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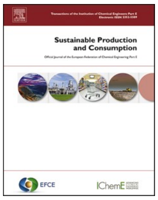

# The impacts of the European chemical industry on the planetary boundaries

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ABSTRACT

The European chemical industry plays a crucial role in the economy, manufacturing thousands of products that find applications across many sectors. On the other hand, the sector is also one of the largest energy consumers, and emits significant amounts of greenhouse gases, together with toxic, bioaccumulative and persistent chemicals. Acknowledging the need for a shift towards a greener industry model, this contribution assesses the absolute sustainability level of the chemical sector by contrasting the impacts it causes with the ecological capacity of the planet, as given by the planetary boundaries framework. Results indicate that impacts incurred by the European chemical industry transgress $CO_2$-based thresholds significantly, with burdens on atmospheric $CO_2$ concentration, energy imbalance, and ocean acidification being 15, 16 and 6 times larger than planetary limits. The biosphere integrity boundary, assessed here based on functional diversity, is also transgressed by 3 %. The five chemicals with the highest production volume, namely ammonia, polypropylene, high-density polyethylene, styrene, and benzene, are responsible for around 50 % of impacts in all the planetary boundaries. This suggests that they should be the target of dedicated research and policies. Finally, the study assesses a set of improvement pathways for the European chemical industry to become sustainable. It is found that the deployment of carbon capture and storage technologies to compensate for the greenhouse gases emitted by the sector would allow the chemical industry to meet all the planetary boundaries concurrently, yet burden-shifting would still cause other planetary boundaries to be deteriorated. This evidences the need to employ holistic approaches to assess the wide implications of any solution adopted within or outside the chemical industry.

## 1. Introduction

Human development is putting unprecedented pressure on the Earth's ability to maintain equilibrium due to a series of factors such as the rapid population increase, climate modification resulting from the emission of greenhouse gases (GHG), and loss of biodiversity caused by ecosystem destruction and alteration. It has been proved that anthropogenic activities have triggered many environmental imbalances which threaten, not only nature, but also the human ecosystem in diverse ways. As a result, once habitable regions are becoming unhabitable due to extreme climate, flooding, or the spreading of diseases (Hellweg et al., 2023; IPCC, 2022; UN Environment, 2019).

A switch to a sustainable development model has become urgent from both a technological and a political point of view (Garrido-Baserba et al., 2022; Keith et al., 2023; Peng et al., 2023). In this study, the focus is set on the European chemical sector: a driving factor of the world's economy bringing significant benefits to our welfare, yet at the expense of high environmental costs. At a global level, the chemical industry has annual revenues worth four trillion euro and has been in continuous growth (CEFIC, 2023). Europe is the second largest chemical manufacturer with sales over 500 billion € per year, and the region exporting the most chemicals in the world (CEFIC, 2023). During the COVID-19 pandemic, the European chemical sector suffered drops of over 5 % of demand, with slight but irregular recovery during 2020 (De Vet et al., 2021). The disrupted sourcing or transport logistics and supply chains, increasingly competitive landscape, and escalating energy prices following the Ukraine crisis, also challenge the development of the European chemical sector and affect trading (Beacham, 2022).

Despite persistent efforts in improving the sustainability level of production processes, the chemical industry is still one of the largest energy consumers and GHG emissions producers. In addition, it is also responsible for impacts related to toxic, bioaccumulative and persistent products, and is linked to major industrial accidents. Overall, the sector's activity is known to heavily alter the natural functioning of Earth systems. Still, there is a significant lack of information on the amount of chemicals released into the environment and their associated impacts. This is especially critical in the case of new entities (OECD, 2001), which

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## Nomenclature

*Acronyms and abbreviations*

| | |
|---|---|
| AAL | Atmospheric aerosol loading |
| aCO2 | Atmospheric $CO_2$ concentration |
| BAU | Business-as-usual |
| BECCS | Bioenergy with carbon capture and storage |
| BII | Biodiversity Intactness Index |
| CBI | Change in biosphere integrity |
| CCS | Carbon capture and storage |
| CDR | Carbon dioxide removal |
| CF | Characterization factor |
| DACCS | Direct air carbon capture and storage |
| DEA | Diethanolamine |
| DQA | Data quality analysis |
| EI | Energy imbalance at top of atmosphere |
| EU | European Union |
| FU | Functional unit |
| FWU | Freshwater use |
| GHG | Greenhouse gases |
| GVA | Gross value added |
| HDPE | High-density polyethylene |
| ISO | International Organization for Standardization |
| LCA | Life cycle assessment |
| LCI | Life cycle inventory |
| LCIA | Life cycle impact assessment |
| LDPE | Low-density polyethylene |
| LLDPE | Linear low-density polyethylene |
| LSC | Land-system change |
| N | Biogeochemical nitrogen flows |
| NACE | Statistical Classification of Economic Activities in the European Community |
| NBL | Natural background level |
| NMVOC | Non-methane volatile organic compounds |
| OA | Ocean acidification |
| ODS | Ozone depleting substance |
| P | Biogeochemical phosphorous flows |
| PB | Planetary boundary |
| PB-LCIA | Planetary boundaries-life cycle impact assessment |
| PE | Polyethylene |
| PP | Polypropylene |
| PV | Production volume |
| RER | European region (ecoinvent) |
| RM | Renewable mix |
| SOD | Stratospheric ozone depletion |
| SOS | Safe operating space |
| SoSOS | Share of safe operating space |
| WIOD | World Input-Output Database |

*Variables and parameters*

| | |
|---|---|
| $CF_{e,b}$ | Characterization factor quantifying the impact caused on control variable *b* by a unit of environmental burden *e* (i.e., substance or resource) |
| $GVA_{ChemInd}$ | Gross value added of the EU-28 chemical industry |
| $GVA_{EU\text{-}28}$ | Gross value added of the EU-28 |
| $IMP_{i,b}$ | Impact incurred by chemical *i* in control variable *b* |
| $LCI_{i,e}$ | Life cycle inventory including the amount of environmental burden *e* (i.e., substance or resource) exchanged with the environment during the life cycle of chemical *i* |
| $Pop$ | Population |
| $Pop_{EU\text{-}28}$ | EU-28 population |
| $Pop_{World}$ | World population |
| $PSh_{i,j}$ | Production share of chemical *i* that is carried out with process *j* |
| $PV_i^{cor}$ | Production volume of chemical *i* corrected by discounting the amount used as feedstock for the production of other chemicals |
| $PV_i^{raw}$ | Gross production volume of chemical *i* |
| $RMT_{i,i',j}$ | Amount of raw material *i* that is required to produce one unit of chemical *i′* with production process *j* |
| $SOS_b$ | Safe operating space for control variable *b* |
| $SoSOS_{b,EG}^{EU-28}$ | Share of safe operating space for control variable *b* corresponding to EU-28 based on an egalitarian perspective |
| $SoSOS_{b,EG+EG}^{ChemInd}$ | Share of safe operating space for control variable *b* corresponding to the European chemical industry based on a fully egalitarian perspective |
| $SoSOS_{b,EG+UT}^{ChemInd}$ | Share of safe operating space for control variable *b* corresponding to the European chemical industry based on a combined egalitarian-utilitarian perspective |
| $SoSOS_{b,GF}^{ChemInd}$ | Share of safe operating space for control variable *b* corresponding to the European chemical industry based on a grandfathering perspective |
| $SoSOS_{b,UT+UT}^{ChemInd}$ | Share of safe operating space for control variable *b* corresponding to the European chemical industry based on a fully utilitarian perspective |
| $\omega_{i,e}$ | Life cycle inventory entry providing the amount of environmental burden *e* (i.e., substance or resource) exchanged with the environment in the life cycle to produce one unit of chemical *i* |

are released too rapidly for society to adequately surveil their potential risks (Persson et al., 2022).

Traditionally, Europe has been one of the regions leading the change towards a more sustainable future, yet actions taken so far remain insufficient. The main challenges the sector currently faces with respect to environmental performance are the need to reduce emissions, hazardous waste, and energy consumption (Environment Agency, 2016). Sticking to business-as-usual (BAU) will prevent the European Union (EU) from complying with the goals of the 2050 EU Green Deal, which calls for a strategic review and a paradigm change in the current production processes. Moreover, increasing environmental consciousness and the appearance of many restricting polices will force the sector to transition to a sustainable business model in the upcoming years. This should include new transformation processes with the ability to close material loops in industrial chains and transition towards a circular economy paradigm (Mancini and Raggi, 2021; Ncube et al., 2023; Rivera et al., 2020). In this context, it is key to identify the main drivers of environmental impacts and the processes that are responsible for them. Then, this information could be used to direct research efforts and investments towards new or improved technologies with the capacity to truly improve the sustainability of our industries.

One important aspect is that the production of raw materials and utilities, notably energy, constitutes a significant share of the impacts that can be attributed to the chemical industry (Chung et al., 2023; Meng et al., 2023). Hence, as many environmental repercussions linked to the sector originate from processes beyond the boundaries of the industry itself, the inclusion of upstream activities is of upmost importance for any fair environmental assessment of the sector. In this context, life cycle assessment (LCA) becomes a valuable tool to perform such assessments (Ganesh et al., 2021; Somoza-Tornos et al., 2020).

LCA allows evaluating the environmental pressures associated with a good or service throughout its life cycle, helping identify strategies balancing environmental and economic efficiency through comparative assessments (CEFIC, 2020). Despite this, traditional LCA stills presents the drawback that it cannot inform about the absolute sustainability level of any activity assessed, since no benchmarks based on the ecological capacity of the planet are provided for impact scores.

In this contribution, we overcome this limitation by capitalising on the planetary boundaries (PB) framework, first proposed by Rockström et al. (2009). The PBs framework identifies nine bio-geophysical processes for the Earth system that are key for the resilience of our planet. For these boundaries, quantitative limits on associated control variables have been established, defining a safe operating space (SOS) for human activities (Richardson et al., 2023). The transgression of these boundaries could cause irreversible damage to our planet, undermining the resilience of the ecosystems that support human well-being at different scales (Lenton et al., 2019; Thomas, 2016). Since its development, the PB framework has been continuously reviewed, with the updated version by Steffen et al. (2015) taken as a reference in the present study.

We also benefit from the planetary boundaries-Life Cycle Impact Assessment (PB-LCIA) damage assessment model introduced by Ryberg et al. (2018a, 2018b), which allows for the expression of LCA data in terms of the control variables of the planetary boundaries, taken as impact categories here. The PB-LCIA bridges traditional LCA with the PB framework, enabling absolute environmental sustainability assessments (AESA) for products and processes (i.e., the chemical industry here). Understanding the stressors posed to the Earth's self-regulating mechanisms, and assessing anthropogenic activities using the PB-LCIA methodology, can provide useful guidelines and targets for all industrial sectors and nations to revert this planetary emergency.

Hence, this study develops a production-oriented quantitative assessment of the impacts caused by the European chemical industry on the planetary boundaries, acknowledging that important contributions could also be made in other regions and sectors. To avoid the use of data altered by the social and economic challenges encountered during the recent years, which are not representative of BAU consumption, manufacturing, or trading patterns, the study uses the best available pre-pandemic data (2018), and, consistently, considers Europe as EU-28. Our model of the European chemical industry is based on the top 19 largest-volume chemicals according to the International Energy Agency, which are responsible for 80 % of energy consumption and 75 % of GHG emissions within the industry (IEA, 2013). Our purpose is to identify, quantify and interpret the environmental impacts associated to the activity of the chemical industry in the context of the planetary boundaries using LCA. Therefore, the aims of this research are two-fold: (1) to evaluate whether the current activity of the chemical industry remains within PBs, identifying the most endangered Earth cycles along the way, and (2) to spot the processes with higher environmental impact in order to suggest priorities for action, specific measures, and recommendations to increase the sustainability level of the sector.

## 2. Literature review

The sustainability level of the chemical industry has long been the subject of a myriad of research works due to the potential of its activity to deteriorate human health and the environment (Ganesh et al., 2021; Gavrilescu and Chisti, 2005; Hursthouse, 1996; Ioannou et al., 2021). While the need to transition towards more sustainable production patterns is approached from a wide range of perspectives, going from risk analysis (Dakkoune et al., 2018) to social and economic studies (He et al., 2018; Hoffman, 1999), the analysis of environmental impacts is most commonly tackled through multi-factor indicators, predominantly based on LCA (Jessop, 2020). In fact, LCA results have been established as a fundamental input for decision-making across industry, academia, and the regulatory scene (Finnveden et al., 2009; Kralisch et al., 2015; Tillman, 2000).

In the fields of green chemistry and industrial ecology, the focus of LCA studies is predominantly set on individual processes, products, or services (Burgess and Brennan, 2001; Santos et al., 2019). Most contributions provide comparative assessments of two or more alternative production pathways (Chen et al., 2019; Delgove et al., 2019; Jens et al., 2019; Zhao et al., 2017), feedstock choices (Kua and Lu, 2016; Rathnayake et al., 2018), catalysts (Benavides et al., 2017), management options (Ahamed et al., 2016), or products (La Rosa et al., 2014). Thus, LCA is well established as a tool for process design, including optimization, selection, and synthesis (Cadena et al., 2019; Jacquemin et al., 2012; Kleinekorte et al., 2020). The scanning of processes for hot-spot identification is another relevant application of LCA in industrial chemistry (Gear et al., 2018; Ott et al., 2014; Phuang et al., 2021; Silva et al., 2015). Overall, the use of LCA, whether as a standalone tool or as a component of wider assessments, offers valuable, quantitative information to support and facilitate the implementation of sustainable practices. Nevertheless, for the chemical industry, the scope of current research is broadly limited to specific activities or actions, lacking a sectorial perspective. Besides, analyses are mostly centred around petrochemicals (Santos et al., 2019), which represent only a fraction of the whole sector.

The PB-LCIA framework complements traditional LCA by comparing the impacts of the activities studied with the Earth's ecological capacity, recognizing the inherent boundaries of the Earth's natural systems and providing more informative results (Rockström et al., 2009; Steffen et al., 2015). The PB-LCIA framework is more often used to assess wider systems than traditional LCA, and many industries have already been scrutinised through this methodology. O'Neill et al. (2018) studied whether society's basic needs can be met while not transgressing the PBs. Sandin et al. (2015) assessed the Swedish clothing sector, while Ali and Ryberg (2023) analysed the energy and transport sectors in Tonga and Oceania. Tunji-Olayeni et al. (2019) studied the construction industry, concluding that it does not remain within all PBs. Ryberg et al. (2018b) also focused on the European region by applying the PB-LCIA damage assessment model to the laundry washing industry, and Europe's complete consumption system was assessed by Sala et al. (2020). When it comes to chemical processes, recent papers assess eco-park design alternatives within the ammonia industry (Samaroo et al., 2020), large-scale hydrogen (Weidner et al., 2023) and methanol (Jaggai et al., 2020) production, or the obtention and use of sustainability-oriented fuels (Charalambous et al., 2023; Ehrenstein et al., 2020; Mahabir et al., 2021) through the concept of the PBs.

A comprehensive study by Galán-Martín et al. (2021) modelled the petrochemical industry based on six platform chemicals to investigate the consequences of replacing traditional fossil carbon with renewable carbon. They found that there is no single solution that can place the sector within the PBs. Additionally, Tulus et al., 2021 quantified the stress posed to the PBs by an extensive selection of chemical products. Their findings provided individualized results for each chemical assessed, and revealed that, for >99 % of them, at least one PB was breached. While their study covers a remarkable amount of chemicals, results were calculated and allocated for each chemical separately.

Targeted assessments of specific aspects are of unquestionable value and offer the chance for in-depth examination, yet a complete evaluation of the collective, absolute, environmental impacts of the whole chemical sector is also needed in the path towards greener chemistry. The chemical industry comprises a multitude of chemicals and an even larger number of production routes, which are interrelated in such a way that can alter the results of individual impact assessments due to double-counting errors, among other reasons. Hence, to address this research gap and broaden the scope of previous research, this study takes three main steps.

Firstly, this contribution is not confined to the assessment of the sustainability level of individual chemical compounds or specific production processes. Instead, calculations rely on a sectorial model based on the interactions between examined processes so that impacts of the principal chemical production routes are assessed simultaneously. The objective is to provide a holistic analysis capable of offering a more comprehensive, sector-wide perspective of the environmental shortcomings of the chemical industry across Europe. The scope adopted encompasses a selection of 19 chemicals deemed representative of the entire chemical sector by the International Energy Agency (IEA, 2013).

Secondly, most research related to the environmental performance of chemical processes involves stand-alone or comparative LCAs of the target activities. By assessing environmental performance in terms of the planetary boundaries, impacts are benchmarked against the ecological capacity of the planet, allowing to provide a valuable, but still under-researched perspective of the absolute sustainability of the processes under study.

Finally, the regional context of the study achieved by focusing on the European region alone allows enriching the depth of the research, as it creates the possibility to quantify impacts on the atmospheric aerosol loading PB. This question lies out of reach of global studies due to the regional nature of aerosol pollution.

Additionally, results obtained with the model of the chemical industry are further analysed to identify the main impact drivers of current (i.e., BAU) practices. This information is then utilized to introduce a set of improvement pathways and study if they can potentially revert the current pressure exerted by the sector on all the PBs concurrently. To our knowledge, no previous study quantifies the absolute sustainability of the European chemical industry and models specific action plans considering a sector-wide perspective.

## 3. Methods

Fig. 1 illustrates the approach used to quantify the impacts of the European chemical industry on the PBs. The core step is an attributional, cradle-to-gate LCA of the chemical industry. Note that this is not a conventional LCA of a single individual product (e.g., benzene production), but rather the assessment of a complete sector (chemical industry) (Goedkoop et al., 2009). To tackle this challenge, we first model the chemical industry as a collection of the most representative chemicals and processes, selected based on their production volumes and environmental impacts. Then, individual cradle-to-gate LCAs for each of these products are consistently combined, while ensuring that impacts are not double-counted in the process. The LCA is performed following the four phases described in 14,044 ISO methodology.

In phase 1, the scope of the study is defined according to data availability in terms of chemicals, production processes, PBs relevant to the research, and system boundaries (i.e., cradle-to-gate).

Then, during phase 2, environmental flows exchanged, in the life cycle, between the chemical industry and the environment are quantified. We do this for selected chemicals based on data retrieved from *ecoinvent* v3.5 (Wernet et al., 2016). Acknowledging that results quality strongly depends on data completeness and reliability, we perform a data quality analysis (DQA) and model uncertainties on these environmental flows based on the so-called pedigree matrix.

In phase 3, environmental flows are translated into impacts on the control variables of the PBs. This is done by means of the PB-LCIA damage assessment model proposed by Ryberg et al. (2018a, 2018b). We note that, in the PBs framework, impacts are quantified in terms of constant fluxes rather than discrete exchanges. Hence, annual production volumes of each chemical for the studied year (2018) are used to obtain the total quantities of each pollutant or resource uptake that are attributed to the activity of the chemical industry.

Then, in phase 4, the results obtained are analysed and interpreted. This is where the PBs framework demonstrates its full usefulness, as it provides quantitative limits to discern whether the activity under analysis can be deemed sustainable or not. Note, however, that PBs are defined at the planet level, providing a SOS for the global economy (i.e., not just a single regional sector) to operate. To address this mismatch in scope, we also compare the impacts of the chemical industry to the assigned share of SOS (SoSOS), obtained by downscaling PBs to different levels. This comparison provides more context on the magnitude of the results obtained, unveiling their true significance.

Finally, three principal improvement pathways are proposed to

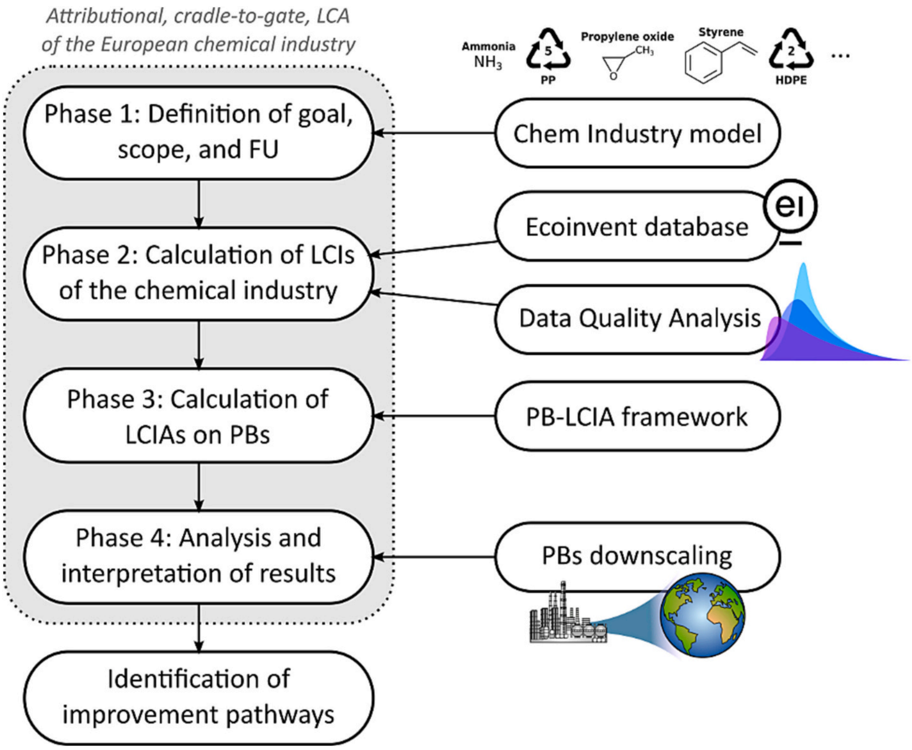


**Fig. 1.** Modelling framework. The PB-LCIA framework allows to quantify the impacts of the European chemical industry into the PBs. FU: functional unit; HDPE: high-density polyethylene; LCA: life cycle assessment; LCI: life cycle inventory; LCIA: life cycle impact assessment; PB: planetary boundary; PB-LCIA: planetary boundaries-life cycle impact assessment; PP: polypropylene.

mitigate the impacts caused by the European chemical industry: (i) powering industrial processes with a more sustainable electricity mix based on renewables; (ii) the deployment of carbon capture and storage technologies to compensate for impacts from the chemical industry; and (iii) the replacement of grey hydrogen with green hydrogen.

### *3.1. Characterization of the European chemical sector*

The European chemical industry is responsible for producing thousands of products, which can be classified between basic inorganics, consumer chemicals, polymers, and speciality chemicals (Thormann et al., 2023). However, huge disparities exist between the production volumes of different chemicals, with some bulk chemicals manufactured massively, while other substances are derivates from basic chemicals or show minor production volumes, mostly related with niche applications.

In this study, we follow the approach by the International Energy Agency and consider the top 19 largest-volume chemicals as representative for the whole European chemical industry (IEA, 2013). We select these chemicals because their manufacture is responsible for 80 % of the total energy consumption and 75 % of GHG emissions within industry. Hence, not only are these chemicals produced in large volumes, but their production processes also show high environmental impacts (IEA, 2013).

We source the production volumes for these chemicals from the *Prodcom* database in Eurostat, and complement them with import and export trade data for the studied region and time (European Union, 2020c). Since this study is production-centred, import data is neglected to avoid the inclusion of environmental damage that is not happening within the studied area (Lucas et al., 2020). Conversely, export data is included since the production of all exported volume does happen within the European territory and the chemical sector (or upstream activities).

In industry, each of these 19 chemicals can be manufactured by means of more than one process. In this study, we include 32 processes for which data were available in the *ecoinvent* 3.5 database, comprised within 23 datasets (see Table 1). The route for the recycling of high-density polyethylene (HDPE) considered in *ecoinvent* involves the sorting and cleaning of waste polyethylene (PE), as well as its subsequent homogenization, shredding and melting. The product of these processes is cooled into final recycled HDPE pellets (Wernet et al., 2016). Total production volumes are provided in *Prodcom* for ammonia, benzene, and HDPE. To split these values between *ecoinvent* activities, the shares of each process in the *ecoinvent* market dataset for each chemical (specified in Table 1) are employed.

Various relationships exist between the chemicals included in this study, with some substances being used as feedstock to produce other chemicals. These interrelations between processes are of critical importance for LCA as, when following a cradle-to-gate scope, impacts for the manufacture of a given chemical include also those caused during the obtention of the raw materials.

An illustrative example of this effect is depicted in Fig. 2, where the aim is to compute the impacts of a piece of the chemical sector comprising two chemicals: ethylene and polyethylene (PE). In this case (Fig. 2a), calculating the impacts of the sector based on the raw production volumes of the two chemicals *i* ($PV_i^{raw}$), independently, would result in an overestimation of the total impacts. This is because the environmental burdens stemming from the production of the ethylene that is used as feedstock for the manufacture of PE (i.e., 0.9 kg of

**Table 1**
Chemicals and production processes considered. RER: European region.

| Chemical | Production processes | Ecoinvent activity |
|---|---|---|
| Acrylonitrile | Sohio process from polypropylene | Acrylonitrile//[RER] Sohio process |
| Ammonia | Steam reforming (84.99 % of market for ammonia) | Ammonia, liquid//[RER] ammonia production, steam reforming, liquid |
| | Partial oxidation (15.00 % of market for ammonia) | Ammonia, liquid//[RER] ammonia production, partial oxidation, liquid |
| | Cocamide diethanolamine production (0.01 % of market for ammonia) | Ammonia, liquid//[RER] cocamide diethanolamine production |
| Benzene | Catalytic reforming (99.23 % of market for benzene) | Benzene//[RER] benzene production |
| | From coke oven (0.77 % of market for benzene) | Benzene//[DE] coking |
| Cumene | Alkylation of benzene and propylene | Cumene//[RER] cumene production |
| Ethylene | Steam cracking out of naphtha | Ethylene, average//[RER] ethylene production, average |
| Ethylene glycol | Hydrolysis of ethylene oxide | Ethylene glycol//[RER] ethylene glycol production |
| Ethylene oxide | Direct oxidation from ethylene | Ethylene oxide//[RER] ethylene oxide production |
| Methanol | Steam reforming | Methanol//[GLO] methanol production |
| Xylenes | Catalytic reforming | Xylene//[RER] xylene production |
| HDPE | Polymerization out of ethylene, gas phase<br>Polymerization out of ethylene, slurry<br>Polymerization out of ethylene, solution<br>(99.92 % of market for HDPE) | Polyethylene, high density, granulate//[RER] polyethylene production, high density, granulate |
| | Recycling of HDPE (0.08 % of market for HDPE) | Polyethylene, high density, granulate//[Europe without Switzerland] polyethylene, high density, granulate, recycled to generic market for high density PE granulate |
| LDPE | Polymerization out of ethylene, autoclave<br>Polymerization out of ethylene, tubular | Polyethylene, low density, granulate//[RER] polyethylene production, low density, granulate |
| LLDPE | Polymerization out of ethylene, autoclave<br>Polymerization out of ethylene, tubular<br>Polymerization out of ethylene, gas phase<br>Polymerization out of ethylene, Slurry<br>Polymerization out of ethylene, solution | Polyethylene, linear low density, granulate//[RER] polyethylene production, linear low density, granulate |
| Polypropylene | Polymerization out of propylene, bulk<br>Polymerization out of propylene, gas phase<br>Polymerization out of propylene, Slurry | Polypropylene, granulate//[RER] polypropylene production, granulate |
| Propylene | Steam cracking of naphtha | Propylene//[RER] propylene production |
| Propylene oxide | Chlorohydrin process | Propylene oxide, liquid//[RER] propylene oxide production, liquid |
| Styrene | Dehydrogenation of ethylbenzene | styrene//[RER] styrene production |
| Terephthalic acid | Oxidation of p-xylene | Purified terephthalic acid//[RER] purified terephthalic acid production |
| Toluene | Catalytic reforming | Toluene, liquid//[RER] toluene production, liquid |
| Vinyl chloride | Direct chlorination and oxychlorination of ethylene | Vinyl chloride//[RER] vinyl chloride production |

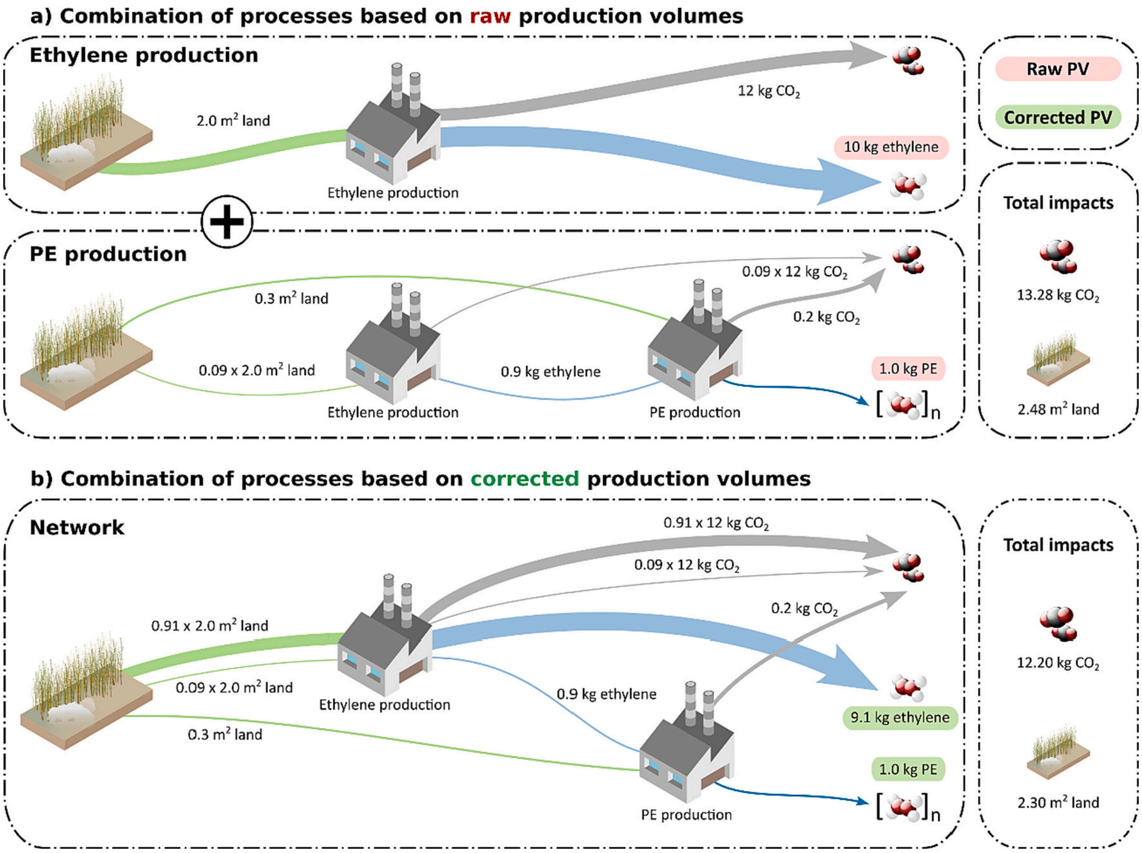


**Fig. 2.** Sankey diagram illustrating the potential double-counting of impacts when studying a system composed by intertwined production processes. Subplot (a) demonstrates an overestimation of impacts resulting from using raw production volumes. Subplot (b) corrects the total impact by disregarding the production of one chemical that is used as raw material to manufacture another chemical also considered within the scope of the study. PE: polyethylene; PV: production volume.

ethylene) would be counted twice.

To avoid this, the total production volume of each chemical $i$ is corrected ($PV_i^{cor}$) by subtracting the amount of it required as feedstock to any of the 23 activities considered within the scope of the study (see Eq. (1)).

$$PV_i^{cor} = PV_i^{raw} - \sum_{i' \neq i} \sum_j PV_{i'}^{raw} PSh_{i',j} RMT_{i,i',j} \quad \forall i \tag{1}$$

Here, $PSh_{i',j}$ provides the share of the production of chemical $i'$ that is carried out with process $j$ (as given by Table 1), while $RMT_{i,i',j}$ indicates the amount of raw material $i$ that is required to produce one unit of chemical $i'$ with production process $j$. Following with the previous example (Fig. 2b), and applying Eq. (1) for ethylene, we would find that $PV_{i=ethylene}^{raw}$ is 10 kg, and that $PV_{i'=PE}^{raw}$ is 1.0 kg. Meanwhile, $PSh_{i',j}$ is equal to 1 as there is only one technology using ethylene as raw material (i.e., $j = PE\ production$, $i' = PE$). Then, $RM_{ii',j}$ equals 0.9, since this is the amount of ethylene needed to produce 1 kg of PE with that technology. Overall, this would result in a $PV_{i=ethylene}^{cor} = 10 - 1.0 \cdot 1 \cdot 0.9 = 9.1$ kg of ethylene.

As the search for links between activities within the system boundaries could be a never-ending task, a threshold of one "step backwards" or "chain echelon" is considered when analysing the input flows for each activity. This approach, studying foreground processes but disregarding background processes, is often adopted in the literature (Bojarski, 2010). It is agreed to be conservative in the sense that overlooked connections, if any, will always lead to an overestimation of impacts owing to a certain degree of double counting. The relationships detected between the studied chemicals by systematic analysis of foreground processes are briefed in Table 2.

### 3.2. Impacts of the European chemical industry

We perform an LCA following four phases, as described in the guidelines of the 14,044 ISO methodology.

#### 3.2.1. Goal and scope definition

In the first phase, the goal and scope of the analysis are defined. Specifically, the goal of the present study is to analyse the environmental impacts caused by the European chemical industry on the PBs, and to propose improvement measures which would increase the sustainability level of the sector. Therefore, an attributional approach is adopted.

Regarding the scope, cradle-to-gate boundaries are considered. These include the acquisition of required feedstocks, their transport to plant, energy generation, and the production of final products (Wernet et al., 2016). This is the most common approach in LCA studies for chemical processes (Santos et al., 2019) as it allows strictly assessing the performance of the chemical industry. In addition, by disregarding the impacts associated with the distribution of the final products, for which the chemical industry could be attributed no responsibility, we avoid introducing significant uncertainties into our analysis (Galán-Martín et al., 2021; Tulus et al., 2021). The only exceptions are the chemicals that are (partially) used as feedstocks within industry itself, for which impacts from the distribution stage will also be quantified, together with other upstream activities of the production chain.

A multiproduct functional unit, based on the (corrected) production volumes for each product or activity for a particular year, is used [kg/yr]. As aforementioned, expressing the functional unit in an annual basis allows the application of the PB-LCIA damage assessment model, since it is based on annual flows rather than on discrete exchanges.

**Table 2**
Interlinks between the studied chemicals. DEA: diethanolamine; HDPE: high-density polyethylene; LDPE: low-density polyethylene; LLDPE: linear low-density polyethylene; PP: polypropylene.

| | Chemical | Main feedstocks | Linked to |
|---|---|---|---|
| 1 | Acrylonitrile, Sohio process | Propylene | 17,1,2 |
| 2 | Ammonia, partial oxidation | Coal heavy fuel oil | – |
| 3 | Ammonia steam reforming | Methane or higher hydrocarbons, catalyst (Ni) | – |
| 4 | Ammonia, from cocamide DEA production | DEA, methyl cocoate/coconut oil/ coconut acids/stripped coconut fatty acids, alkaline catalyst | 8 |
| 5 | Benzene | Chain hydrocarbons | – |
| 6 | Benzene, coking | Coal | – |
| 7 | Cumene | Benzene and propylene | 3,4,17 |
| 8 | Ethylene glycol | Ethylene oxide | 8 |
| 9 | Ethylene oxide | Ethylene | 9,17 |
| 10 | Ethylene, average | Chain hydrocarbons | |
| 11 | HDPE, granulate | Ethylene | 9,17 |
| 12 | HDPE, granulate, recycled to generic market for HDPE | Ethylene | 9,17 |
| 13 | LDPE, granulate | Ethylene | 9,17 |
| 14 | LLDPE, granulate | Ethylene | 9 |
| 15 | Methanol | Natural gas, coal, $CO_2$, other natural resources (e.g., wood, solid waste, etc.) | – |
| 16 | PP, granulate | Propylene | 17 |
| 17 | Propylene oxide | Propylene, chlorine | 17 |
| 18 | Propylene | Chain hydrocarbons | – |
| 19 | Purified terephthalic acid | Xylene, acetic acid | 23 |
| 20 | Styrene | Ethylbenzene | 9, 3, 4 |
| 21 | Toluene, liquid | Chain hydrocarbons | – |
| 22 | Vinyl chloride | Ethylene, chlorine | 9 |
| 23 | Xylene | Chain hydrocarbons | – |

### 3.2.2. *Life cycle inventories*

The second phase of the LCA consists of the quantification of the so-called life cycle inventories (LCI). LCIs, defined for every chemical *i* and environmental burden *e* ($LCI_{i,e}$), include the amount of every substance (e.g., $e =$ benzene, $CO_2$) and resource (e.g., $e =$ land, water) exchanged with the environment during the life cycle of chemical *i*. Typically, these can be obtained from LCA databases, which contain the so-called LCIs entries, providing the amount of substances and resources exchanged with the environment, in the life cycle, to produce one unit of chemical *i* (i.e., $\omega_{i,e}$). Hence, LCIs are built based on LCI entries from *ecoinvent* v3.5, as illustrated in Eq. (2). Exceptions are the exchanges with the technosphere for PE, PP, and vinyl chloride, which are obtained from the same datasets (i.e., same activities), but from v.3.7.1, since these LCIs are not provided by v3.5. Exchanges with the ecosphere for these chemicals are still modelled from v3.5. In all cases, the "Allocation at the point of substitution" system model is used, which allocates impacts derived from the treatment of waste generated in the target processes. Additional information regarding the modelling using *ecoinvent* activities can be found in Section 1.1 of the Supplementary material.

$$LCI_{i,e} = PV_i^{cor}\omega_{i,e}\ \forall i,e \tag{2}$$

LCI entries in databases might not always align with the region or the time period for which the analysis is performed. To address these potential disparities, we consider the uncertainty associated with LCI entries, assuming these follow log-normal distributions (i.e., $\omega_{i,e} \sim LogNormal(\mu_{i,e}, \sigma_{i,e})$) (Weidema and Wesnaes, 1996). Two parameters, $\mu_{i,e}$ and $\sigma_{i,e}$, are required to characterize (quantitatively) the probability distribution of every LCI entry. The former ($\mu_{i,b}$) can be directly obtained by log-transforming the nominal LCI entries provided by *ecoinvent* (i.e., the values that would be used if uncertainties were neglected). Conversely, the latter ($\sigma_{i,e}$) requires additional calculations, as explained next.

First of all, a DQA is carried out through the completion of the so-called pedigree matrix, a rubric developed by Weidema and Wesnaes (1996) to determine the adequacy of LCA datasets to the aims of the study. Specifically, we apply the revised version by Ciroth et al. (2016), which assigns scores ranging from 1 to 5 for five different categories called data quality indicators. These are: (i) reliability, (ii) completeness, and (iii) temporal, (iv) geographical and (v) technological coverage. In this exercise, low-ranking scores do not necessarily imply poor quality of the data, but simply lower relationship with the goals and scope of the particular LCA study. Therefore, the DQA must be consistent with the goals of the study, collected in the so-called data quality goals.

Then, scores assigned to the pedigree matrix are translated into a quantitative estimation of the standard deviation of the corresponding LCI entry ($\sigma_{i,e}$). Hence, a different standard deviation is obtained for each of the 163 LCI entries (i.e., fluxes) involved in the study for each of the 23 activities, which results in total of 3749 uncertainty values.

Finally, probability distributions for LCI entries are discretized into a set of 100 scenarios, generated through Monte Carlo sampling. This allows considering, not only a single (nominal) estimation of impacts, but rather a myriad of possibilities based on potential realization of the underlying uncertainties.

Further details on the overall procedure followed to estimate uncertainties of LCI data can be found in Section 1.2 in the Supplementary material.

### 3.2.3. *Planetary boundaries-life cycle impact assessment*

The PBs framework is based on the scientific evidence that the Earth is not a combination of isolated processes but rather a single, integrated system. Consistently, this study includes the quantification of the impacts on 10 control variables that have been defined for the PBs. These include energy imbalance at top of atmosphere, atmospheric $CO_2$ concentration, stratospheric ozone depletion, ocean acidification, the nitrogen and phosphorus cycles, land-system change, freshwater use, aerosol loading, and (functional) biosphere integrity.

In this phase, LCIs need to be expressed in terms of their impact towards the control variables of the PBs, helping portray the severity of the environmental damage in a clearer and more direct way. This can be done through the PB-LCIA methodology presented by Ryberg et al. (2018b), which considers the control variables of the PBs as impact categories. Hence, LCIs obtained in the previous section are multiplied by the corresponding characterization factors (CF) to calculate the impact incurred by chemical *i* in every control variable *b* ($IMP_{i,b}$), as illustrated in Eq. (3). Note that this equation needs to be applied to each of the 100 scenarios developed for each LCI, therefore providing a distribution of impacts for each chemical *i* and control variable *b*, instead of a single value.

$$IMP_{i,b} = \sum_e LCI_{i,e}CF_{e,b}\ \forall i,b \tag{3}$$

CFs developed by (Ryberg et al., 2018a, 2018b) are used for all control variables except for the biosphere integrity boundary, which is assessed through the methodology presented by Galán-Martín et al. (2021). Biosphere integrity, as defined in the PB framework, has two facets: functional and genetic diversity. Bearing this in mind, Galán-Martín et al. (2021) provided a way to assess functional diversity based on the estimation of the Biodiversity Intactness Index (BII), and then use it as a proxy for biosphere integrity. Indeed, this method provides a lower bound on the real impacts incurred on biosphere integrity for two main reasons. First, the impacts caused on genetic diversity, the other facet of biosphere integrity, are left out of the scope of the analysis. In addition, the method proposed computes the mean species abundance loss based on two stressors only (i.e., direct land use and $CO_2$-eq emissions), thus, disregarding the effect that other environmental pressures have in diminishing functional diversity. Note, however, that this approach has already been used in previous studies (Bachmann et al., 2023; Cabrera-Jiménez et al., 2023; Weidner et al., 2023).

In addition, we also note that no global limit has been quantified yet for the atmospheric aerosol loading boundary. However, data availability allows for the assessment of this boundary at a regional level. Consistent with the research scope, we use CFs specifically developed by Ryberg et al. (2018b) for the European region, since these allow for a more adequate assessment than if global averages were employed. These CFs reflect the fact that the circulation of aerosols between regions is highly limited, therefore giving more importance to regionally emitted aerosols, and assigning a lower weight to aerosols transported to other regions.

#### 3.2.4. *Results interpretation*

The final step is to interpret and analyse the impacts caused by the chemical industry on the different PBs. To this end, LCA results are compared against absolute limits derived from the PB framework, which define the level to which the principal Earth-system processes can be disturbed before triggering irreversible damage. These limits are linked to the global perception of what environmental damage is acceptable, and what risks and changes we are willing to take and make.

While some Earth-system processes have a clear threshold where a critical change would happen, others do not. However, the latter still show a point after which increased stress would cause growing, and at some point, irreversible damage and chained effects to other systems. Hence, an uncertainty zone is defined for the boundary on each control variable.

In addition, the planet itself has a natural contribution towards each control variable of the PBs. This so-called natural background level (NBL) has to be subtracted from the corresponding threshold before the SOS can be calculated. It is the SOS which provides the available "environmental budget" for each Earth system that can be "consumed" by anthropogenic activities. Table 3 shows the PBs that are selected for the present study, together with their control variables, units, NBL, their SOS, and, finally, their current status. In the case of aerosol loading, no global threshold has been defined, as the boundary is studied at a regional level. The threshold employed in this study was originally proposed by Steffen et al. (2015) for South Asia (as a case-study), yet has already been used for Europe in the past (Ryberg et al., 2018a, 2018b).

### 3.3. *Downscaling the planetary boundaries*

When comparing the impacts from the European chemical industry with the SOS defined at the planet level, two situations might arise. If impacts transgress the limits of the SOS, we can irrefutably conclude that the chemical industry is unsustainable. However, if all impacts lie within the PBs, it still not possible to assert that the chemical industry is sustainable, since the question of whether there is enough room left for economic activities in other regions and sectors would remain unanswered.

To address this mismatch and provide more context to the results, the SOS has to be downscaled from a global level to the studied sector using an allocation factor, obtaining this way the assigned "share of SOS" (SoSOS).

The criterion chosen for the allocation step can widely influence the results and the conclusions of the study, as different criteria will give rise to different values for the SoSOS (Sandin et al., 2015). In this contribution, and without loss of generality, we consider four different downscaling principles, three of which are addressed at two different scope levels.

The main downscaling method is based on a combined egalitarian-utilitarian perspective performed at two scope levels, since this is the prevalent approach for downscaling the SOS to the sector level in the PBs literature (Ryberg et al., 2020). According to this approach, an egalitarian perspective is used in the first level to allocate a share of the SOS to the EU-28 (i.e., $SoSOS_{b,EG}^{EU-28}$), proportional to the share of inhabitants residing within this area (see Eq. (4)) (Häyhä et al., 2016; Hjalsted et al., 2021). The egalitarian perspective is based on the idea that all people should have the same right to the ecological space, and is the most common practice to downscale the SOS to the country level in current studies using the PB-LCIA framework (Algunaibet et al., 2019; Dao et al., 2018; Fang et al., 2015; Fanning and O'Neill, 2016; O'Neill et al., 2018; Ryberg et al., 2018a, 2018b; van den Berg et al., 2020). Note that this step is not necessary for the aerosol loading control variable, which is already a regional boundary. Therefore, the SOS defined for this boundary can be taken as the SoSOS for the EU-28 without any further allocation.

$$SoSOS_{b,EG}^{EU-28} = SOS_b \frac{Pop_{EU-28}}{Pop_{World}} \ \forall b \neq Atmospheric\ aerosol\ loading \tag{4}$$

In this equation, $Pop_{EU-28}$ and $Pop_{world}$ refer to the population of the countries conforming EU-28 (thus, before United Kingdom's exit) and the world, respectively. Data regarding Europe are gathered from Eurostat and information about the world's population is obtained from the World Population Prospects (European Union, 2020b; United Nations, 2019).

The $SoSOS_{b,EG}^{EU-28}$ calculated with Eq. (4) provides an environmental budget for all economic activities within Europe and, therefore, is not specific for the chemical sector therein. Hence, when comparing impacts obtained with Eq. (3) with these boundaries, there will still be uncertainty concerning the environmental feasibility of the remaining economic activities within the EU-28. To address this mismatch, we further

**Table 3**

Briefing of the Earth-system processes linked to a planetary boundary (PB) considered in the present study. N: Biogeochemical nitrogen flows; NBL: Natural background level; P: Biogeochemical phosphorous flows; SOS: safe operating space.

| Earth-system process | Control variable | Boundary | Unit | NBL | SOS | Current |
|---|---|---|---|---|---|---|
| Climate change | Energy imbalance at top-of-atmosphere | 1.0–1.5 | $W \cdot m^{-2}$ | 0 | 1.0–1.5 | 2.3 |
| | Atmospheric $CO_2$ concentration | 350–500 | ppm | 278 | 72–172 | 412.5[a] |
| Stratospheric ozone depletion | Stratospheric $O_3$ concentration | 275–261 | DU | 290 | 15–29 | 283[b] |
| Ocean acidification | Carbonate ion concentration: average global surface ocean aragonite saturation state | 2.75–2.41 | $\Omega_{arag}$ | 3.44 | 0.69–1.03 | 2.89 |
| Biogeochemical flows | N Global: Industrial and intentional biological fixation of nitrogen | 62–82 | $Tg\ N \cdot yr^{-1}$ | 0 | 62–82 | 150 |
| | P Global: phosphorus flow from freshwater systems into the ocean | 11–100 | $Tg\ P \cdot yr^{-1}$ | 1.1 | 9.9–98.9 | 22 |
| Land-system change | Global: Area of forested land as fraction of potential forest | 75–54 | % | 100 | 25–46 | 62 |
| Freshwater use | Global: Maximum amount of consumptive blue water use | 4000-6000 | $km^3 \cdot yr^{-1}$ | 0 | 4000-6000 | 2600 |
| Atmospheric aerosol loading | Regional: AOD as seasonal average over a region | 0.25–0.5 | AOD | 0.14 | 0.11–0.36 | 0.3[c] |
| Biosphere integrity | Biodiversity Intactness Index | 10–70 | % | 0 | 10–70 | 26.8 |

[a] Updated from Matlin et al. (2022).

[b] Updated from Sala et al. (2020).

[c] Regional boundary.

allocate the $SoSOS^{EU-28}_{b,EG}$ among the different economic sectors of the EU-28 to estimate the part of it that could be assigned to the chemical industry alone (i.e., $SoSOS^{ChemInd}_{b,EG+UT}$). This is done following a utilitarian perspective, where the objective is to maximize the sum of welfare of individuals. For simplicity, we assume that the economic output of industries is a proxy for the human welfare added (Ryberg et al., 2020), and further downscale the $SoSOS^{EU-28}_{b,EG+UT}$ based on the fraction of gross value added (GVA) generated by the chemical industry, as shown in Eq. (5) (Brejnrod et al., 2017; Sandin et al., 2015; Wolff et al., 2017).

$$SoSOS^{ChemInd}_{b,EG+UT} = SoSOS^{EU-28}_{b,EG}\frac{GVA_{ChemInd}}{GVA_{EU-28}}\ \forall b \tag{5}$$

In this case, the total GVA ($GVA_{EU-28}$) is obtained from the Prodcom database (European Union, 2020a), while the fraction of it corresponding to the sector under study ($GVA_{ChemInd}$) is calculated through the World Input-Output Database (WIOD) (Timmer et al., 2015). The WIOD contains economic information of different sectors of an economy, classified according to NACE (Statistical Classification of Economic Activities in the European Community) codes. In this case, the chemical industry is represented within the tables through category R-11, which corresponds to NACE C20 (manufacture of chemicals and chemical products).

Although the combination of the egalitarian and utilitarian principles is widely used for downscaling the SOS to the sector level, we acknowledge that any allocation method would be controversial and far from perfect (Hjalsted et al., 2021). In this case, the $SoSOS^{ChemInd}_{b,EG+UT}$ is based on the economic value of the whole European chemical industry, not only on the 19 selected chemicals. This could be solved by further allocating the $SoSOS^{ChemInd}_{b,EG+UT}$ based on the share of the total annual value of the sector corresponding to the specific chemicals considered. However, this could also be deemed unfair, since by considering life cycle (instead of direct) impacts, we are overestimating the impacts of the chemical industry alone (i.e., our assessment also includes impacts taking place in other related industries such as the energy sector). Hence, in the absence of better data to refine the downscaling, we expect the two mismatches to (partially) cancel out, thus providing a fairer allocation.

Regardless of this, we explore the sensitivity of our results to the downscaling method, by resorting to other distributive justice principles for assigning a SoSOS to the chemical industry. Specifically, we consider three more approaches, two of which include two downscaling levels (see Table 4).

On the one hand, we employ a full egalitarian perspective at two different levels. In the first one, we downscale the SOS to the EU-28 level using the share of population, as done before in the combined egalitarian-utilitarian approach. Then, we further downscale the SoSOS to the scope of the chemical industry based on the number of indirect jobs generated by this industry in 2018 ($SoSOS^{ChemInd}_{b,EG+EG}$). Note that we resort to indirect (instead of direct) jobs for consistency with the scope of the LCA. This approach differs from the main downscaling method in the second step.

Analogously, we also adopt a full utilitarian perspective at two different downscaling levels. In the first one, the GVA of the EU-28 zone is used to downscale the SOS at the regional level. Subsequently, we employ the same allocation factor as in the combined egalitarian-utilitarian approach, which is also based on the GVA, to obtain the SoSOS that can be assigned to the chemical industry ($SoSOS^{ChemInd}_{b,UT+UT}$). The difference between the full utilitarian perspective and the egalitarian-utilitarian approach relies in the SoSOS assigned to the EU-28.

Finally, we also explore the use of the grandfathering principle to downscale the SOS to the European chemical industry level ($SoSOS^{ChemInd}_{b,GF}$). This principle, assigns a share of the SOS which is proportional to the *status quo* impacts and, therefore, is based on the acquired rights to pollute (i.e., all economic activities should reduce their impacts in the same proportion, as necessary to avoid the transgression of any PB). Note that, opposite to all previous downscaling methods, the allocation factor for the grandfathering principle is different for each PB, as so is their current situation at the global level. Further discussion on these downscaling methods can be found in Section 1.2.1 of the Supplementary information.

### 3.4. *Improvement pathways*

Due to the high production volumes and environmental consequences of the chemicals studied, improvements on any of the processes considered are bound to have substantial impacts. Hence, after assessing the performance of the chemical industry in the PBs, we investigate potential scenarios to enhance it. The aim is to determine the magnitude of the improvement they could allow for, and whether burden shifting occurs due to collateral impacts of their deployment. Three groups of measures are considered.

The first action proposed is the switch to a more sustainable electricity mix based on renewables (RM). The mix relies on the technology shares presented in the World Energy Outlook 2019, in accordance with the Sustainable Development Scenario (IEA, 2019). It is mostly composed of renewable energies, while carbon capture and storage (CCS) is installed in coal and natural gas plants as an aid to reduce their $CO_2$ emissions. This mix would allow curbing GHG emissions and mitigating the impacts of the sector on the $CO_2$-based boundaries (i.e., climate change, ocean acidification and, partially, biosphere integrity), but it is also expected to reduce the stratospheric ozone depletion and atmospheric aerosol emissions through reduced methane, dinitrogen monoxide, sulphate, and particulate matter emissions. Note that this is not a prospective LCA, which we leave for future work, but rather a *ceteris paribus* change on electricity supply for foreground activities only.

Following, the capacity of CCS technologies to position the chemical

**Table 4**

Briefing of methods used to downscale the safe operating space (SOS) to different scope levels: the European Union with 28 countries (EU-28), and the European chemical industry (ChemInd). GVA: Gross Value Added.

| Approach | Sharing principles | Downscaling level | Allocation variables | Data sources |
|---|---|---|---|---|
| Egalitarian + utilitarian (EG + UT) | Egalitarian | EU-28 | Population | EU-28 (European Union, 2020b)<br>World (United Nations, 2019) |
| | Utilitarian | ChemInd | GVA | ChemInd (Timmer et al., 2015)<br>EU-28 (European Union, 2020a) |
| Egalitarian (EG + EG) | Egalitarian | EU-28 | Population | EU-28 (European Union, 2020b)<br>World (United Nations, 2019) |
| | Egalitarian | ChemInd | Indirect jobs | EU-28 (Oxford Economics, 2019) |
| Utilitarian (UT + UT) | Utilitarian | EU-28 | GVA | EU-28 (European Union, 2020a)<br>World (World Data Bank, 2023) |
| | Utilitarian | ChemInd | GVA | ChemInd (Timmer et al., 2015)<br>EU-28 (European Union, 2020a) |
| Grandfathering (GF) | Grandfathering | ChemInd | Current impacts (*status quo*) | ChemInd (using Eq. (3))<br>World (Steffen et al., 2015) |

industry within the safe zone of the climate change and ocean acidification boundaries is investigated. Acknowledging that appealing opportunities for the deployment of CCS in industry might also exist (Thonemann and Pizzol, 2019), life cycle data lacks the necessary resolution to identify these point sources. Hence, instead, we consider the deployment of carbon dioxide removal (CDR) technologies to offset the impacts incurred by the chemical industry, as an interim measure that could help during the transitioning of the sector towards a more sustainable model (Pozo et al., 2020). Specifically, we assess the potential of two of such technologies, namely direct air carbon capture and storage (DACCS) and Bioenergy with carbon capture and storage (BECCS). Four scenarios are presented for each of these two CDR technologies. The first one, is a nominal scenario where the aim is to obtain net zero $CO_2$ emissions. The second one is an improvement over the first scenario, which replaces the conventional electricity mix by the RM studied in the previous action. Then, two additional scenarios are defined, where the aim is to cancel, not only $CO_2$ emissions, but the total contribution on the energy imbalance control variable by capturing the equivalent amount of $CO_2$. The difference between these last two scenarios stem from the use of the BAU electricity mix or the RM.

Finally, grey hydrogen production is replaced by green hydrogen obtained through the electrolysis of water powered by wind power (Weidner et al., 2023). This mainly affects the production of all types of PE, PP, vinyl chloride, ammonia, and methanol. While the focus of this scenario is the substitution of grey hydrogen, the chlor-alkali process, producing yellow or white hydrogen as a by-product, is also addressed (Arcos and Santos, 2023). Specifically, the electricity mix of the chlor-alkali electrolysis (foreground process) is changed to the RM in aims to alleviate the impacts caused by the high electricity consumption of this process (Liu and Elgowainy, 2019). This influences the manufacturing of all chemicals using feedstocks from the chlor-alkali process (i.e., propylene oxide, benzene, terephthalic acid, and vinyl chloride).

Further details on the modelling of each of these scenarios can be found in Section 1.3 of the Supplementary material.

## 4. Results and discussion

### 4.1. Performance of the European chemical industry on the planetary boundaries

We start by analysing the BAU situation, plotting the current impacts of the whole economy, as given in Table 3, onto the PBs at the global level (Fig. 3a). At the time of writing, only three of these boundaries are met: stratospheric ozone depletion, ocean acidification and freshwater use. Two of the remaining PBs lie in the uncertainty zone (i.e., land-system change, and biosphere integrity), while the other two are severely transgressed, reaching the high-risk zone. For the latter, climate change is transgressed owing to the energy imbalance control variable (i.e., impacts on atmospheric $CO_2$ concentration lie in the uncertainty zone), while the limit on biogeochemical flows is surpassed due to nitrogen flows (phosphorous flows remain in the uncertainty zone, too). Recall that no impacts are plotted for the atmospheric aerosol loading PB, since it has not been quantified at the global level, yet.

In this plot (Fig. 3a), we also depict the contributions of the European chemical industry with respect to the current impacts of the whole global economy (grey sectors and labels). As can be seen, the European chemical industry has minor contributions at the global scale, with impacts below 3 % in all the cases, and smaller than 0.1 % in many cases. Even when the contributions from the European chemical industry are compared against the SOS at the global level, the SOS occupied ranges from <0.1 % to 5.3 %. This is not a surprising result considering that the European chemical industry is just a sector of a single region, and therefore, its contribution should, ideally, be small in the global context.

A different situation emerges when the impacts from the European chemical industry are compared against the share of SOS allocated to the EU-28 region using an egalitarian approach (i.e., $SoSOS_{b,EG}^{EU-28}$, see Fig. 3b). Still no single boundary on control variables is transgressed, yet important contributions of 68 % [57 %–79 %] and 72 % [61 %–80 %] of the SoSOS are observed, respectively, for energy imbalance and atmospheric $CO_2$ concentration (note that grey labels in this and next subplots provide the ratio between the impacts and the corresponding SoSOS). This highlights an unsustainable situation since it is hard to envision that the remaining economic activities within the EU-28 region can successfully operate within the spare SoSOS for these control variables. The other $CO_2$-driven PB, i.e., ocean acidification, stands next, with an impact of 23 % [20 %–25 %] of the SoSOS. Impacts on the remaining PBs are generally small (i.e., below 1 %), including that for the atmospheric aerosol loading (regional) PB, which is quantified here. The only exception is the biosphere integrity boundary, where impacts contribute a non-negligible 5 % [4 %–6 %] of the SoSOS. This is also due to GHG emissions, which are responsible for 97 % of the impacts on this PB.

To provide more context, we further downscale the SoSOS to the appropriate region (EU-28) and sector (chemical industry), using a utilitarian perspective as explained in Section 3.3 ($SoSOS_{b,EG+UT}^{ChemInd}$), and use it as a benchmark for the impacts from the European chemical industry. This comparison, arguably the fairest considering the scope of the LCA, unveils a more concerning situation, with boundaries on three out of 10 control variables transgressed significantly. The chemical industry is an energy intensive sector and a primary emitter of GHG emissions, undoubtedly trespassing climate change limits: energy imbalance (1413 % [1180 %–1644 %]) and atmospheric $CO_2$ concentration (1492 % [1269 %–1660 %]). Although 45 types of GHGs have been analysed, between 98.0 % and 99.8 % of all GHG emissions in kilograms correspond to $CO_2$, and between 99.8 and 100.0 % of these come from the combustion of fossil fuels. The ocean acidification boundary, highly related to GHG emissions, is also transgressed, reaching levels of 473 % [416 %–526 %] the SoSOS. These results suggest that the European chemical industry is an important threat for these three Earth systems, which is particularly dangerous considering that that these boundaries are also transgressed at the global level.

In addition, the biosphere integrity boundary is also affected by the high levels of GHG emissions (contributions of 104 % [90 %–118 %] of the SoSOS). Consistent with the significantly low impact of the industry on the land-system change PB (<1 %), the contribution of the land use stressor to biodiversity loss is low (3 %).

The sector remains below the threshold for all other boundaries, although they demonstrate disparate contributions from the European chemical industry. For instance, aerosol emissions are dominated by non-methane volatile organic compounds (NMVOCs), sulphur dioxide, and nitrogen oxides, positioning the sector at 18 % [15 %–22 %] of the assigned SoSOS. Then, the nitrogen cycle shows approximately half of this contribution (9 % [6 %–15 %]). In this case, part of the total nutrient fluxes attributed to the industry end up stemming from waste treatment processes, rather than from direct emissions. Nevertheless, industrial activity is also directly responsible for nitrate and phosphate point source pollution due to wastewater effluents poured to surface waters (Zhang et al., 2015), when no or insufficient treatment is applied.

For the remaining control variables, contributions from the chemical industry are always below 2 % of the assigned SoSOS. Continuing with biochemical cycles, the impact on the phosphorus cycle remains under the limit and takes up only 1 % [1 %–2 %] of the SoSOS after downscaling. Meanwhile, recent regulations on the use of ozone depleting substances (ODS) cause the chemical industry to lie 99 points below the limit, with an occupation of the assigned SoSOS of only 1 % [0 %–1 %]. Out of all ODS that contribute to damaging the ozone layer, dinitrogen monoxide accounts for 99 % of overall emissions once total volumes are considered.

The chemical industry occupies <1 % of the allocated environmental budget for the land-system change boundary, which is the Earth system

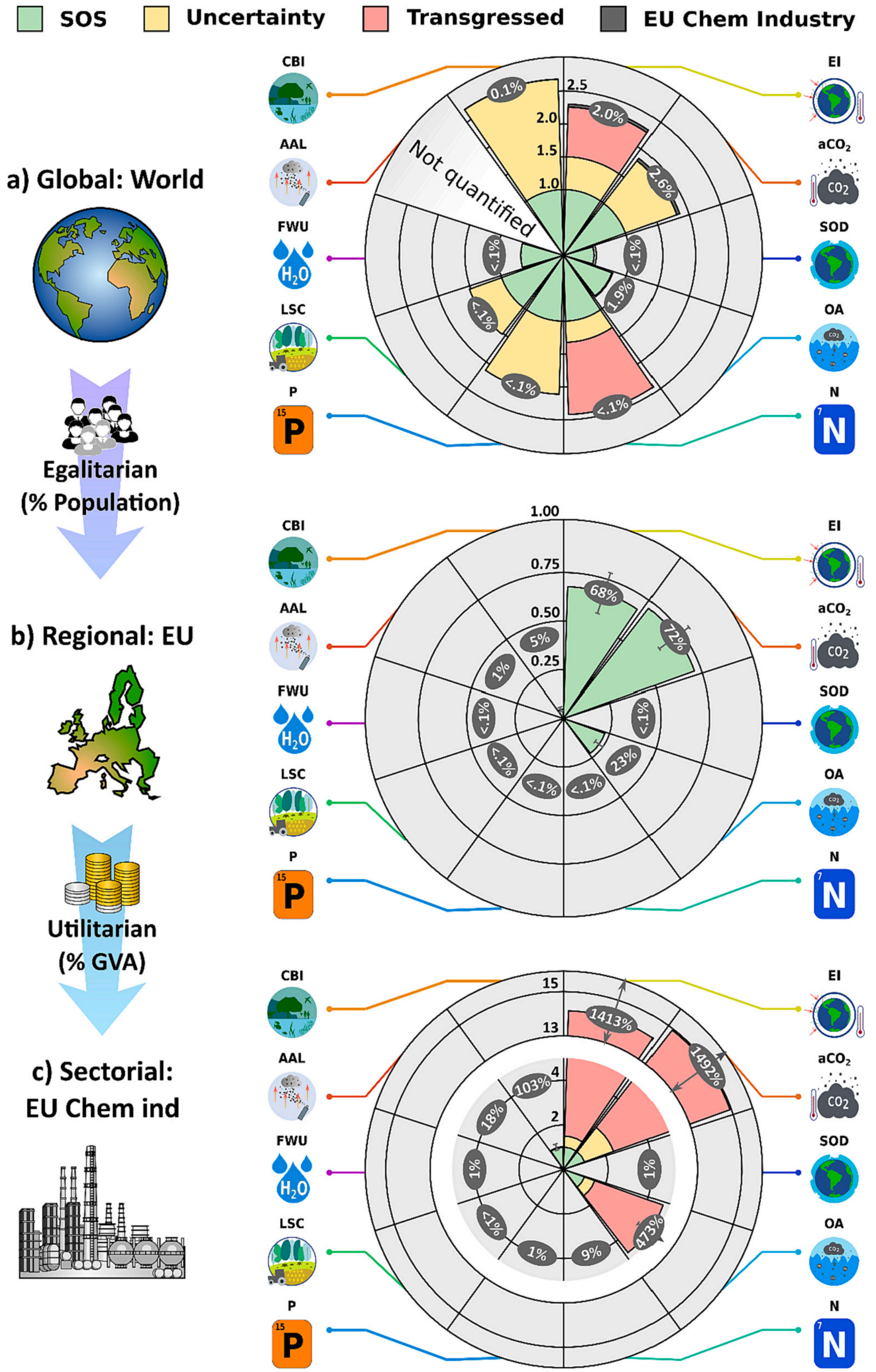


**Fig. 3.** Impacts of the European chemical industry onto the PBs. In subplot (a), current impacts of the whole economy are depicted against boundaries on the different control variables, with different colours depending on whether they lay within the SOS (green), in the uncertainty zone (yellow), or in the high-risk zone (red). The contribution from the European chemical industry is also highlighted with grey sectors, with labels providing their contribution to current impacts. In subplot (b), impacts from the European chemical industry alone are plotted against the SoSOS$^{\text{EU-28}}$ obtained following an egalitarian approach, with labels providing the exact number and error bars providing the variability among the 100 scenarios modelled. In subplot (c), impacts from the European chemical industry alone are plotted against the SoSOS$^{\text{ChemInd}}$ obtained following an egalitarian + utilitarian approach, with labels and error bars as in subplot (b). Error bars topped with arrows indicate that uncertainties extend beyond the plottable region. GVA: Gross Value Added; EI: energy imbalance at top of atmosphere; aCO$_2$: atmospheric CO$_2$ concentration; SOD: Stratospheric ozone depletion; OA: Ocean acidification; N: Biogeochemical nitrogen flows; P: Biogeochemical phosphorous flows; LSC: Land-system change; FWU: Freshwater use; AAL: Atmospheric aerosol loading; CBI: Change in biosphere integrity.

receiving the smallest pressure out of all the assessed control variables. Agriculture is the primary cause of land use (Food and Agriculture Organization, 2016), which has no direct link with the chemical industry. Another important cause of land change, however, is biomass consumption. If biomass becomes more important in the future industrial and energy sectors, it could cause an increase of the land attributed to the chemical sector. In addition, some industries resort to reforestation and afforestation projects as a mean to stay below their emission limits by compensation (UNFCCC, 2013). These carbon trading mechanisms are still in place after COP27 (UNFCCC, 2022). In *ecoinvent*, reforestation projects for industrial activities are reflected in LCI entries labelled “land transformation to forest”, which are counted as negative contributions (i.e., environmental credits) to the land-system change PB. Fig. S2-1 in the Supplementary material shows the comparison between deforested and reforested area calculated per activity and separated by type of transformation. If reforestation projects were not considered (by the omission of their respective CFs), the impact on the land-system change boundary would be incremented by 220 %. This difference would not cause the threshold to be transgressed, and the contribution to the final SoSOS would still remain below 1 %.

Results indicate that the use of freshwater derived from chemical plants does not pose a threat to the water cycle, as only 1 % [1 %–1 %] of the total downscaled boundary is occupied. If adequate treatment of effluents is carried out, water can be returned to the environment. As with reforestation, the treatment and return of water has been quantified as a negative contribution to the PB (see Fig. S2-2). A total of 89 % of returned water is discharged to surface water bodies, while the remaining 11 % goes to underground reservoirs. The total impact to the freshwater use boundary would be 19 % larger if no water return was considered, still insufficient to trespass the corresponding boundary.

Overall, we find more urgency in addressing impacts of the chemical industry on biosphere integrity and $CO_2$-based and PBs, since these are not only transgressed by the chemical industry post-allocation, but also at the global level. Other PBs currently transgressed globally, such as biogeochemical flows, show minor contributions from the chemical industry, which suggests they are less significant for this sector with current technologies.

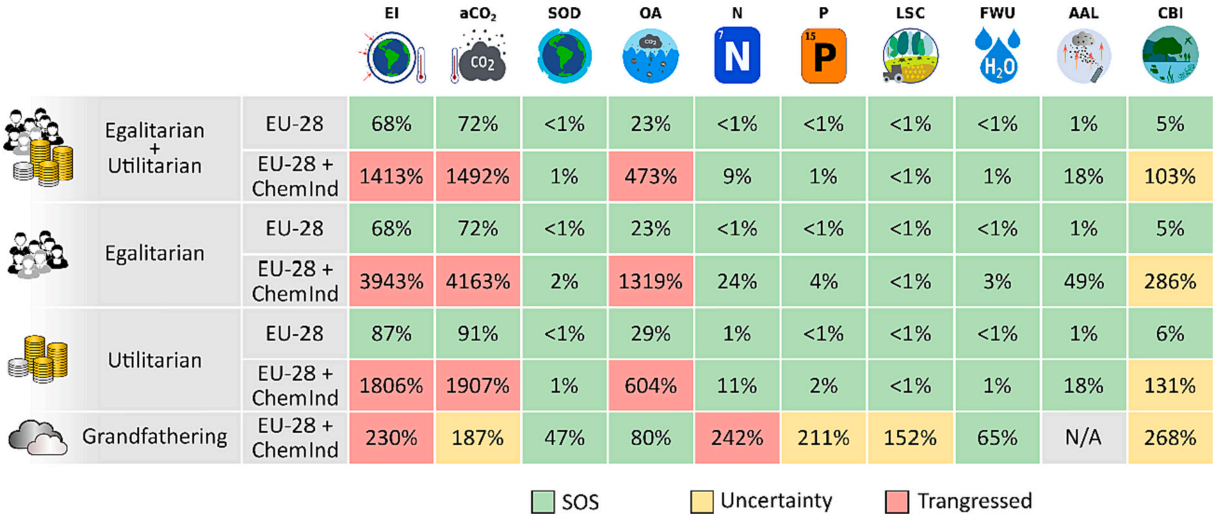
### *4.1.1. Influence of the downscaling methods*

Previous results were obtained considering a SoSOS derived from a combined egalitarian-utilitarian approach ($SoSOS_{b,EG+UT}^{ChemInd}$). However, it is well-known that the outcome of any study could vary depending on the downscaling method used to assign a SoSOS to the activity assessed (Hjalsted et al., 2021). Hence, we next test the robustness of our results by contrasting the impacts incurred by the European chemical industry against the SoSOS that would be obtained under three additional downscaling principles: full egalitarian ($SoSOS_{b,EG+EG}^{ChemInd}$), full utilitarian ($SoSOS_{b,UT+UT}^{ChemInd}$), and grandfathering ($SoSOS_{b,GF}^{ChemInd}$). In turn, for the first two methods, we consider two downscaling levels: the EU-28 region, and the European chemical industry itself (Fig. 4).

We find that both, full egalitarian and full utilitarian methods, mirror the pattern of the combined egalitarian-utilitarian approach discussed in the previous section. In the three cases, the European chemical industry transgresses the $CO_2$-based PBs: climate change, through both energy imbalance and atmospheric $CO_2$ concentration control variables, and ocean acidification. This transgression is significantly larger for the full egalitarian principle than for the other two approaches, suggesting that the current impacts of this sector are disproportional to the number of people indirectly employed in it. Impacts on the other control variables remain at relatively low levels: between 0 and 49 % for full egalitarian and between 1 and 18 % for full utilitarian. The only exception is change in biosphere integrity, where impacts reach the uncertainty zone, mainly owing to contributions from $CO_2$ emissions. For this control variable, the high-risk zone is never attained, not even under the full egalitarian approach (transgression of 286 %, while the high-risk zone lies at 700 %).

On the other hand, results at the regional level suggest that the utilitarian approach assigns a smaller SoSOS than the egalitarian principle. This indicates that the EU-28 region represents a smaller share of the world’s economy than in terms of population. As a result, following a utilitarian perspective, the European chemical industry already occupies 87–97 % of the SoSOS assigned to the whole economy of the region for climate change PBs, and a non-negligible 29 % of the SoSOS for ocean acidification, evidencing an unsustainable situation that would leave almost not room for other economic sectors.

Finally, the grandfathering principle behaves different to all other downscaling methods. As explained in Section 1.2.1 of the Supplementary material, according to this method, the activity used for downscaling will always result in the same transgression levels as the world economy. Hence, results obtained for this principle are analogous to



| | | EI | $aCO_2$ | SOD | OA | N | P | LSC | FWU | AAL | CBI |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Egalitarian + Utilitarian | EU-28 | 68% | 72% | <1% | 23% | <1% | <1% | <1% | <1% | 1% | 5% |
| | EU-28 + ChemInd | 1413% | 1492% | 1% | 473% | 9% | 1% | <1% | 1% | 18% | 103% |
| Egalitarian | EU-28 | 68% | 72% | <1% | 23% | <1% | <1% | <1% | <1% | 1% | 5% |
| | EU-28 + ChemInd | 3943% | 4163% | 2% | 1319% | 24% | 4% | <1% | 3% | 49% | 286% |
| Utilitarian | EU-28 | 87% | 91% | <1% | 29% | 1% | <1% | <1% | <1% | 1% | 6% |
| | EU-28 + ChemInd | 1806% | 1907% | 1% | 604% | 11% | 2% | <1% | 1% | 18% | 131% |
| Grandfathering | EU-28 + ChemInd | 230% | 187% | 47% | 80% | 242% | 211% | 152% | 65% | N/A | 268% |

🟩 SOS 🟨 Uncertainty 🟥 Trangressed

**Fig. 4.** Transgression levels of the European chemical industry considering different downscaling methods. The transgression level achieved is given as a % of the corresponding SoSOS, depicted in different colours depending on whether impacts lay within the SoSOS (green), in the uncertainty zone (yellow), or in the high-risk zone (red). EI: energy imbalance at top of atmosphere; $aCO_2$: atmospheric $CO_2$ concentration; SOD: stratospheric ozone depletion; OA: ocean acidification; N: biogeochemical nitrogen flows; P: biogeochemical phosphorous flows; LSC: land-system change; FWU: freshwater use; AAL: atmospheric aerosol loading; CBI: change in biosphere integrity.

those shown for the whole economy in Fig. 3a. This can be interpreted as if all economic activities should reduce their impacts in the same proportion to avoid transgressing the PBs, and is consistent with the principle of “acquired rights to pollute” (Banuri et al., 1995). Note that, since no global limit has been established on the atmospheric aerosol loading, no downscaling is possible for this boundary using the grandfathering principle.

Overall, we can conclude that, in this case, results are robust and the same conclusions can be derived from the study regardless of the downscaling principle employed (with the argued exception of the grandfathering approach), namely that there is an urgency to reduce $CO_2$ emissions stemming from the chemical industry. Reducing impacts to other PBs, although always desirable, seems less of a priority for the sector since the chemical industry exhibits less significant contributions to the corresponding Earth-system processes.

### 4.2. Impact breakdown

Fig. 5 breakdowns the impacts of the European chemical industry on the PBs by the 19 chemicals considered. Chemicals are displayed on the left-hand side of the figure, sorted from higher (ammonia, bottom) to lower (xylenes, top) corrected production volumes, i.e., including exports and discounting feedstock uses for other chemicals. Propylene does not explicitly appear in the figure because its corrected production volume is zero (i.e., its impacts are accounted for in the burdens of its derived products), reason why only 18 chemicals are displayed. Their contributions onto the different control variables of the PBs are represented by ribbons connecting the corresponding segments, with the width of the ribbons being proportional to the impact contributions.

As seen, the three $CO_2$-based control variables (i.e., energy imbalance at top of atmosphere, atmospheric $CO_2$ concentration, and ocean

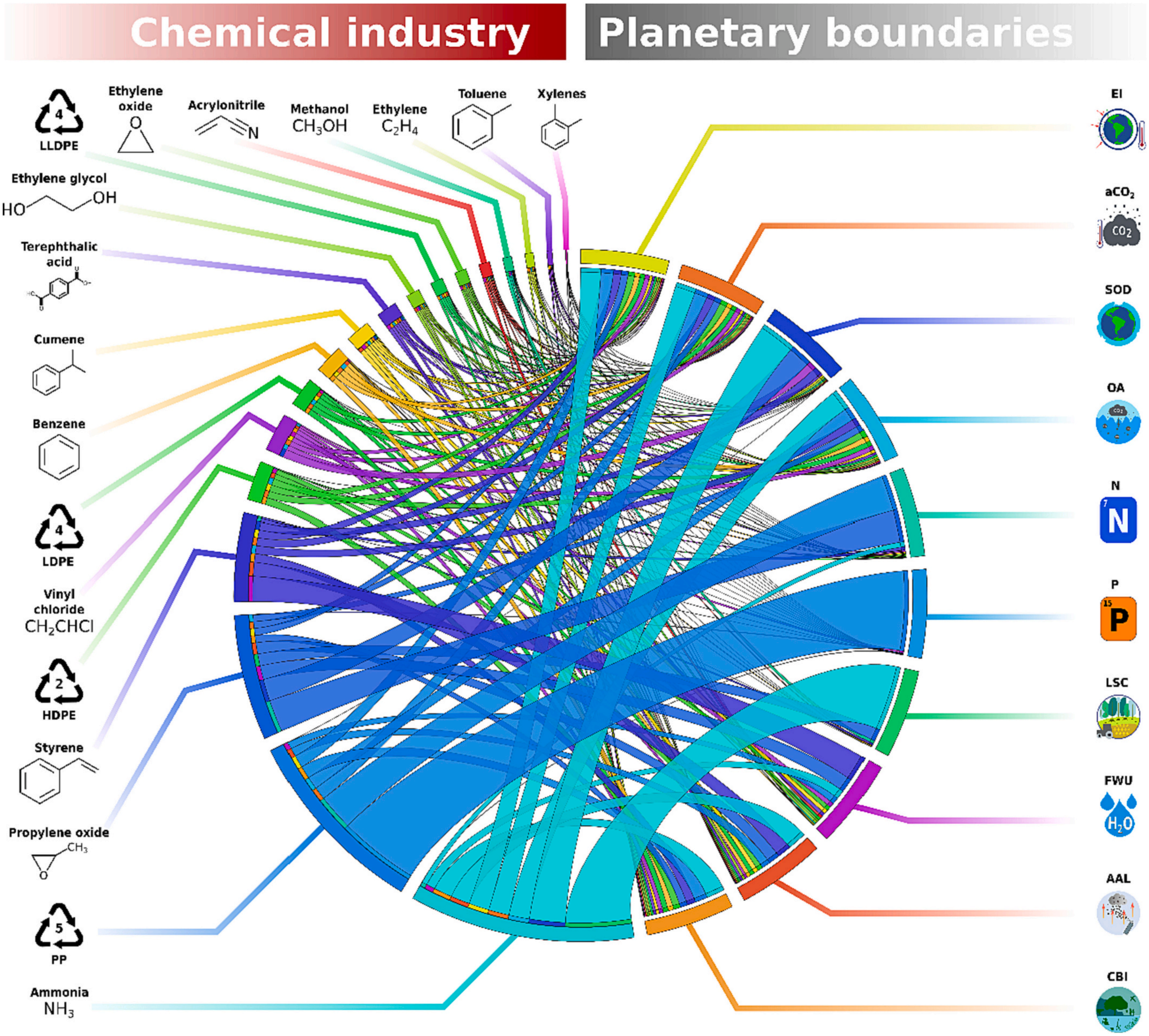


**Fig. 5.** Breakdown of the impacts of the European chemical industry onto PBs. Chemicals (left-hand side) are sorted according to their corrected production volume, from largest (ammonia) to lowest (xylenes). Propylene is not depicted as its corrected production volume is zero. The right-hand side provides the control variables for the PBs. EI: energy imbalance at top of atmosphere; $aCO_2$: atmospheric $CO_2$ concentration; SOD: stratospheric ozone depletion; OA: ocean acidification; N: biogeochemical nitrogen flows; P: biogeochemical phosphorous flows; LSC: land-system change; FWU: freshwater use; AAL: atmospheric aerosol loading; CBI: change in biosphere integrity.

acidification) show a similar pattern, with impacts highly proportional to the production volumes of the different chemicals. This suggests that no significant differences exist between the carbon intensities of the different products. Ammonia and polypropylene (PP) are the two largest contributors to these control variables, precisely because of their large production volumes, accounting for 25 % and 15 % of the overall impacts on these boundaries, respectively. In the case of ammonia, two production routes are considered, with the partial oxidation one being more carbon intense. This is because coal or heavy oils are used as raw materials instead of natural gas or light carbon fuels, as in the other route (i.e., the steam reforming process). In addition, the energy demand of the partial oxidation processes is also higher than for steam reforming. However, both processes produce $CO_2$ as part of the reaction sequence in more than one stage, generating high quantities of residual GHGs. Therefore, the production of green hydrogen for the manufacturing of green ammonia could help mitigate these impacts (Rostami et al., 2022). In turn, these would allow companies to partially exploit current infrastructure for downstream activities (e.g., the Haber-Bosch process). For PP, 69 % of the impacts can be attributed to propylene production due to the energy intensity of the process. In this case, recycling or substitution of polymers (including PP), could reduce the pressure exerted on $CO_2$-based control variables. Considering the current momentum towards circular economy, business opportunities are expected for companies aimed at transforming residues such as plastic waste into valuable chemicals (Somoza-Tornos et al., 2020). Electrification, and the switch to a greener electricity mix, could also benefit the industry as a whole and improve its sustainability level (Mallapragada et al., 2023; Van Geem and Weckhuysen, 2021). Some of these routes are explored in Section 4.3 of this study.

The fact that these three control variables are at high-risk zone in Fig. 3c, and transgressed at the global level, calls for a deeper analysis. For instance, inspection of GHG emissions reveals that 99 % of the total correspond to fossil $CO_2$. The main source of unitary $CO_2$ emissions (i.e., per kg of chemical) are propylene oxide plants operating with the chlorohydrin process, mainly due to the obtention of the reagents (52 %) and the electricity and thermal energy used (25 %), with additional contributions from the treatment of wastes and the production process itself. The more sustainable "hydrogen peroxide to propylene oxide" process, combined with the use of innovative catalysts to increase selectivity, pose an opportunity to fully eliminate the highly damaging chlorohydrin route while achieving a high conversion (Alvear et al., 2023; Aquino et al., 2023). Styrene also appears to have significantly high unitary $CO_2$ emissions, incurred in the dehydrogenation of ethylbenzene (see Fig. S2-4). Finally, ammonia also stands out as a primary emitter of $CO_2$, causing acrylonitrile, which uses it as feedstock, to have high specific emissions as well.

The other PB transgressed in some scenarios (Fig. 3c) is the change in biosphere integrity. In this case, contributions also mimic those of the $CO_2$-based control variables, consistent with the small contribution expected from the non-$CO_2$ stressors (i.e., land use, see Section 4.1). As land use takes little relevance in the final impact (just slightly above 3 %), the remaining share of impacts is directly related to GHG emissions. Even if 30 % of the chemicals contributing to the change in biosphere integrity are not considered in other carbon-based control variables, their contribution to the total score in biosphere integrity is limited to only 0.02 %. Thus, the breakdown of the total impact on biosphere integrity is almost identical to that of any other $CO_2$-based indicator, showing ammonia and polypropylene as the main contributors.

For the remaining control variables, the distribution of impacts is more independent from production volumes, thus revealing that some activities are especially responsible for the alteration of specific Earth mechanisms.

When analysing the impacts on stratospheric ozone depletion, ammonia and propylene oxide stand out again, dwarfing the impacts from all other chemicals. Despite having a modest unitary impact (Fig. S2-5), ammonia alone accounts for 43 % of the total impacts on this boundary (30 % from the steam reforming process plus 13 % attributed to partial oxidation). Conversely, propylene oxide, ultimately contributing with a 26 % of the total impacts on this boundary, widely outweighs all other chemicals in terms of unitary impacts (Fig. S2-5). The reason behind the high impact of propylene oxide production is the chlor-alkali electrolysis, found to account for nearly 80 % of all $N_2O$ emissions. Another chemical with significant unitary emissions of ODS is vinyl chloride, as plants operating with the direct chlorination and oxychlorination of ethylene require chlorine as a baseline reagent. Hence, $N_2O$ from the obtention of chlorine through the chlor-alkali process, combined with emissions originating from waste treatments, result in an overall significant contribution (see Supplementary results). All the LCI values for the principal waste types produced in chemical plants (i.e., average incineration residue, municipal solid waste, waste plastic, and waste wood) are higher for vinyl chloride than for any other chemical studied.

Processes manufacturing chemicals derived from propylene account for most phosphorus emissions and a great fraction of nitrate emissions (see also Figs. S2-6 and -7). Specifically, PP and propylene oxide make up for 80 % and 96 % of the impacts on the nitrogen and phosphorus control variables, respectively. For instance, 95 % of nitrate emissions from propylene oxide originate from impurities found in the raw materials for the electrolytic production of chlorine and NaOH. On the other hand, phosphorus emissions are most likely attributed to wastewater management since the chlorohydrin process requires intense post-treatment of waste effluents. These plants can produce a waste consisting of a dilute calcium chloride brine, which requires phosphate compounds for its treatment (Dingwen and Changhui, 1989). Further discussion on the origin of these emissions is provided in the Supplementary results.

The land system change boundary is not transgressed globally, and, similarly, no critical or large impacts are caused by any manufacturing process of the chemical industry. The main contributor to land use is ammonia (85 %), followed by propylene oxide (5 %) and methanol (4 %). As previously explained, the final impact each activity has on this boundary is calculated considering the possibility to counteract deforestation practices with reforestation projects, which can reduce the total area transformed by the action of the different enterprises. Hence, this managerial decision can help companies reduce their land footprint through ecosystem services. On the other hand, chemicals such as terephthalic acid, acrylonitrile, and styrene, despite associated with higher land transformation, are also accredited for contributing to the recovery of other areas back to forest (see Fig. S2-1). Conversely, methanol is identified as the third largest contributor to land use, despite not having a high impact on land. The reason is that methanol-producing industries are barely involved in reforestation projects. We even found some chemicals with net negative impacts on land change because their participation in reforestation programmes offsets the deforestation they incur. These are the cases of ethylene and PE, PP, vinyl chloride, xylene, and toluene. Note, however, that these practices might not fully recover the initial ecosystems that the industry perturbs, since old, undisturbed forests hold environmental functions and present characteristics that young plantations may take years to achieve and develop (Luyssaert et al., 2008; Wohlleben, 2020).

Regarding freshwater use, processes show a much more homogeneous distribution of impacts. Still, styrene and propylene oxide do take up 30 % and 18 % of the impacts, respectively, mainly due to the use of water as a reagent and/or as a heating or cooling agent. This is particularly critical for styrene production via the dehydrogenation of ethylbenzene, which requires large quantities of steam to maintain the reaction temperature (Zarubina, 2015). Ammonia (10 %) and polypropylene (8 %) are next in terms of contribution to the freshwater use PB, but these cannot be attributed to high unitary impacts, but rather to their large production volumes (Fig. S2-9). In addition, some processes return a fraction of water to the environment (Fig. S2-2). However, there is no processes returning more water than they withdraw, not even in cases where water is formed as a by-product in the reaction (e.g., the chlorohydrin process or the direct oxidation of ethylene). Overall, one recursive observation is that steam production is one of the main stressors for this boundary in the chemical industry, which suggests that increasing energy efficiency and exploiting heat-integration opportunities could further reduce its use.

Analogously to the climate change and ocean acidification control variables, the impacts on aerosol loading are mainly dependent on the production volumes, with similar unitary emissions between all chemicals (Fig. S2-10). Actually, many flows are classified as both GHGs and aerosols (e.g., NMVOCs). The primary aerosols emitted by the chemical industry are sulphur dioxides (almost 39 % of total mass emissions), nitrogen oxides (29 %), NMVOCs (24 %), and particulates (8 %). Despite this, propylene oxide is the chemical showing the largest pollution rate (Fig. S2-10), mainly due to the chlor-alkali employed to obtain the necessary chlorine, which is responsible for 72 % of aerosol emissions. It is important to reduce environmental pressures on atmospheric aerosol loading since, among non-transgressed boundaries, this is the Earth-system where a larger part of the SoSOS is occupied (18 %, Fig. 3c). For Europe, the circulation of aerosols between regions is highly limited. Thus, they primarily have an impact within the region where they are emitted (Ryberg et al., 2018b), which can facilitate control and regulation. Measures would need to focus on the three principal aerosols emitted, i.e., NMVOCs, sulphur dioxide, and nitrogen oxides.

Table 5 presents a summary of the impact breakdown, showing the top four chemicals with the highest contribution to each control variable in terms of both absolute and unitary impacts. Additional insight is provided in Section 2.2 of the Supplementary material.

**Table 5**

Top contributors to PBs considering absolute and unitary impacts. HDPE: high-density polyethylene; LDPE: low-density polyethylene; LLDPE: linear low-density polyethylene, PB: planetary boundary.

| PBs: control variables | Absolute impact | Per kg of chemical |
|---|---|---|
| Climate change: energy imbalance at top of atmosphere | Ammonia<br>Polypropylene<br>Propylene oxide<br>HDPE | Propylene oxide<br>Acrylonitrile<br>Styrene<br>Ammonia |
| Climate change: atmospheric $CO_2$ concentration | | |
| Stratospheric ozone depletion | Ammonia<br>Propylene oxide<br>Vinyl chloride<br>Styrene | Propylene oxide<br>Vinyl chloride<br>Ethylene glycol<br>Styrene |
| Ocean acidification | Ammonia<br>Polypropylene<br>Propylene oxide<br>HDPE | Propylene oxide<br>Acrylonitrile<br>Styrene<br>Ammonia |
| Biogeochemical flows: Nitrogen cycle | Polypropylene<br>Propylene oxide<br>Ammonia<br>Styrene | Propylene oxide<br>Polypropylene<br>Ethylene glycol<br>Styrene |
| Biogeochemical flows: Phosphorus cycle | Polypropylene<br>Vinyl chloride<br>Propylene oxide<br>Ammonia | Polypropylene<br>Vinyl chloride<br>Propylene oxide<br>LDPE |
| Land-system change | Ammonia<br>Propylene oxide<br>Methanol<br>Styrene | Propylene oxide<br>Acrylonitrile<br>Terephthalic acid<br>Styrene |
| Freshwater use | Styrene<br>Propylene oxide<br>Ammonia<br>Polypropylene | Propylene oxide<br>Styrene<br>Acrylonitrile<br>Ethylene glycol |
| Atmospheric aerosol loading | Ammonia<br>Styrene<br>Polypropylene<br>HDPE | Propylene oxide<br>Styrene<br>Cumene<br>LDPE |
| Biosphere integrity | Ammonia<br>Polypropylene<br>Propylene oxide<br>HDPE | Propylene oxide<br>Acrylonitrile<br>Styrene<br>Ammonia |

### 4.3. Improvement pathways

We next analyse the results obtained through the application of the different improvement pathways introduced in Section 3.4. Note that these pathways prioritize corrective measures for impacts affecting PBs that are transgressed at the global level or by the European chemical industry after allocation. This choice is motivated by the urgency on addressing these environmental problems in a timely manner. The results obtained are summarised in Fig. 6, where we illustrate improvements (in green circles) or deteriorations (in red circles) produced in the control variables of the PBs as a result of the application of the proposed actions. Red or green outlines indicate whether the boundary ends up being transgressed (or not) after the modifications, taking as reference the $SoSOS^{ChemInd}_{b,EU+UT}$. For the DACCS and BECCS cases, only the models where the contribution to the energy imbalance control variable is cancelled are represented in the figure. The results for the cancellation of $CO_2$ emissions are provided in the Supplementary material, together with further methodological details on the application of the improvement pathways (see Section 2.3 therein).

#### 4.3.1. Energy mix

The BAU mix based mainly on coal, natural gas, and oil is replaced by a new mix which relies widely on hydropower, solar, wind and nuclear energy, and includes carbon capture at coal and natural gas plants. This causes $CO_2$ and total GHG emissions per kWh of electricity to be reduced by 67.8 % and 67.7 %, respectively. However, since the change in the electricity mix can only be applied to foreground activities due to data availability, the carbon-based control variables see a pressure reduction of 8–9 %, which is insufficient to meet the corresponding PBs. The biosphere integrity PB also benefits from the mix change, showing a similar reduction to the rest of carbon-based Earth-system processes (8 %). Importantly, this improvement is sufficient to avoid the transgression.

The greatest improvements are seen in the freshwater use and the stratospheric ozone depletion PBs, with reductions of 24 and 20 % on the final impacts, respectively. Coal, natural gas, and nuclear energy were found to require water volumes from 1 to 6 orders of magnitude larger than any other energy type included in the renewable mix (RM). Therefore, the substitution of these technologies causes the water requirements of the processes to drop dramatically. On the other hand, the reduction of methane and dinitrogen monoxide emissions stemming from the RM (from $7{\cdot}10^{-4}$ to $4{\cdot}10^{-4}$ and from $1.85{\cdot}10^{-5}$ to $3.7{\cdot}10^{-6}$ kg per kWh, respectively) has a beneficial effect on the stratospheric ozone depletion PB.

Even if the mix change does not cause its transgression, the nitrogen cycle is slightly deteriorated (0.6 %). Nitrate emissions to surface water of concentrated solar power plants are significantly higher than those of the conventional mix ($1.42{\cdot}10^{-5}$ vs $6.4{\cdot}10^{-6}$ $m^3$ of water per kWh). These emissions are most likely due to the salt mixtures containing nitrates utilized as energy storage media in concentration solar power installations (Fernández and Cabeza, 2019; Villada et al., 2019). Thermal energy storage is used to enable plants to produce electricity when solar radiation is low, even during the night. Molten salts commonly used for this purpose include potassium and sodium nitrate. The results indicate that, while concentrating solar power is seen as an attractive alternative to fossil fuels (Villada et al., 2019), its widespread use could damage the nitrogen cycle and may thus require attention. Additionally, wind and solar photovoltaic installations, and natural gas plants

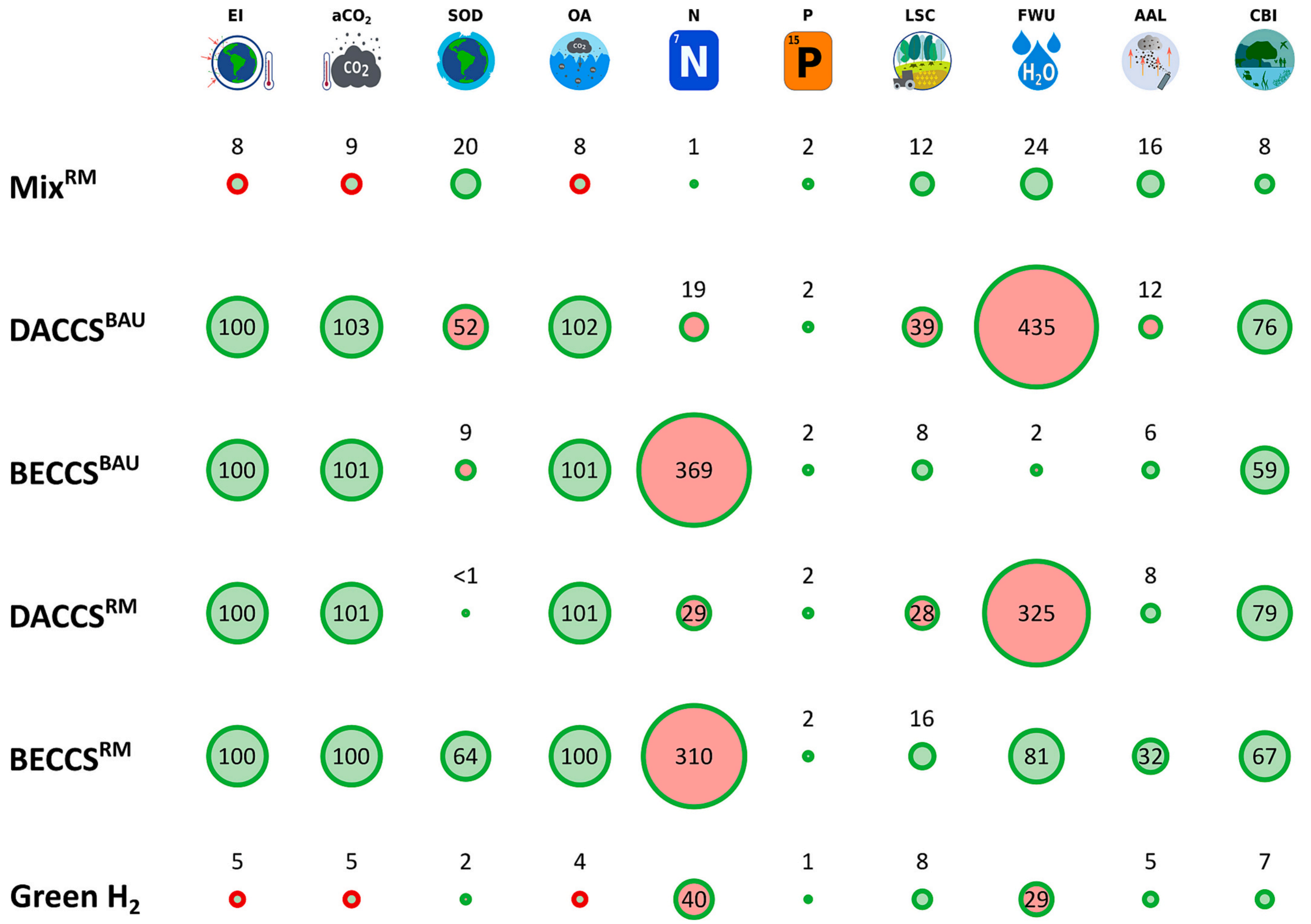


**Fig. 6.** Summary of improvement pathways. Improvement (or worsening) of the occupied SoSOS is represented for each scenario with a green (or red) circle, whose size is proportional to the change in this occupation. The colour of the outer ring provides whether the limit on the corresponding control variable ends up being transgressed in the scenario. EI: energy imbalance at top of atmosphere; aCO$_2$: atmospheric CO$_2$ concentration; SOD: stratospheric ozone depletion; OA: ocean acidification; N: biogeochemical nitrogen flows; P: biogeochemical phosphorous flows; LSC: land-system change; FWU: freshwater use; AAL: atmospheric aerosol loading; CBI: change in biosphere integrity. BAU: business as usual; BECCS: bioenergy with carbon capture and storage; DACCS: direct air carbon capture and storage; RM: renewable mix.

operating with CCS also have nitrate emissions one order of magnitude above the conventional mix. The former arise from the use of sorbent to collect CO$_2$, which is typically an amine (diethanolamine or ethanolamine).

### *4.3.2. Carbon capture and storage*

The DACCS and BECCS capacity required to attain the proposed goals is calculated when (i) the total amount of CO$_2$ released wants to be sequestered and (ii) the total impact on energy balance wants to be cancelled out. In the second case, any of the three CO$_2$-based control variables could have been chosen as objective for cancellation, yet we opted for the energy imbalance control variable since it is the one receiving the highest pressure at the global level, and the one that better represents the impact of all non-CO$_2$ GHGs. In both cases, two options are studied to power the CDR technologies: the BAU mix, and a renewable mix (superscripts BAU and RM in the figure). In all the scenarios, the CDR capacity that needs to be installed is calculated considering the additional emissions stemming from the CDR technologies themselves.

When the BAU mix is used, 140 Mt. of CO$_2$ must be removed with DACCS to obtain a total balance of CO$_2$ emissions equal to zero. This allows to achieve a significant reduction in the impacts on the climate change, ocean acidification, and biosphere integrity control variables, which are now respected. In the case of BECCS, the volume to sequester is slightly below that of DACCS, standing at 136 Mt. The cause is the volume of additional CO$_2$ emitted by the technology itself, which is higher per kg of captured CO$_2$ in the case of DACCS.

To cancel the impact on the energy imbalance control variable, 147 and 127 Mt. of CO$_2$ need to be sequestered through DACCS and BECCS, respectively (see Fig. 2-11 in the Supplementary material). In the case of BECCS, the volume to sequester is lower when aiming to cancel the impact on energy imbalance than when trying to cancel all CO$_2$ emissions. The cause are the CO$_2$ emissions of the technology itself, a 95 % of which (in volume) fall under the “carbon dioxide, from soil or biomass stock” ecoinvent category, which has an insignificant contribution to energy imbalance, but must be captured regardless in the CO$_2$ scenario. For DACCS, the capture volume is incremented with respect to the CO$_2$ scenario because the technology emits significant amounts of non-CO$_2$ GHGs and, therefore, requires the capture of more CO$_2$ to compensate for its own emissions.

The combination of these CDR technologies with the RM allows for a non-negligible reduction in their required capacity: 13 % for DACCS and 8 % for BECCS.

The deployment of DACCS with the BAU mix causes the pressure on all non-carbon related PBs to increase, except for the phosphorus cycle control variable, which receives insignificant improvements of <2 %.

Impact increments are in the range of 12 %–52 %, except for freshwater use, where impacts rise as much as 435 % owing to the use of liquid solvents with high water demand. This number might seem very high, yet it only causes the chemical industry to occupy 6 % of the $SoSOS_{b,EU+UT}^{ChemInd}$, since the original impacts on this PB were small. When the renewable mix is used to power DACCS, the same trends persist, although most impacts are generally smaller. In both cases (i.e., BAU and RM), DACCS allows to obtain negative contributions on the control variables for atmospheric $CO_2$ concentration and ocean acidification, generating additional environmental budget for other economic activities that might be harder to abate.

In the case of BECCS, patterns are also similar to those of DACCS, but in this case, no significant deterioration is observed on the freshwater use PB (lower than 2 % with the BAU mix, and even improving 81 % with the RM). Instead, the nitrogen cycle emerges as the most critical control variable since the additional damage incurred causes the occupation of 36–43 % of the $SoSOS_{b,EG+UT}^{ChemInd}$. Still, none of the impacts that increased due to burden shifting cause the transgression of any additional PB.

If a correct management of nitrogen losses is achieved, BECCS offers the most promising results. However, in the best-case scenario (BECCS using the RM), 117 million tonnes of $CO_2$ still need to be removed from the atmosphere to cancel the contribution on the energy imbalance control variable.

The storage of the $CO_2$ captured does not pose a significant immediate threat, since it would imply the annual occupation of only 0.01–0.02 % of the EU-28's geological onshore storage capacity if no additional uses of $CO_2$ are considered (e.g., carbon capture and utilisation strategies). However, considering the $CO_2$ captured would be attributed solely to the chemical industry and is an annual requirement, any rate maintained over long periods would eventually become problematic. With the same downscaling method that was applied to assign the SOS correspondent to the EU-28's chemical industry, the fraction of total storage available is 0.32 %. Thus, the chemical industry would consume that fraction before 2050 if no measures were applied.

On the other hand, the amount of land required to annually grow the biomass necessary in the BECCS scenarios would be that of 20,750–24,120 $km^2$, which is close to the size of 4 million football fields. This is based on poplar, considering a carbon content of 49.4 % and a $CO_2$ capture efficiency of 90 % (Galán-Martín et al., 2021; Gasol et al., 2009). Still, this is smaller than land requirements for DACCS facilities, which need to be located at least 250 m apart from each other to prevent dual depleted air intake (McCollum and Ogden, 2006).

In the BECCS scenarios, significant amounts of electricity are produced. As an example, when BECCS is powered with the BAU mix and the aim is to sequester the total volume of $CO_2$ emissions from the chemical industry, the electricity generated could cover 7.6 % of Europe's electricity demand. Although we assign no environmental credits to this electricity, we do highlight the value of this by-product which could be employed in a variety of applications. For instance, this energy could be partially used in the industry itself to lower fossil fuel consumption if further electrification had been deployed, or to produce green hydrogen through water electrolysis.

Hence, the deployment of BECCS and DACCS could help hard-to-abate companies to compensate for their GHG emissions, thus emerging as a promising option for managers.

### *4.3.3. Green hydrogen*

Modest improvements are seen on $CO_2$-related control variables, with impact reductions of 5 % in energy imbalance and atmospheric $CO_2$ concentration, 4 % in ocean acidification, and 7 % in biosphere integrity. The land-system change boundary also shows an impact decrease of 8 %, while a 5 % improvement is observed for aerosol loading. Changes in stratospheric ozone depletion and the phosphorus cycle stand below 2 %.

In line with findings in González-Garay et al. (2019), the freshwater use and nitrogen inputs are the main impaired control variables (29 % and 40 %, respectively), even if none of them is transgressed in this case. It could be argued that the slight improvements in the benefited boundaries seem too small to compensate for the large quantities of freshwater needed in the electrolysis process, and the nitrogen flows associated with the renewable mix powering it. On the other hand, we note that these results are based on replacing the activities used in *ecoinvent* 3.5 database to produce the hydrogen inputs required for the manufacturing of the 19 chemicals considered. In this version of the database, the main hydrogen production route in Europe is the cracking of fossil fuels, which includes, but is not limited to, steam methane reforming. This may explain why the improvements we observed through substitution of grey hydrogen are modest compared to what is found in other studies (Weidner et al., 2023).

## 5. Conclusions

Although the European chemical industry shows marginal contributions to the global burden exerted on PBs, the situation changes when contrasting impacts with the share of safe operating space that can be allocated to this regional economic sector. In this case, four of the 10 control variables assessed are transgressed, including those for the energy imbalance at top of atmosphere, atmospheric $CO_2$ concentration, ocean acidification, and biosphere integrity. This situation is repeatedly obtained for different downscaling methods, which suggests that it is indeed representative of the current landscape of this sector. Ultimately, this reveals a critical situation where it urges to mitigate impacts on these control variables, as boundaries on them are also surpassed at the global level.

The climate change PB suffer the greatest damage, with the contribution of the industry being an order of magnitude larger than the established limit on the corresponding control variables (15 and 16 times larger, respectively). Meanwhile, the ocean acidification PB receives impacts 6 times above the threshold, while the biosphere integrity boundary is transgressed by 3 %, lying at the uncertainty zone. This urges policy-makers to develop effective mechanisms to curb $CO_2$ emissions associated with the chemical industry. Land-system change receives the least pressure from the industry's activity, followed by freshwater use, stratospheric ozone depletion, and the phosphorus cycle.

The top five highest volume chemicals (i.e., ammonia, PP, HDPE, styrene, and benzene) take up almost 50 % of the impacts on all PBs despite not having especially high unitary (per kg) contributions (except for styrene, which does classify as one of the top contributors to nine out of 10 control variables). The struggle to meet chemical demands while respecting the PBs underscores the urgency to achieve more sustainable consumption patterns. Referent institutions, including the United Nations, the European Union, or the World Economic Forum, advocate for the adoption of a circular economy concept to help close the loop in industrial production chains and enhance the efficiency and durability of resource use. Increased life-cycle thinking combined with green chemistry concepts give the industry a chance to operate sustainably acknowledging the rising resource limitations and environmental challenges. This situation offers business opportunities for companies dedicated to emerging technologies, such as waste valorisation or carbon capture utilisation and storage. For the former, chemical recycling of polymers allows to close material loops, yet at the expense of significant energy consumption. Further research is needed to develop effective catalysts or biological routes that can achieve similar results as the more widespread pyrolysis, yet at a lower environmental cost. Regarding $CO_2$ capture, efforts on advancing adsorption technologies using metal-organic frameworks or zeolites, or absorption in ionic liquids, could help to bring the cost of these option down until they gain enough momentum to penetrate the market. Meanwhile, research on traditional amines still continues.

It is to be highlighted how the chlorohydrin technology for the manufacturing of propylene oxide yields especially high unitary impacts to all PBs, significantly standing out among all processes. The adoption of environmentally preferable alternatives to this route has already started and is of upmost importance given the critical impacts of the production of this chemical. The more sustainable "hydrogen peroxide to propylene oxide" process, combined with the use of innovative catalysts to increase selectivity, pose an opportunity to fully eliminate the highly damaging chlorohydrin route while achieving a high conversion. This gives a good example of a green chemistry concept, as research on catalysts is key in the path towards optimized processes.

The deployment of non-fossil energy and decarbonization of the sector, as well as the switch to greener production routes, are also actions that fall within the green chemistry and circular economy frameworks. These all were investigated in this research to some extent. Our results show how a significant amount of the impacts stem from sectors beyond the boundaries of the chemical industry itself. Any improvement measures in the chemical industry must be coupled and planned in accordance with progress made in related sectors. A clear example and the main underlying system responsible for the positioning of the industry above the PBs is the energy sector. Despite rising research on the use of hydrogen, electrochemistry, or plasma, curbing carbon emissions through the electrification of the chemical industry is only possible through collaboration and integration with the power sector. This poses a challenge for policy-makers, who might need to develop regulations with a wider-scope, or carefully balance their actions across different sectors.

In an effort to illustrate the implications of deploying some potential solutions to mitigate impacts for the European chemical industry, we studied a set of improvement pathways combining different options: the use of a renewable electricity mix, the deployment of DACCS and BECCS to cancel out $CO_2$ (or GHG) emissions, and the replacement of conventional with green $H_2$ obtained from water electrolysis. Our results evidence that there is no "silver bullet" which would allow to solve the climatic problem without causing havoc in other environmental categories. On the one hand, the mere adoption of a cleaner mix or green hydrogen fail to bring the European chemical industry to the safe operating space. On the other hand, the use of BECCS and DACCS can indeed allow the chemical industry to meet all PBs concurrently, emerging as a promising strategy for managers of hard-to-abate companies. However, burden-shifting still causes other PBs to be deteriorated, which calls for additional research to improve the performance of these technologies. Meanwhile, a holistic assessment of the impacts caused by any proposed action is needed to identify the potential shifts in burdens between Earth-systems processes and sectors. The need for improvements in activities outside the industry, such as the energy sector, also advocates for holistic approaches.

Finally, the temporal dimension, currently overlooked in present allocation methods, is not to be taken lightly. From an egalitarian perspective, the per-capita share of each PB will decrease as global population increases. This is in addition to the need to allocate impacts from larger production volumes unless per-capita consumption of chemicals is reduced. Indeed, the demand for chemical products will probably increase with population unless a paradigm shift is experienced in per-capita consumption rates. Meanwhile the allocation factor, calculated as a share of global population, will remain similar for many regions but could increase or reduce further owing to different factors (e.g., despair birth rates or migration).

While we have provided a sector-wide assessment including life cycle impacts and possible improvement pathways, a recommendation for subsequent research would be to broaden the scope of the study, currently limited to an environmental perspective, to also encompass impacts on human health. This holistic approach could help further prioritize future actions considering both environmental and public health concerns. Even from a purely environmental perspective, methods are required to express life cycle data as impacts onto the novel entities planetary boundary, for which the chemical industry is expected to exert significant pressure.

## Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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## Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.spc.2023.12.006.

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