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Perspective

Toward Assessing Absolute Environmental Sustainability of Chemical Pollution

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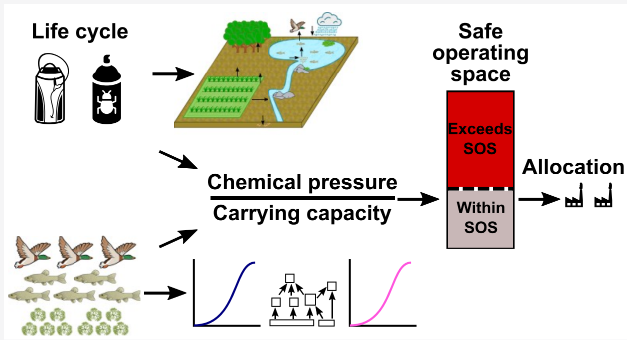

ABSTRACT: Chemicals are widely used in modern society, which can lead to negative impacts on ecosystems. Despite the urgent relevance for global policy setting, there are no established methods to assess the absolute sustainability of chemical pressure at relevant spatiotemporal scales. We propose an absolute environmental sustainability framework (AESA) for chemical pollution where (1) the chemical pressure on ecosystems is quantified, (2) the ability for ecosystems to withstand chemical pressure (i.e., their carrying capacity) is determined, and (3) the "safe space" is derived, wherein chemical pressure is within the carrying capacity and hence does not lead to irreversible adverse ecological effects. This space is then allocated to entities contributing to the chemical pressure. We discuss examples involving pesticide use in Europe to explore the associated challenges in implementing this framework (e.g., identifying relevant chemicals, conducting analyses at appropriate spatiotemporal scales) and ways forward (e.g., chemical prioritization approaches, data integration). The proposed framework is the first step toward understanding where and how much chemical pressure exceeds related ecological limits and which sources and actors are contributing to the chemical pressure. This can inform sustainable levels of chemical use and help policy makers establish relevant and science-based protection goals from regional to global scale.

KEYWORDS: *sustainability assessment, pesticides, biodiversity, ecotoxicity, carrying capacity, safe operating space*

1. INTRODUCTION

Over the past several decades, the number of chemicals on the market has grown with some estimates as high as 350000 chemicals registered for production and use globally.[1] Chemicals serve as the building blocks of modern society with diverse usage in agriculture, product manufacture, and medicine.[2] However, the growing number of marketed compounds also increases the potential for chemical pollution and negative pressure on human and ecosystem health. For example, pesticides are hazardous by design, have intentional, widespread environmental release, and easily migrate beyond their area of use, which can result in exposure of nontarget organisms and potential bioaccumulation in ecological food webs.[3] Chemicals can be released into the environment along their entire life cycle, from resource extraction, chemical synthesis, material and product manufacturing, to product use and end-of-life treatment, including recycling.[2] Despite the apparent risk chemicals pose to both human and ecosystem health, the combined chemical pressure exerted on the natural environment by different chemical classes and across the whole chemical universe is unknown.

The European Green Deal was initiated to tackle the climate change and environmental degradation challenges of the European Union (EU).[4] To meet the zero-pollution ambition, the European Commission published a Chemicals Strategy for Sustainability, outlining a roadmap for chemical production and use that maximizes chemicals' contribution to society while avoiding adverse environmental impacts.[5] As a part of this roadmap, chemicals that are 'safe and sustainable-by-design' across their life cycles are promoted, and greater consideration is taken for the adverse long-term and large-scale impacts chemical pollution has on the natural environment. These EU ambitions are strongly aligned with the United Nation's global Sustainable Development Goals (SDGs) to halt biodiversity loss, promote sustainable resource use, and ensure environmentally sound management of toxic chemicals and waste.[6] Together, these European and global goals promote sustainable chemical practices and require a systems approach to consider the totality of chemical pollution impacts in the context of ecosystems' natural limits to withstand negative chemical pressure.

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Due to the potential for chemicals to exert long-standing adverse effects on ecosystems, chemical pollution is recognized both as its own planetary boundary (introduction of novel entities) and to affect other boundaries.[7] While few chemicals are considered to have global effects, the combination of local-to-regional impacts across the wide range of released chemicals may irreversibly disrupt biodiversity at the global scale.[8,9,10] Therefore, a sustainable chemicals management requires consideration of local and regional chemical impacts.[11] Figure 1 outlines some of the planetary boundaries that chemicals affect, along with the adverse outcomes they contribute to. Persson et al. 2022 suggest that the safe operating space related to the planetary boundary for novel entities has been exceeded, mainly because the rate of chemical production has outpaced the global capacity to conduct chemical safety assessments and monitoring.[12] They report that the production, diversity, and global release of novel entities have consistently increased, while the state of chemical pollution and the related effects on ecosystems at the global level can currently not be fully quantified. Consequently, no boundary—at a planetary or other scale—is currently defined for chemical pollution's contribution to disruption of essential ecosystem functions. Relevant metrics are needed to link the cumulative chemical pressure to the capacity of ecosystems to absorb such pressure, and these need to be determined for explicit regions and times of chemical usage and ecological exposures to capture spatiotemporally differentiated ecosystem effects. Further, methods are needed to allocate the chemical pressure to actors contributing to chemical pollution to enable efficient chemical management and reduction of chemical pressure below levels that may cause irreversible adverse effects. However, such methods are currently lacking.

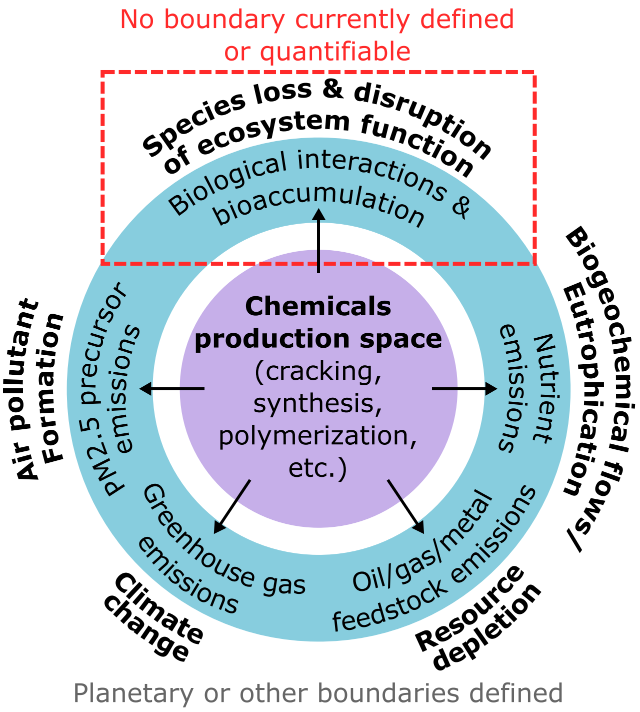

Figure 1. Overview of chemical contributions to planetary boundary threats and other adverse effects. $PM_{2.5}$ = particulate matter.

To address this gap, we introduce a conceptual framework for assessing chemical pollution in an absolute environmental sustainability context, and explore existing approaches that can be used as starting points. We then use practical examples from pesticide use in Europe to discuss challenges and ways forward to operationalize this framework to build the foundation for an eco-effective and sound management of chemicals.

2. METHODOLOGICAL STARTING POINTS

We propose that an absolute environmental sustainability assessment (AESA) framework should be developed to determine levels of chemical pollution pressure that should not be exceeded. Similar approaches have been proposed to assess life cycle impacts of various activities and sectors against finite environmental limits, including global-level limits represented by certain planetary boundaries, such as climate change.[13,14] However, no methods exist to evaluate absolute environmental sustainability for chemical pollution, nor have the methodological components and requirements for developing such an approach been clarified.

To determine thresholds that protect ecosystems against chemical exposure that may lead to irreversible changes in structure or function, we are interested in assessing how chemical pollution contributes to species loss and disruption of ecosystem functions (Figure 1). To develop an AESA framework for chemical pollution, we propose that three methodological steps should be considered. First, the cumulative chemical pressure needs to be quantified at the relevant spatiotemporal scales. Second, absolute environmental sustainability targets beyond which chemical pressure leads to irreversible adverse effects on ecosystems need to be identified at the appropriate scale based on ecological carrying capacities. Third, the chemical pressure needs to be linked to related carrying capacities to define a "safe space" for chemicals, which can then be allocated to individual chemicals, activities, and sectors to monitor sustainable practices for chemical use against science-based targets for chemical pollution. An outline of these methodological steps is presented in Figure 2.

2.1. Quantifying Chemical Pollution Pressure. The first step in implementing an AESA for chemical pollution is to determine the various pathways of chemicals, from chemical production and use to life cycle emissions, environmental fate, and corresponding ecosystem exposures and damages. To link chemical emissions to ecological impacts, the level of ecosystem damage should also address different organisms' and communities' response to chemical levels within the exposed ecosystems.[2,15] A generalized impact pathway for chemical pollution is illustrated in Figure 2.

Chemical footprinting approaches have been proposed to assess chemical impacts on ecosystems.[11,16] The concept of footprinting is to quantify the impacts of human activities on an area (e.g., carbon footprint from fossil fuel burning). By applying this approach to chemical emissions (either individually or across chemicals), the intensity of chemical pressure on ecosystems following environmental release can be determined. For example, chemical emissions can be related to species sensitivity distributions (SSDs), which reflect inter-species sensitivity to a compound and are frequently used to assess biodiversity impacts.[17] Zijp et al. 2014[16] conducted two case studies for chemicals emitted in Europe to determine cumulative impacts of mixtures, with exposure quantified from the concentration of released compounds across environmental compartments through multimedia fate models and ecological impacts quantified as the percent of species affected. In both case studies, the chemical pressure was aggregated over the

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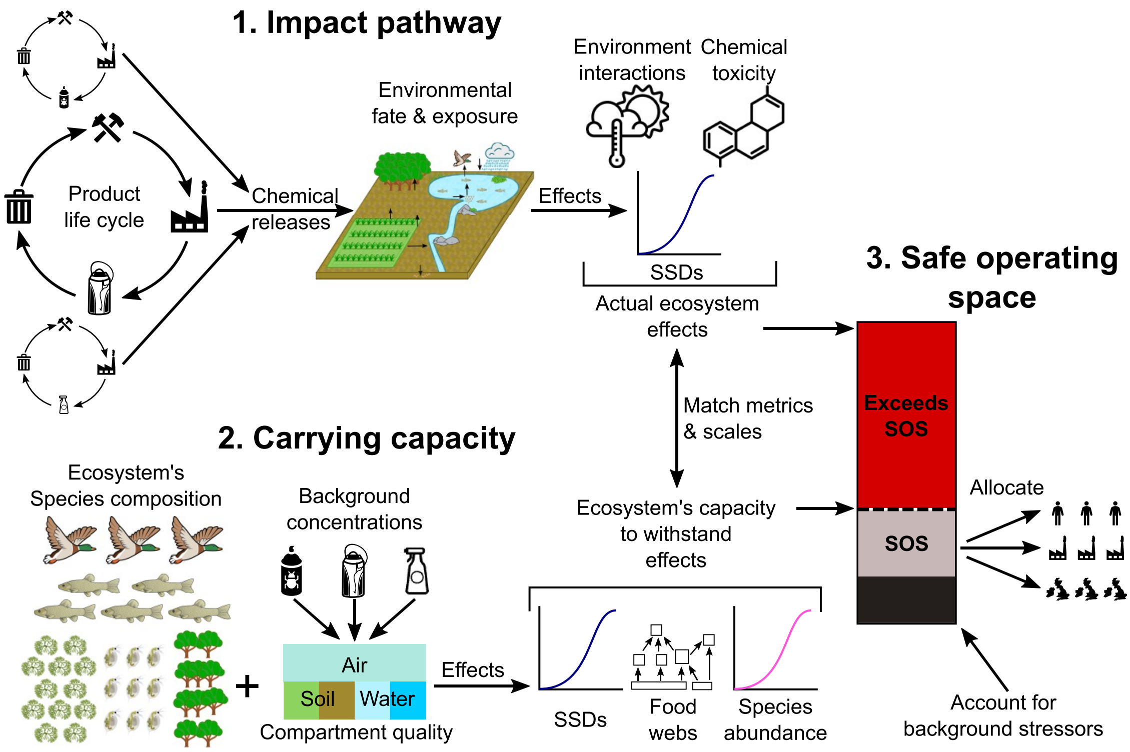

Figure 2. Proposed framework for assessing absolute environmental sustainability of chemical pressure. Chemical emissions can occur along all product and technology life cycle stages, including resources extraction, manufacturing, use, and end-of-life treatment. SSDs = species sensitivity distributions. Source allocation levels include different actors, including individuals, sectors, and nations.

environmental compartments, ultimately calculating the mixture toxic pressure as the multisubstance potential affected fraction of species (msPAF). This approach was also followed by Posthuma et al. 2020[19] in an analysis of 24 priority substances of EU-wide concern.

While these examples measured the expected cumulative impacts of chemicals on aquatic ecosystems, one limitation is that they do not link pollution levels to relevant emissions during the mixture components' life cycles (e.g., releases during chemical production). To assess chemical pollution in an absolute environmental sustainability context, a combination of life cycle thinking and human and ecological risk assessment is necessary to assess the intensity of chemical pressure and potential environmental harm.[11,18] Life cycle impact assessment (LCIA) starts from the emission inventory of all stages in a chemical, product or technology life cycle, and derives characterization factors (CFs) to express the relationship between these emissions and their environmental impacts based on mathematically represented cause-effect chains.[9,20] Bjørn et al. 2014[20] assessed the total pressure from chemical life cycle emissions on freshwater ecosystems in a case study for 173 compounds emitted at the country level in Europe and a case study of field emissions of pesticide use in Denmark.

While the discussed analyses represent starting points for chemical impact quantification, they also highlight some of the prevailing challenges. For example, spatially resolved multimedia mass balance models and time variability were not considered by Zijp et al. 2014,[16] and emissions data for European countries in Bjørn et al. 2014[20] were largely based on extrapolation from a country's GDP and chemical sales. Further, the calculated CFs are nonspatial, only describing generic global averages of species effects. Determining chemical pressure on an ecosystem should also extend beyond the level of a given effect and translate it into damages on genetic diversity (e.g., species loss) and functional diversity (i.e., damage on ecosystem functions). While LCIA methods and mixture toxicity pressure calculations represent viable approaches to determine chemical pressure, there are still many limitations to overcome in order to operationalize such methods for evaluating absolute environmental sustainability impacts of chemicals at the appropriate spatiotemporal scales.

2.2. Defining Ecological Carrying Capacities for Chemical Pollution. To link chemical usage and emissions to the limits of an ecosystem to withstand chemical pressure, absolute environmental sustainability targets for chemical pollution need to be defined. Numerous adverse effects from chemical pollution have been identified for both environmental health (e.g., loss of biodiversity[5]) and human health (e.g., increased disease burden[21]), and measures are required to determine related targets.[11] Figure 2 outlines the steps to develop such absolute environmental sustainability targets, which in many ways mirror the steps for quantifying chemical pressure (defining chemical effects on species, chemical fate in an ecosystem, etc.) but following a different perspective. Rather than calculating the chemical impacts on an ecosystem from a set of emissions, absolute environmental sustainability targets determine the capacity for an ecosystem to withstand chemical exposures.

To develop such targets, global or regional boundaries can be based on existing policies, expert opinions, identified through scientific literature review, or a combination of these approaches.[22] Many studies use planetary boundaries as targets, but analyses incorporating the introduction of a boundary for novel entities are comparatively scarce. Bjørn et al. 2020[14] reviewed 34 approaches for absolute environmental sustainability target development and found that only two studies included chemical pollution. Butz et al. 2018[23] set the global control variable for introduction of novel entities around a set of selected average emission intensities and scaled up to three times the current emission levels, while Meyer and Newman 2018[24] described Planetary Quotas for human activities that are derived from planetary boundaries, with chemical pollution set as a target of net imperishable waste at zero kg/year. However, both of these boundaries were defined around economically sustainable applications, and neither analysis was spatially resolved nor incorporated potential ecotoxicity effects into the proposed target.

Ecological carrying capacities represent the maximum persistent impacts an environment can sustain without impairing the integrity of the natural systems, and can serve as thresholds beyond which chemical pollution causes irreversible damage.[14,25] Compared to chemical impact quantification, approaches to quantify related carrying capacities are less developed. We focus on freshwater ecosystems as a starting point because chemicals are frequently released in this environmental compartment, the volume of the water in a region is straightforward to characterize, and aquatic ecotoxicity data are available for many substances.[17] One approach implemented by Bjørn et al. 2014[20] sets the volume of surface freshwater available (e.g., a catchment near an area of pesticide application) as the target.[20] In contrast, Zjip et al. 2014[16] set a policy-based target around the fraction of species above which the analyzed ecosystems were expected to be affected by chemicals to an irreversible extent, based on the level where 0.1% of species were affected, as determined from SSDs. While this approach does account for species effects, a challenge in relating chemical impacts to dilution capacity is that, when the spatial scale is larger (e.g., a country), the calculated dilution capacity may not be representative as the actual chemical impacts may be more focused within a single region (meaning the dilution capacity is overestimating the available target space). Further, limiting the calculated effects to species sensitivity does not account for ecosystem functions. Therefore, expanded methods are necessary to define appropriate targets for the high volume of chemicals emitted from innumerable sources (globally or regionally) across the diversity of ecosystems.[8,26]

2.3. Identifying and Allocating a "Safe Space" for Chemicals. By relating the chemical pressure to the potential for an ecosystem to absorb such pressure, it is possible to determine if the target for absolute environmental sustainability of chemicals has been transgressed. So long as the chemical pressure is below the cutoff for the ecological carrying capacity, the related chemical usage is within a so-called "safe operating space" (SOS).[7] However, parameters for defining the SOS at any scale for chemical pollution have not yet been defined.

To develop the SOS from the absolute environmental sustainability target (e.g., ecological carrying capacity), the space available for the specific chemicals under study should first be determined from the entire available target space occupied by both these and competing stressors. Competing stressors could be additional chemical classes or other types of environmental stressors like phosphorus load in a water body, contributing to its eutrophication with accompanying change in the carrying capacity for chemical pressure. After defining the SOS, the ratio between the actual quantified chemical pressure and the SOS derived from ecological carrying capacities can be derived. Generally, if the ratio is below 1, then chemical pressure is considered within the safe limits. Additionally, once the SOS is defined, a share of the available SOS can be allocated to individual actors contributing to the chemical pressure (e.g., chemical users, manufacturers, etc.).[27] The SOS development and allocation is the third step of the framework illustrated in Figure 2.

Some common methods for allocating the SOS to relevant actors include utilitarianism (distribution of environmental impacts should maximize the sum of welfare across actors),[28] egalitarianism (actors should be equal in terms of what is being allocated),[29] prioritarianism (maximize the sum of welfare such that a benefit has greater moral value the worse the situation of the actor to whom it accrues, e.g., a country had a historical injustice and thus gets a greater share of the SOS than other countries),[30] and sufficientarianism (equality matters less than all actors having "enough").[31] For determining the share of the SOS for a sector contributing to (or even exceeding) it, sharing principles need to be able to consider the value that different contributing entities (e.g., products or sectors) have for humans. Both utilitarian and prioritarian approaches can apply to individuals, countries, products, or different sectors by aiming to maximize the utility (contribution to economic value, contribution to happiness, etc.) that an industry or product can have to individuals. However, allocating the SOS according to these methods requires forming outcome-based sharing principles (e.g., increasing individual welfare) rather than determining the more attainable means to reach the outcome (e.g., equal resource distribution to increase individual welfare).[27] Therefore, utilitarian methods are challenged by a lack of methods and models to describe how welfare can be maximized among individuals, while prioritarian assessments require more outcome-based methods and data to determine the "worse situation" of the actors accruing the welfare.[32]

In contrast to utilitarianism and prioritarianism, the data needed for calculating equal per-capita sharing (meaning the SOS is allocated to individuals based on an equal right to the resource under study) is more straightforward, as it only considers the population of the geographic region under analysis. Ryberg et al. 2020[27] reviewed 18 studies allocating planetary boundary SOSs to actors and found that 34 different allocation principles were used. Across these studies, the country level was the most commonly allocated geographic scale, followed by the sector level. Most analyses followed an egalitarian allocation principle utilizing the equal per capita sharing of the SOS. However, while this review provides an overview of different allocation approaches taken in the literature, none of these studies included the allocation of a safe space for chemical pollution. Therefore, these allocation approaches need to be expanded to determine the SOS for chemical pollution (i.e., subtract background stressors) and distribute the SOS among actors contributing to chemical pressure in a given spatiotemporal setting.

3. CHALLENGES AND WAYS FORWARD

Several challenges across the different methodological steps have prevented development of absolute environmental sustainability methods for evaluating chemical pollution. These include availability of relevant data, incorporation of adequate spatiotemporal granularity, and determining the most relevant chemical, geographic, or sector levels for assessment.

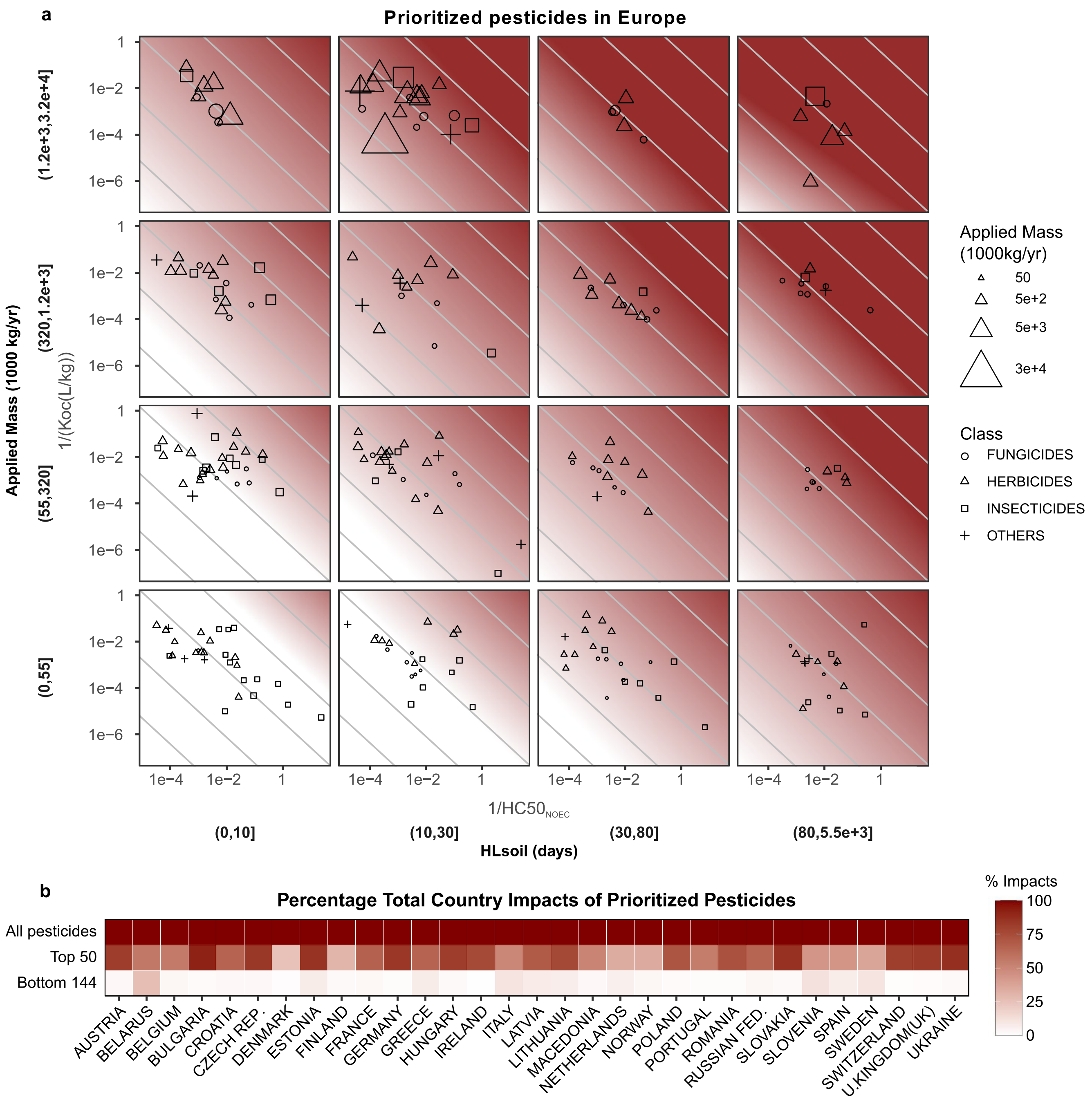

Figure 3. Prioritization of pesticides for chemical impact quantification in Europe. a) 255 prioritized pesticides. The outer *y*-axis bins the annual pesticide usage, and the outer *x*-axis bins the pesticide soil half-life. Each individual plot shows the $1/HC50_{NOEC}$ on the *x*-axis and the $1/K_{oc}$ on the *y*-axis. The size of each point reflects the cumulative applied mass per year. Pesticides farther in the top right of the overall figure have the greatest potential for ecosystem threat. b) The percentage of total chemical impacts per country in Europe covered by all 255 pesticides, the top 50 prioritized pesticides, and the bottom 144 pesticides.

Similar challenges have been identified that currently limit quantification of a planetary boundary for novel entities (e.g., need for global data sets with sufficiently high spatiotemporal granularity).[12] We will illustrate these challenges through a set of practical examples structured around pesticide use in Europe, where "pesticides" refer to the active ingredients in plant protection formulations. According to FAOSTAT data, global pesticide use nearly doubled between 1990 and 2018 (http://fao.org/faostat), and pesticide use is likely to increase with population growth and climate change.[33] Pesticides also encapsulate both the challenges and ways forward for implementing an AESA framework for chemical pollution. Agricultural pesticides have straightforward impact pathways (from direct field application to ecosystem exposure) compared to other chemical classes (e.g., chemicals in consumer products released into indoor environments), are well-regulated in many regions around the world, and have comparatively high data availability. However, the conditions

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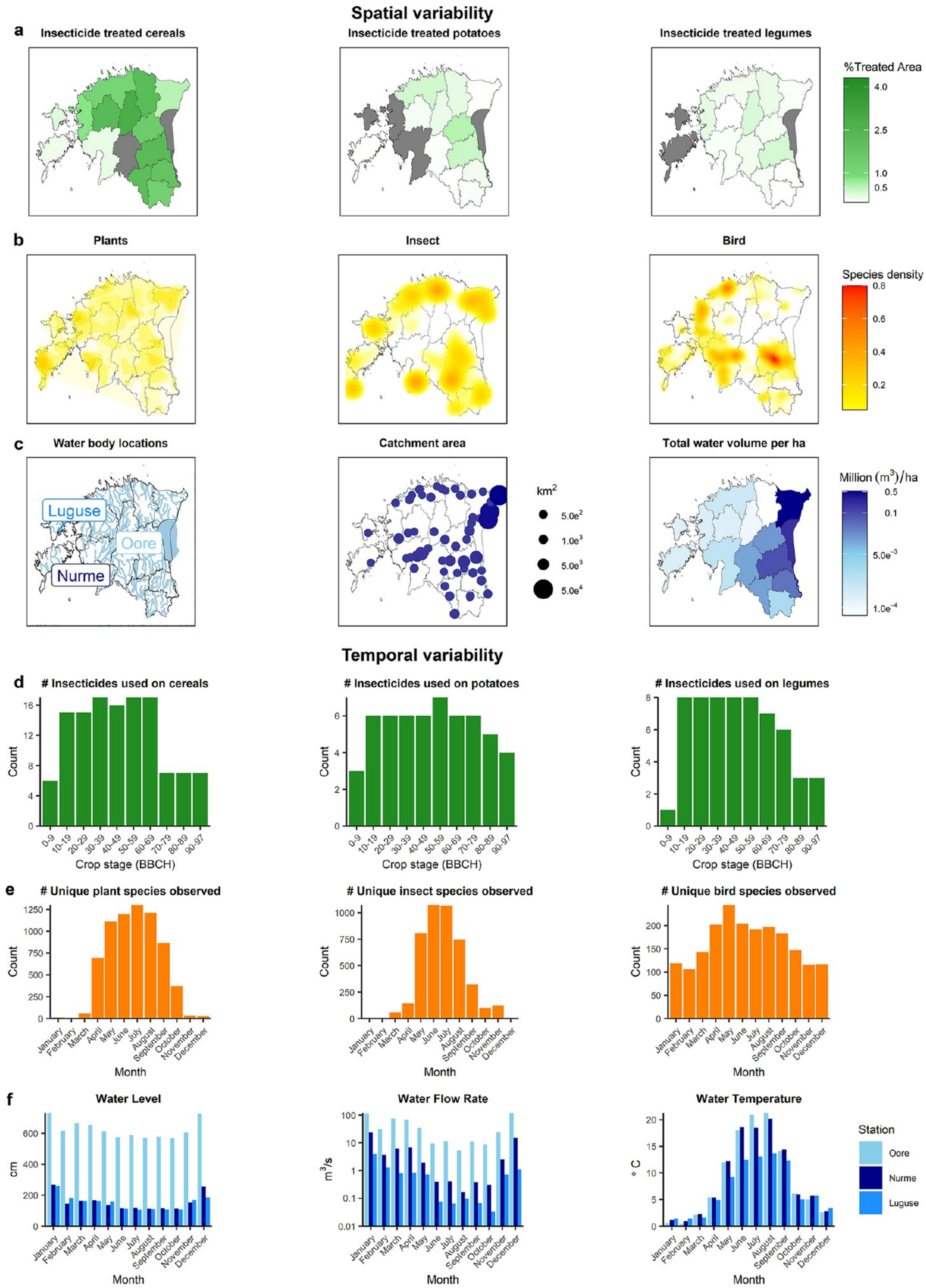

Figure 4. Spatiotemporal challenges in ecological carrying capacity calculation for Estonia in 2015. a) Percentage of total hectares for each county in Estonia that grows the respective crop and are treated with insecticides. Gray regions do not have that crop treated with that pesticide class. b) The density of unique species observations for each organism group across counties in Estonia. c) The spatial variability in water across Estonia, including locations of water bodies and hydrologic stations, catchment area, and total water volume per county. d) The number of insecticides that can be applied to each crop growth stage class (BBCH). e) The number of unique species observed each month in 2015. f) Water levels, flow rates, and temperatures measured at hydrologic sampling stations in Estonia in 2015 (corresponding to labeled stations in c).

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for their use (e.g., variable application times and patterns as a function of pest occurrence) create spatiotemporal challenges for their assessment.

3.1. Identifying Relevant Chemicals. Conducting AESA for all chemicals is not straightforward. Developing complete chemical emission inventories, elucidating appropriate effect endpoints, and allocating the SOS among the most relevant actors require copious data and modeling approaches. Prioritization methods can help identify those chemicals that pose the greatest threat to ecosystems. Through this, the compounds responsible for the majority of chemical pollution pressure can be identified, reducing the data requirements and associated assessment challenges. Once these methods are fully developed and chemical impacts are quantified at the appropriate level of spatiotemporal resolution, future research can use the relationship between chemical properties and impacts to identify features driving ecological damages from chemical pressure.

As an example, we prioritized 255 pesticides applied across countries in Europe for chemical pressure quantification and determined the percentage of the total chemical impacts covered by the top and bottom subsets of pesticides. From this priority list, we demonstrate that the top-prioritized pesticides explain the majority of total pesticide-related impact. By creating prioritized subsets of chemicals for analysis, the most relevant chemicals for a given spatial scale can be identified based on their potential to cause adverse ecosystem effects to help reduce data needs when quantifying chemical pressure. Figure 3 shows the results of this illustrative analysis. Details and full results on the data integration, prioritization, and impact quantification are found in SI Sections S-1−S-4. Additional discussion of chemical selection challenges (e.g., chemical interactions, metabolism) and suggested ways forward is found in SI Section S-5.

3.2. Spatiotemporal Considerations. Limitations in data availability, model refinement, and aggregation methods can affect spatiotemporal granularity for chemical pressure quantification and carrying capacity development. To outline some spatiotemporal challenges in carrying capacity development, we generated an example around pesticides applied in Estonia. We integrated publicly available data on regional, crop-specific pesticide usage, species density, and water characteristics for Estonia for the year 2015 (details in SI Sections S-6−S-13), with results presented in Figure 4.

There are several different spatial considerations for calculating regional impacts and related carrying capacities. Different crops are grown in different regions, and even for the same crop, different pesticides are used in variable quantities (Figure 4a). As seen through our example for Estonia, there is variability in species distribution and species richness across geographic regions, with a fairly even distribution of unique plant species observed, while the distribution of insect and bird species is sparser, with dense pockets of greater species richness (Figure 4b). This variability in species distribution and richness is important, because if pesticides are applied in a region with low species richness, then loss of one species may be significant compared to a region with greater species richness overall. Therefore, in addition to toxicity-based considerations of species sensitivity to compounds, species richness and ecosystem functions should be considered. One approach developed by Hoeks et al.[34] uses species-specific exposure-response models with population growth concepts to assess the effects of chemical exposures on mean species abundance. While this approach is more constrained by data availability than traditional SSD-based approaches, it shows promise for incorporating species richness into chemical effect endpoints. Other spatial features of a region like the locations of waterbodies and the available water volume also need to be considered as this affects the environmental fate and eventual dilution of applied pesticides per region (Figure 4c). For discussion of temporal differences identified in our case study (e.g., pesticide application times, water flow rate, species occurrence), see SI Section S-14.

To reduce data needs for chemical pressure quantification and carrying capacity development, the most relevant geographic regions and timeframes can be prioritized. For example, if freshwater ecosystems are most relevant for the compounds under study (as is the case with many pesticides), key watersheds likely to be heavily impacted by pesticide pollution (e.g., a watershed receiving multiple chemical emissions or a watershed with species that are particularly sensitive toward exposure to certain pesticides) can be prioritized rather than needing to characterize all surrounding regions a chemical is released in. Further, depending on when pesticides are applied and/or when the most sensitive species are present, the analysis can be focused on specific timeframes. Additionally, when allocating the SOS, background concentrations of the chemical under study may be present following emissions in different spatial regions. For example, if the area under study is downstream of an area where the same pesticide is used, then the remaining fraction of the upstream pesticide emission also has to be considered and subtracted from the available carrying capacity.

3.3. Aligning Metrics and Scales. To develop the outlined framework for chemical pollution, data need to be aligned so the calculated metrics and spatiotemporal granularity match between the quantified chemical pressure and related absolute environmental sustainability targets. This requires methods for data aggregation that do not lose relevance or interpretability. For example, if the pesticide emission data for Estonia resulted in chemical pressure quantified at the country level over the course of a year, then the carrying capacity also has to be developed at the country level and cover the whole year, meaning data may need to be aggregated. For a discussion of these challenges and ways forward in the context of the Estonia case study, see SI Section S-15.

In addition to aligning spatiotemporal granularity and aggregation levels, the metrics for each step have to match and be relevant for allocation of the SOS to relevant actors. For example, if the chemical pressure is quantified as the potentially affected fraction (PAF) of species in an ecosystem but the carrying capacity is presented as a dilution volume, then these metrics need to be aligned. This becomes more complicated when allocating the SOS to relevant actors. If the absolute environmental sustainability target is set based on dilution volume, then the share of the SOS allocated to actors can be designated in cubic meters of water per year. Further, when determining the available SOS for the chemicals under study, the background stressors (e.g., competing chemicals) that occupy the same SOS need to be calculated in such a way that they can be removed from the available dilution volume. A discussion of aggregation challenges for the SOS is provided in SI Section S-16.

3.4. Data Challenges. The most relevant limitation for implementing this framework for AESA of chemical pollution

Table 1. Data Needs, Challenges, and Ways Forward for Developing an Absolute Environmental Sustainability Assessment (AESA) Framework for Chemical Pollution Based on a Case Study of Pesticide Use in Europe

data needs	data sources and types	data challenge	potential ways forward
quantifying chemical pressure and developing a SOS: pesticide application data	pesticide usage data (e.g., FAOSTAT pesticide use data[a])	data reported in aggregate by country, year, and pesticide class (e.g., insecticides−carbamates), partly outdated and reporting sales instead of actual use	integrate data across country pesticide reporting agencies[b,c]
quantifying chemical pressure and developing carrying capacity: chemical fate data	chemical properties data (e.g., Pesticide Properties Database[d])	missing data (e.g., many chemicals do not have reported soil/water half-lives) and wide variability in reported values	complement with additional data sets (e.g., CompTox Chemicals Dashboard[e]) and incorporate predictive approaches[f]
quantifying chemical pressure and developing carrying capacity: species effects data	species sensitivity distributions data (e.g., Posthuma et al. 2019[g])	limited by *in vivo* ecotoxicity tests, do not account for species relationship and functions within ecosystems	incorporate *in vitro* bioassays to fill gaps (Neale et al. 2017[h]), incorporate mean species abundance approach (Hoeks et al. 2020[i])
quantifying chemical pressure, developing carrying capacity, and developing a SOS: land use data	agricultural land cover data (e.g., CORINE[j])	land cover descriptors in aggregate (fruit trees and berry plantations)	integrate with other land use resources (e.g., EarthStat[k]) and/or complement with country reports (e.g., Statistics Estonia[l])
quantifying chemical pressure and developing carrying capacity: species distributions data	species monitoring data (e.g., GBIF[m])	data primarily based on human observations, do not reference species' sensitivity/richness	merge across lat/longs to assess richness, integrate with data on vulnerable species (e.g., IUCN Red list[n])
developing carrying capacity: water characteristics data	water monitoring/characteristics data (e.g., HydroBASINS[o])	data are not temporally resolved for a given year, there may be inconsistencies between river and lake data sets	complement with country hydrologic reports (e.g., Estonian Weather Service[p])
developing a SOS: data for allocation	population data (e.g., FAOSTAT global population data[q])	a per capita approach is not sufficient for determining allocation to a company	upscale data from individual level (e.g., final consumption expenditure[r], green incentives[s])

[a]https://fao.org/faostat/en/#data/RP. [b]https://ec.europa.eu/eurostat/cache/metadata/en/aei_fm_salpest09_esms.htm. [c]https://www.eppo.int/ACTIVITIES/plant_protection_products/registered_products. [d]https://sitem.herts.ac.uk/aeru/ppdb/. [e]https://comptox.epa.gov/dashboard. [f]Scheringer et al. 2009.[35] [g]Posthuma et al. 2019.[17] [h]Neale et al. 2017.[36] [i]Hoeks et al. 2020.[34] [j]https://land.copernicus.eu/pan-european/corine-land-cover. [k]http://www.earthstat.org. [l]https://andmed.stat.ee/en/stat. [m]https://www.gbif.org. [n]https://www.iucnredlist.org. [o]https://www.hydrosheds.org/page/hydrobasins. [p]http://www.ilmateenistus.ee/?lang=en. [q]https://fao.org/faostat/en/#data/OA. [r]Ryberg et al. 2018.[13] [s]Hjalsted et al. 2020.[32]

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will be the data available. Each of the three steps is challenged by the state of the science with detailed information on chemical emissions, species effects, spatiotemporal features of chemical usage and ecosystems, and relevant allocation information scarce or nonexistent. For specific examples and expanded detail of these data challenges, see SI Section S-17.

There are two main ways forward: reduce data needs for each step and integrate underutilized and disparate data sets. We have already mentioned several approaches to reduce data needs at each methodological step, including chemical prioritization approaches and focusing analyses on regions and time scales for the most sensitive species/vulnerable ecosystems under study. While reducing data needs can address some challenges in our proposed framework, these methods can only be implemented with increased focus on data integration. There are numerous publicly available sources spread across agency repositories, policy documents, and the literature that could be used to begin addressing the challenge of data scarcity. Table 1 gives examples of the necessary data types for our illustrative AESA case study of pesticide pollution in Europe, potential sources for the methodological steps we outlined, some of the typical challenges for each data type, and possible ways forward. In addition to integrating across repositories, incorporating underutilized data types (e.g., *in vitro* data) and underexplored fields can help to fill some of the presented gaps, both in the data available and the methods to address the challenges outlined. Ultimately, integrating these data will require interpolation methods to address gaps in spatiotemporal species effects, chemical property, and chemical inventory data (e.g., kriging, machine learning), as well as advanced data extraction (e.g., web scraping, PDF extraction) and integration techniques (e.g., fitting variable data formats and ontologies, translating across numerous countries' native languages).

4. POLICY IMPLICATIONS AND OUTLOOK

Our outlined framework is the first step toward determining spatiotemporally resolved levels of chemical pollution as well as related carrying capacities in an absolute environmental sustainability perspective, which can help realize the assessment of local-to-global boundary transgressions for novel entities.[12] The Organisation for Economic Co-operation and Development (OECD),[37] United Nations,[38] and European Commission[39] have all developed outlooks and strategies calling for reduction of harmful chemicals in products, but a challenge in implementing sustainable chemical strategies is the ability to quantify and monitor the chemical pressure on ecosystems as a consequence of different chemical management activities.[40] Our approach will address this challenge for several reasons. First, the framework is designed to relate the actual chemical pressure on ecosystems to their carrying capacity, enabling direct progress measurement of pollution reduction strategies. Further, since the quantified chemical pressure covers life cycle emissions for a given product or technology, progress at all stages of chemical development and management can be considered to determine the necessary combination of pollution mitigation activities to reduce and maintain chemical pressure at sustainable levels. Green chemistry approaches are of growing interest to industries, businesses, and governmental organizations,[41] and our framework can be used to identify absolutely sustainable chemical replacements that minimize trade-offs and guide reduction of the chemical pollution impacts toward meeting absolute environmental sustainability targets. Finally, by allocating shares of the SOS for chemicals among relevant actors, individual actors' progress toward SDGs (i.e., goals for a sustainable development) can be measured. This provides a consistent framework that can be used to elucidate requirements for pollution managers across actors (e.g., individual farmers, companies) and geographic scales (e.g., advising regional planners, developing management strategies at the national level for cross-border catchments, e.g., Lake Peipus shared between Estonia and Russia) informing them not just what is better than the current practice but what is required to reduce the pressure to actually sustainable levels. This can also ease implementation of the criteria set by policy makers for stakeholders (e.g., chemical pollution targets for mitigation/reduction) who can base chemical production and design on their share of the safe operating space by incorporating the AESA framework into research and development workflows.

The use of benchmarks or thresholds to assess chemical pollution or other ecological stress is not new. An example is to compare predicted environmental concentrations (PECs) of individual chemicals to predicted no-effect concentrations (PNECs) for certain species.[42] However, such approaches do not consider carrying capacity-based effects of entire ecosystems that are cumulatively exposed to various chemicals, while keeping track of emission sources and release locations, but instead focus on specific species and make use of arbitrary "safety" factors. With that, these approaches are unable to link actual chemical pressure to available ecosystem-level safe operating space for chemical pollution and allocate this space back to contributing sources and actors, rendering our proposed AESA framework unique in its ability to address these aspects. Another example is to determine total maximum daily loads (TMDLs) of nutrient loading. TMDLs represent the maximum amount of a pollutant (e.g., nutrients, microbial contaminants) that can enter a waterbody while maintaining water quality standards, and the pollutant load is allocated among sources to guide control actions to achieve necessary water quality.[43] These water quality standards outlined by the United States Clean Water Act and used in the development of TMDLs could serve as a starting point for carrying capacity development in implementation of the AESA framework, but additional information related to ecosystem function would need to be incorporated. TMDLs also differ from the AESA framework because AESAs relate the actual chemical pollution pressure (including cumulative emissions) to carrying capacities for ecosystems of variable scope (e.g., waterbodies and/or terrestrial ecosystems), with consideration of emissions and related impacts along entire product and technology life cycles.

Our analysis identified areas where future funding activities need to focus to enable chemical pollution assessment in an absolute environmental sustainability context. First, new and better resolved data are necessary to capture relevant spatiotemporal granularity. This can be accomplished through expanded environmental monitoring (e.g., covering diverse ecosystems and geographic regions, identifying what time periods different species' offspring are born, etc.), chemical monitoring (e.g., collecting more detailed chemical usage data), and more consistent data reporting, both in what information is reported (e.g., universal pesticide application data reporting that includes the amount of applied active ingredient, crop growth stage, application time, etc.) and the format the data are provided in (e.g., easily accessible and

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downloadable tabular data files). Further, increased efforts to integrate existing published data are necessary. Agency documents containing data on chemical use are frequently published as lengthy PDFs, making discovery and utilization of relevant information challenging. An enhanced focus should be put on extracting pertinent information from these existing documents and providing it in an accessible way that enables data reuse and can better clarify data gaps.

We outline an analytical framework to assess absolute environmental sustainability of chemical pollution and discuss approaches to overcome the related challenges using pesticide use in Europe as an example. While other chemical classes may have greater data limitations (e.g., emissions data), other challenges are likely to be lower (e.g., industrial chemicals tend to be emitted year round, yielding fewer temporal variability challenges than pesticides). Therefore, this analysis of pesticides represents a uniquely challenging case. While global targets related to AESA have been assessed for several planetary boundaries (climate change, biogeochemical flows, etc.), numerous challenges have impeded progress in assessing chemical pollution, either globally or at other scales. The present work is the first step in moving toward sustainable chemical usage by addressing long-standing questions around incorporating spatiotemporal granularity into chemical impact quantification and carrying capacity development, and addressing challenges in data availability. With that, our outlined approach can serve as a methodological foundation to support policy ambitions and meet local-to-global goals for sustainable chemical use.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.est.1c06098.

Prioritization of pesticides at national scale (Sections S-1−S13), temporal challenges (Section S-14), metrics and scales alignment (Sections S-15 and S-16), and data challenges (Section S-17) (PDF)

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Notes

The authors declare no competing financial interest.

Biography

Dr. Peter Fantke is Professor and head of the Quantitative Sustainability Assessment (QSA) section at the Technical University of Denmark. In 2012, he obtained his Ph.D. in technology assessment and environment for work conducted at the University of Stuttgart (Germany) and University of Michigan (United States). His current research and teaching focus on assessing life cycle chemical emissions, far- and near-field exposures and impacts on humans and the environment, and evaluating alternatives to hazardous chemicals in products and technologies. He is director of USEtox, the scientific consensus model for characterizing chemical toxicity and ecotoxicity developed under the auspices of the UN Environment's Life Cycle Initiative. He coordinates global task forces under UN Environment on quantifying pesticide impacts and assessing impacts from exposure to toxic chemicals and fine particulate matter. Together with his colleagues, Dr. Michael Hauschild, Professor in life cycle assessment, and Dr. Marissa Kosnik, computational toxicologist, he is pioneering the development of methods for Absolute Environmental Sustainability Assessment (AESA) of chemical pollution.

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