E-06	4.3E-06	-1.6E- 05	-1.6E-05	4.0E-06	4.0E-06	5.9E-07	-1.9E-07	-1.4E-06	-1.4E-06	8.6E-06	5.8E-06
Marine eutrophication	kg N eq	1.1E-04	1.6E-04	1.1E-05	1.0E-05	1.6E-04	1.6E-04	1.1E-05	6.1E-06	7.8E-07	7.9E-07	2.4E-04	1.9E-04
Terrestrial ecotoxicity	kg 1,4-DCB	2.9E-01	3.8E-01	4.9E-01	5.0E-01	3.5E-01	3.5E-01	8.9E-02	5.2E-02	2.4E-02	2.7E-02	4.9E-01	4.1E-01
Freshwater ecotoxicity	kg 1,4-DCB	1.7E-04	4.1E-04	4.9E-04	5.0E-04	3.8E-04	3.8E-04	9.9E-05	5.5E-05	3.4E-06	4.1E-06	4.8E-04	4.3E-04
Marine ecotoxicity	kg 1,4-DCB	3.2E-04	4.2E-04	4.4E-04	4.5E-04	3.9E-04	3.9E-04	1.1E-04	6.3E-05	1.8E-05	2.1E-05	5.5E-04	4.6E-04
Human carcinogenic toxicity	kg 1,4-DCB	4.5E-04	5.8E-04	6.3E-04	6.8E-04	5.1E-04	5.1E-04	1.1E-04	6.8E-05	2.6E-05	2.6E-05	6.7E-04	5.8E-04
Human non-carcinogenic toxicity	kg 1,4-DCB	2.2E-02	3.0E-02	3.8E-02	4.0E-02	2.7E-02	2.7E-02	2.8E-03	1.7E-03	2.5E-04	2.2E-04	3.9E-02	3.2E-02
Land use	m2a crop eq	7.6E-02	1.1E-01	-4.0E- 02	-4.1E-02	1.1E-01	1.1E-01	1.9E-03	1.2E-03	-1.4E-04	-2.8E-04	1.7E-01	1.3E-01
Mineral resource scarcity	kg Cu eq	3.4E-04	4.6E-04	7.6E-04	7.7E-04	4.3E-04	4.3E-04	9.1E-05	5.2E-05	1.7E-05	1.7E-05	6.1E-04	5.0E-04
Fossil resource scarcity	kg oil eq	1.7E-02	2.1E-02	2.6E-02	2.5E-02	2.0E-02	2.0E-02	9.8E-03	5.6E-03	3.2E-03	3.2E-03	2.6E-02	2.3E-02
Water consumption	m3	7.2E-03	1.0E-02	5.1E-03	4.9E-03	1.0E-02	1.0E-02	7.7E-04	4.3E-04	-1.1E-05	-8.5E-06	1.6E-02	1.2E-02
GTP100	kg CO2 eq	7.7E-02	9.5E-02	1.3E-01	1.2E-01	9.8E-02	9.8E-02	3.7E-02	2.1E-02	4.5E-03	4.7E-03	1.4E-01	1.2E-01
MCTPs	ppt	7.4E-04	9.5E-04	1.1E-03	8.9E-04	1.2E-03	1.2E-03	5.2E-04	3.0E-04	4.7E-05	4.8E-05	1.6E-03	1.3E-03

Table S14. Characterized impact scores in category-specific units excluding long-term emissions for sensitivity scenarios 3-53

		S15	S16	S17	S18	S19	S20	S21	S22	S23	S24	S25	S26
Climate change	kg CO2 eq	5.3E-02	5.3E-02	5.3E-02	5.3E-02	1.7E-02	1.7E-02	1.7E-02	1.7E-02	1.7E-02	1.7E-02	1.7E-02	2.1E-02
Stratospheric ozone depletion	kg CFC11 eq	6.0E-07	5.2E-07	4.4E-07	3.9E-07	2.3E-07	1.8E-07	1.6E-07	1.4E-07	1.2E-07	1.1E-07	9.6E-08	3.0E-07
Ionizing radiation	kBq Co-60 eq	2.6E-04	2.5E-04	2.4E-04	2.3E-04	6.1E-05	5.4E-05	5.1E-05	4.9E-05	4.6E-05	4.4E-05	4.3E-05	7.9E-05
Ozone formation, Human health	kg NOx eq	1.8E-04	1.7E-04	1.5E-04	1.4E-04	6.3E-05	5.3E-05	4.8E-05	4.5E-05	4.2E-05	3.9E-05	3.6E-05	8.0E-05
Fine particulate matter formation	kg PM2.5 eq	8.4E-05	7.8E-05	7.3E-05	6.9E-05	2.7E-05	2.3E-05	2.1E-05	2.0E-05	1.9E-05	1.8E-05	1.7E-05	3.4E-05
Ozone formation, Terrestrial ecosystems	kg NOx eq	1.9E-04	1.7E-04	1.6E-04	1.5E-04	6.6E-05	5.6E-05	5.1E-05	4.7E-05	4.4E-05	4.1E-05	3.9E-05	8.4E-05
Terrestrial acidification	kg SO2 eq	2.5E-04	2.2E-04	2.0E-04	1.9E-04	8.2E-05	6.9E-05	6.2E-05	5.8E-05	5.3E-05	4.9E-05	4.6E-05	1.0E-04
Freshwater eutrophication	kg P eq	3.6E-06	2.6E-06	1.8E-06	1.2E-06	1.0E-06	4.8E-07	1.9E-07	1.9E-08	-1.7E-07	-3.4E-07	-4.7E-07	1.7E-06
Marine eutrophication	kg N eq	1.4E-04	1.2E-04	1.0E-04	9.2E-05	5.1E-05	3.9E-05	3.4E-05	3.0E-05	2.6E-05	2.3E-05	2.0E-05	6.5E-05
Terrestrial ecotoxicity	kg 1,4-DCB	3.5E-01	3.2E-01	3.0E-01	2.8E-01	1.2E-01	1.0E-01	9.2E-02	8.7E-02	8.2E-02	7.7E-02	7.4E-02	1.5E-01
Freshwater ecotoxicity	kg 1,4-DCB	3.8E-04	3.6E-04	3.5E-04	3.3E-04	1.1E-04	1.0E-04	9.4E-05	9.0E-05	8.7E-05	8.3E-05	8.1E-05	1.4E-04
Marine ecotoxicity	kg 1,4-DCB	3.9E-04	3.6E-04	3.3E-04	3.1E-04	1.3E-04	1.1E-04	1.0E-04	9.5E-05	8.9E-05	8.4E-05	8.0E-05	1.6E-04
Human carcinogenic toxicity	kg 1,4-DCB	5.1E-04	4.8E-04	4.5E-04	4.4E-04	1.6E-04	1.4E-04	1.3E-04	1.3E-04	1.2E-04	1.2E-04	1.1E-04	2.0E-04
Human non-carcinogenic toxicity	kg 1,4-DCB	2.6E-02	2.3E-02	2.1E-02	1.9E-02	8.5E-03	7.0E-03	6.3E-03	5.8E-03	5.3E-03	4.8E-03	4.5E-03	1.1E-02
Land use	m2a crop eq	9.6E-02	8.3E-02	7.0E-02	6.1E-02	3.5E-02	2.7E-02	2.2E-02	2.0E-02	1.7E-02	1.5E-02	1.3E-02	4.5E-02
Mineral resource scarcity	kg Cu eq	4.1E-04	3.8E-04	3.4E-04	3.2E-04	1.4E-04	1.2E-04	1.0E-04	9.8E-05	9.0E-05	8.4E-05	7.9E-05	1.8E-04
Fossil resource scarcity	kg oil eq	2.1E-02	2.0E-02	2.0E-02	1.9E-02	6.9E-03	6.4E-03	6.1E-03	6.0E-03	5.8E-03	5.7E-03	5.6E-03	8.7E-03
Water consumption	m3	9.4E-03	8.1E-03	7.0E-03	6.1E-03	3.4E-03	2.6E-03	2.2E-03	2.0E-03	1.8E-03	1.5E-03	1.4E-03	4.3E-03
GTP100	kg CO2 eq	9.5E-02	8.7E-02	8.0E-02	7.4E-02	3.4E-02	2.9E-02	2.6E-02	2.5E-02	2.3E-02	2.2E-02	2.0E-02	4.3E-02
MCTPs	ppt	1.1E-03	1.0E-03	9.7E-04	9.1E-04	3.9E-04	3.4E-04	3.2E-04	3.0E-04	2.8E-04	2.7E-04	2.6E-04	7.2E-05

		S27	S28	S29	S30	S31	S32	S33	S34	S35	S36	S37	S38
Climate change	kg CO2 eq	2.1E-02	2.1E-02	2.1E-02	2.1E-02	2.1E-02	2.1E-02	3.2E-02	3.2E-02	3.2E-02	3.2E-02	3.2E-02	3.2E-02
Stratospheric ozone depletion	kg CFC11 eq	2.3E-07	2.0E-07	1.8E-07	1.6E-07	1.4E-07	1.2E-07	5.7E-07	4.4E-07	3.8E-07	3.3E-07	2.9E-07	2.5E-07
Ionizing radiation	kBq Co-60 eq	7.0E-05	6.6E-05	6.2E-05	5.9E-05	5.7E-05	5.5E-05	1.7E-04	1.5E-04	1.4E-04	1.3E-04	1.3E-04	1.2E-04
Ozone formation, Human health	kg NOx eq	6.8E-05	6.2E-05	5.7E-05	5.3E-05	4.9E-05	4.6E-05	1.5E-04	1.2E-04	1.1E-04	1.0E-04	9.3E-05	8.5E-05
Fine particulate matter formation	kg PM2.5 eq	2.9E-05	2.7E-05	2.6E-05	2.4E-05	2.3E-05	2.2E-05	6.3E-05	5.4E-05	4.9E-05	4.6E-05	4.3E-05	4.0E-05
Ozone formation, Terrestrial ecosystems	kg NOx eq	7.1E-05	6.5E-05	6.0E-05	5.6E-05	5.2E-05	4.9E-05	1.5E-04	1.3E-04	1.2E-04	1.1E-04	9.8E-05	9.0E-05
Terrestrial acidification	kg SO2 eq	8.8E-05	7.9E-05	7.4E-05	6.8E-05	6.2E-05	5.8E-05	2.0E-04	1.6E-04	1.5E-04	1.3E-04	1.2E-04	1.1E-04
Freshwater eutrophication	kg P eq	9.5E-07	6.1E-07	3.6E-07	1.2E-07	-1.0E-07	-2.7E-07	4.1E-06	2.7E-06	2.0E-06	1.5E-06	1.0E-06	5.7E-07
Marine eutrophication	kg N eq	5.1E-05	4.4E-05	3.9E-05	3.4E-05	3.0E-05	2.6E-05	1.3E-04	9.9E-05	8.5E-05	7.5E-05	6.5E-05	5.6E-05
Terrestrial ecotoxicity	kg 1,4-DCB	1.3E-01	1.2E-01	1.1E-01	1.0E-01	9.8E-02	9.3E-02	2.7E-01	2.3E-01	2.1E-01	2.0E-01	1.8E-01	1.7E-01
Freshwater ecotoxicity	kg 1,4-DCB	1.3E-04	1.2E-04	1.2E-04	1.1E-04	1.1E-04	1.0E-04	2.6E-04	2.3E-04	2.2E-04	2.1E-04	2.0E-04	1.9E-04
Marine ecotoxicity	kg 1,4-DCB	1.4E-04	1.3E-04	1.2E-04	1.1E-04	1.1E-04	1.0E-04	3.0E-04	2.5E-04	2.3E-04	2.2E-04	2.0E-04	1.9E-04
Human carcinogenic toxicity	kg 1,4-DCB	1.8E-04	1.7E-04	1.6E-04	1.5E-04	1.5E-04	1.4E-04	3.7E-04	3.2E-04	3.0E-04	2.8E-04	2.7E-04	2.6E-04
Human non-carcinogenic toxicity	kg 1,4-DCB	9.0E-03	8.1E-03	7.4E-03	6.7E-03	6.2E-03	5.7E-03	2.1E-02	1.7E-02	1.5E-02	1.4E-02	1.3E-02	1.1E-02
Land use	m2a crop eq	3.4E-02	2.9E-02	2.6E-02	2.2E-02	1.9E-02	1.6E-02	8.9E-02	6.8E-02	5.8E-02	5.1E-02	4.4E-02	3.7E-02
Mineral resource scarcity	kg Cu eq	1.5E-04	1.3E-04	1.2E-04	1.2E-04	1.1E-04	1.0E-04	3.3E-04	2.7E-04	2.5E-04	2.3E-04	2.1E-04	1.9E-04
Fossil resource scarcity	kg oil eq	8.1E-03	7.8E-03	7.6E-03	7.3E-03	7.1E-03	7.0E-03	1.5E-02	1.3E-02	1.3E-02	1.2E-02	1.2E-02	1.2E-02
Water consumption	m3	3.4E-03	2.9E-03	2.6E-03	2.3E-03	2.0E-03	1.7E-03	8.5E-03	6.6E-03	5.6E-03	5.0E-03	4.3E-03	3.7E-03
GTP100	kg CO2 eq	3.7E-02	3.4E-02	3.1E-02	2.9E-02	2.7E-02	2.6E-02	7.7E-02	6.5E-02	5.9E-02	5.4E-02	5.0E-02	4.6E-02
MCTPs	ppt	5.9E-05	4.1E-04	3.8E-04	3.6E-04	3.4E-04	3.3E-04	8.8E-04	7.5E-04	6.9E-04	6.5E-04	6.0E-04	5.6E-04

		S39	S40	S41	S42	S43	S44	S45	S46	S47	S48	S49	S50
Climate change	kg CO2 eq	3.2E-02	4.3E-02	4.3E-02	4.3E-02	4.3E-02	4.3E-02	4.4E-02	4.4E-02	6.5E-02	6.5E-02	6.5E-02	6.6E-02
Stratospheric ozone depletion	kg CFC11 eq	2.2E-07	8.3E-07	6.4E-07	5.5E-07	4.8E-07	4.2E-07	3.6E-07	3.1E-07	1.4E-06	1.0E-06	8.9E-07	7.8E-07
Ionizing radiation	kBq Co-60 eq	1.2E-04	2.5E-04	2.3E-04	2.1E-04	2.0E-04	1.9E-04	1.9E-04	1.8E-04	4.3E-04	3.8E-04	3.6E-04	3.4E-04
Ozone formation, Human health	kg NOx eq	7.9E-05	2.1E-04	1.8E-04	1.6E-04	1.5E-04	1.3E-04	1.2E-04	1.1E-04	3.5E-04	2.9E-04	2.6E-04	2.3E-04
Fine particulate matter formation	kg PM2.5 eq	3.8E-05	9.2E-05	7.8E-05	7.2E-05	6.7E-05	6.2E-05	5.8E-05	5.5E-05	1.5E-04	1.3E-04	1.2E-04	1.1E-04
Ozone formation, Terrestrial ecosystems	kg NOx eq	8.4E-05	2.2E-04	1.8E-04	1.7E-04	1.5E-04	1.4E-04	1.3E-04	1.2E-04	3.6E-04	3.0E-04	2.7E-04	2.5E-04
Terrestrial acidification	kg SO2 eq	1.0E-04	2.9E-04	2.4E-04	2.1E-04	2.0E-04	1.8E-04	1.6E-04	1.5E-04	4.7E-04	3.9E-04	3.5E-04	3.2E-04
Freshwater eutrophication	kg P eq	2.3E-07	6.6E-06	4.4E-06	3.4E-06	2.6E-06	1.9E-06	1.2E-06	7.4E-07	1.1E-05	7.9E-06	6.2E-06	4.9E-06
Marine eutrophication	kg N eq	5.0E-05	1.9E-04	1.5E-04	1.3E-04	1.1E-04	9.6E-05	8.3E-05	7.3E-05	3.1E-04	2.4E-04	2.1E-04	1.8E-04
Terrestrial ecotoxicity	kg 1,4-DCB	1.6E-01	3.9E-01	3.3E-01	3.0E-01	2.8E-01	2.6E-01	2.4E-01	2.3E-01	6.3E-01	5.3E-01	4.8E-01	4.5E-01
Freshwater ecotoxicity	kg 1,4-DCB	1.9E-04	3.8E-04	3.4E-04	3.2E-04	3.0E-04	2.9E-04	2.8E-04	2.7E-04	6.2E-04	5.5E-04	5.2E-04	4.9E-04
Marine ecotoxicity	kg 1,4-DCB	1.8E-04	4.3E-04	3.7E-04	3.3E-04	3.1E-04	2.9E-04	2.6E-04	2.5E-04	7.0E-04	5.9E-04	5.4E-04	5.0E-04
Human carcinogenic toxicity	kg 1,4-DCB	2.4E-04	5.3E-04	4.6E-04	4.3E-04	4.1E-04	3.9E-04	3.6E-04	3.5E-04	8.6E-04	7.5E-04	6.9E-04	6.6E-04
Human non-carcinogenic toxicity	kg 1,4-DCB	1.1E-02	3.1E-02	2.5E-02	2.2E-02	2.0E-02	1.8E-02	1.7E-02	1.5E-02	5.1E-02	4.1E-02	3.7E-02	3.3E-02
Land use	m2a crop eq	3.2E-02	1.3E-01	1.0E-01	8.6E-02	7.5E-02	6.5E-02	5.5E-02	4.8E-02	2.2E-01	1.7E-01	1.4E-01	1.3E-01
Mineral resource scarcity	kg Cu eq	1.8E-04	4.8E-04	4.0E-04	3.6E-04	3.3E-04	3.0E-04	2.7E-04	2.5E-04	7.9E-04	6.5E-04	5.8E-04	5.3E-04
Fossil resource scarcity	kg oil eq	1.1E-02	2.1E-02	1.9E-02	1.8E-02	1.7E-02	1.7E-02	1.6E-02	1.6E-02	3.3E-02	3.0E-02	2.8E-02	2.7E-02
Water consumption	m3	3.3E-03	1.3E-02	9.7E-03	8.4E-03	7.4E-03	6.4E-03	5.5E-03	4.9E-03	2.1E-02	1.6E-02	1.4E-02	1.2E-02
GTP100	kg CO2 eq	4.3E-02	1.1E-01	9.2E-02	8.3E-02	7.7E-02	7.0E-02	6.4E-02	6.0E-02	1.8E-01	1.5E-01	1.3E-01	1.2E-01
MCTPs	ppt	5.3E-04	1.3E-03	1.1E-03	9.7E-04	9.1E-04	8.4E-04	7.8E-04	7.4E-04	2.0E-03	1.7E-03	1.5E-03	1.4E-03

		S51	S52	S53
Climate change	kg CO2 eq	6.6E-02	6.6E-02	6.6E-02
Stratospheric ozone depletion	kg CFC11 eq	6.7E-07	5.7E-07	5.0E-07
Ionizing radiation	kBq Co-60 eq	3.3E-04	3.2E-04	3.1E-04
Ozone formation, Human health	kg NOx eq	2.1E-04	1.9E-04	1.8E-04
Fine particulate matter formation	kg PM2.5 eq	1.0E-04	9.4E-05	8.9E-05
Ozone formation, Terrestrial ecosystems	kg NOx eq	2.2E-04	2.0E-04	1.9E-04
Terrestrial acidification	kg SO2 eq	2.9E-04	2.6E-04	2.4E-04
Freshwater eutrophication	kg P eq	3.7E-06	2.6E-06	1.7E-06
Marine eutrophication	kg N eq	1.6E-04	1.4E-04	1.2E-04
Terrestrial ecotoxicity	kg 1,4-DCB	4.2E-01	3.8E-01	3.6E-01
Freshwater ecotoxicity	kg 1,4-DCB	4.7E-04	4.5E-04	4.3E-04
Marine ecotoxicity	kg 1,4-DCB	4.6E-04	4.2E-04	4.0E-04
Human carcinogenic toxicity	kg 1,4-DCB	6.2E-04	5.8E-04	5.6E-04
Human non-carcinogenic toxicity	kg 1,4-DCB	3.0E-02	2.7E-02	2.5E-02
Land use	m2a crop eq	1.1E-01	9.2E-02	7.9E-02
Mineral resource scarcity	kg Cu eq	4.8E-04	4.4E-04	4.1E-04
Fossil resource scarcity	kg oil eq	2.6E-02	2.5E-02	2.4E-02
Water consumption	m3	1.1E-02	9.1E-03	8.0E-03
GTP100	kg CO2 eq	1.1E-01	1.0E-01	9.4E-02
MCTPs	ppt	1.3E-03	1.2E-03	1.2E-03


Figure S2. Comparison of impact scores when testing the influence of geographic location at pilot and large scale (S1, S2, S3 and S4). The impact scores are normalized to the highest score in each impact category.



Figure S3. Comparison of impact scores when testing the influence of avoided treatment of molasses waste at large scale in Italy and Germany (S2, S4, S5 and S6). Impact scores

are normalized to the highest score in each impact category. Bars for freshwater eutrophication for S5 and S6 are cut off to fit the figure (their values are -358 and -359%, respectively)

## **S5. References**

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