An effect factor approach for quantifying the impact of plastic additives on aquatic biota in life cycle assessment

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Abstract
Purpose Plastic pervades now almost every aspect of our daily lives, but this prosperity has led to an increasing amount of plastic debris, which is now widespread in the oceans and represents a serious threat to biota. However, there is a general lack of consideration regarding marine plastic impacts in life cycle assessment (LCA). This paper presents a preliminary approach to facilitate the characterization of chemical impacts related to marine plastic within the LCA framework.

Methods A literature review was carried out first to summarize the current state of research on the impact assessment of marine plastic. In recent years, efforts have been made to develop LCA-compliant indicators and models that address the impact of marine littering, entanglement, and ingestion. The toxicity of plastic additives to marine biota is currently a less understood impact pathway and also the focus of this study. Relevant ecotoxicity data were collected from scientific literature for a subsequent additive-specific effect factor (EF) development, which was conducted based on the USEtox approach. Extrapolation factors used for the data conversion were also extracted from reliable sources.

Results and discussion EFs were calculated for six commonly used additives to quantify their toxicity impacts on aquatic species. Triclosan shows an extremely high level of toxicity, while bisphenol A and bisphenol F are considered less toxic according to the results. Apart from additive-specific EFs, a generic EF was also generated, along with the species sensitivity distribution (SSD) illustrating the gathered data used to calculate this EF. Further ecotoxicity data are expected to expand the coverage of additives and species for deriving more robust EFs. In addition, a better understanding of the interactive effect between polymers and additives needs to be developed.

Conclusions This preliminary work provides a first step towards including the impact of plastic-associated chemicals in LCA. Although the toxicity of different additives to aquatic biota may vary significantly, it is recommended to consider additives within the impact assessment of marine plastic. The generic EF can be used, together with a future EF for adsorbed environmental pollutants, to fill a gap in the characterization of plastic-related impacts in LCA.

Keywords Characterization factor · Ecotoxicity · Industrial ecology · LCA · Marine plastic · Plastic additives

1 Introduction
Plastic, with a wide variety of forms and application fields, has become an essential component of our daily lives. The global plastics industry has been growing dramatically since the beginning of massive plastic production in the 1950s (Geyer et al. 2017). Meanwhile, poor waste management and inappropriate human behavior have resulted in the ubiquity and profusion of plastic debris (Barnes et al. 2009). Mismanaged plastic waste can eventually end up in the marine environment through multiple pathways, including atmospheric and river transport (Lebreton et al. 2017), beach littering (Bravo et al. 2009), and sea-based activities such as aquaculture and fishing (Bugoni et al. 2001). Plastic debris has been observed on the world’s most remote islands and within every marine habitat (STAP 2011; do Sul and Costa 2014). It is estimated that 4.8–12.7 million metric tons of plastics enter the ocean per annum, and this figure will continue increasing sharply if there are no improvements in waste management (Jambeck et al. 2015). As the growing amount
of plastic litter is causing serious pollution in terrestrial and aquatic ecosystems, there is universal agreement that this issue needs to be addressed urgently (Koelmans et al. 2014).

Litter around the globe has been reported to affect over 3800 terrestrial, freshwater, and marine species (https://litterbase.awi.de/interaction_detail; Accessed: 20 January 2022). Specifically, the potential risks of plastic litter to human health and the environment have drawn increasing public attention in recent years (Koelmans et al. 2017). To tackle these concerns, various regional and international instruments and initiatives have been established, such as the International Coastal Cleanup and the Plastic Leak Project (Ocean Conservancy 2020; Quantis 2020). In the ocean environment, the impact of plastic debris can be divided into physical impacts (e.g., entanglement and ingestion) (Gall and Thompson 2015), chemical impacts (caused by the build-up or release of toxic substances) (Amec Foster Wheeler 2017), and other impacts such as dispersal via rafting and transport of alien species (SCBD 2016).

As regards the chemical impacts, plastic-associated chemicals pose potential hazards to marine organisms and can eventually affect human health through the food chain. Plastic contains a great diversity of functional additives incorporated during manufacture, such as antioxidants, stabilizers, and plasticizers (Hermabessiere et al. 2017). Plastic can also adsorb persistent organic pollutants from the environment (SCBD 2016). Wiesinger et al. (2021) established a comprehensive database of chemical substances used in plastic production based on an extensive review of industrial, scientific, and regulatory sources. The database covers over 10,000 substances, of which more than 2400 were identified as substances of potential concern. Recent studies have indicated that plastic additives may have significant toxicity impacts on aquatic species (Beiras et al. 2020; Capolupo et al. 2020).

Life cycle assessment (LCA) is a sustainability assessment methodology commonly used by decision-makers for quantifying the environmental impact of human activities (Woods et al. 2018). Life cycle impact assessment (LCIA), the third phase of LCA, links inventory data with specific impact categories and indicators with the aim of understanding the significance of the environmental impact throughout a product’s life cycle (ISO 14040 2006). As stated in the Medellin Declaration, the impact of marine plastic is not adequately addressed in the LCA methodology (Sonnemann and Valdivia 2017). Hence, there is an urgent need for LCA-compliant impact assessment models and characterization factors. The LCA community also recommends the development of species sensitivity distribution (SSD)-based models and metrics that can be used in LCIA (Woods et al. 2019). In the next sections, we first summarize the existing research on the impact assessment of marine plastic within LCA. Afterwards, we introduce the data collection and the EF calculation in detail. Finally, we discuss how the results of this work can make a contribution in practical contexts and put forward recommendations for further methodological development.

### 2 State of the art

A number of recent LCA studies have considered the potential amount of plastic littered into the sea. In a comparative LCA of carrier bags conducted in Spain, Civancik-Uslu et al. (2019) introduced a novel indicator to evaluate the impact of discarded waste in marine waters. Similarly, Stefanini et al. (2020) evaluated the impact of empty bottle littering in the Mediterranean Sea within an LCA study on pasteurized milk bottles. Regarding the impact of marine plastic on biota, Woods et al. (2019) proposed a preliminary EF approach for quantifying the entanglement of marine species in macroplastic debris. Starting from this approach, McHardy (2019) made significant improvements by developing region- and taxon-specific SSD models to better link marine plastic quantities to species entanglement rates. Saling et al. (2020) developed a midpoint characterization model for assessing the impact of microplastic ingestion by organisms.

Founded in 2019, the scientific working group MarILCA (Marine Impacts in LCA) is actively supporting the development of methodologies to incorporate marine impacts in LCA, with a focus on marine plastic litter (Boulay et al. 2021). In the modeling framework proposed by the group (Woods et al. 2021), the ecotoxicity of plastic-associated chemicals will be assessed separately from the impacts caused by the presence of polymers. In line with this framework, Lavoie et al. (2021) developed EFs regarding the physical impact (resulting from the intake by organisms) of micro- and nanoplastics (MNs) in aquatic environments. Data were acquired from experiments based on virgin polymers (i.e., without consideration of additives). EFs were derived for a common scenario (the ALL EF using all data points), a best possible scenario (the BEST EF using almost only chronic EC50s), and seven other subgroups according to particle size, particle shape, and polymer type. Lavoie et al. (2021) also highlighted the need for future ecotoxic EFs that account for the impact of additives and the impact of toxic substances adsorbed onto plastic debris.

One suitable option to address this research need is presented in USEtox, a scientific consensus model for characterizing human- and ecotoxicological impacts of chemical emissions (Rosenbaum et al. 2008). USEtox can be applied in the context of LCA, and its main purpose is to compare alternatives instead of calculating absolute risks (Fanette et al. 2017). At midpoint level, a USEtox characterization factor provides an estimate of the potentially affected fraction of species (PAF) integrated over time and volume per
unit mass of a chemical released. The model results can be further extended to determine endpoint effects expressed as the potentially disappeared fraction of species (PDF), applying a translation factor of 0.5 (Jolliet et al. 2003). The SSD-midpoint is HC50EC50 and it denotes the concentration at which 50% of species are exposed above their EC50 values (Fantke et al. 2017). In the current USEtox database (USEtox version 2.12, https://usetox.org/), ecotoxicity EFs are available for some additives (e.g., bisphenol A and dibutyl phthalate). However, as USEtox EFs are derived using effect data for freshwater species only, the toxicity impact of these additives on marine biota is not considered.

The methodological review shows that some LCAs have addressed marine littering impacts and attempts have been made to quantify macroplastic entanglement and microplastic ingestion within LCIA. However, the toxicity of plastic-related chemicals to biota is not yet considered in any impact assessment methods associated with marine plastic. Inspired by Lavoie et al. (2021), this study focuses on the ecotoxicity of plastic additives and aims to reflect the environmental significance of these substances. Results of recent aquatic ecotoxicity tests were collected for a subsequent additive-specific EF development.

3 Methods

3.1 Data acquisition

A literature search was conducted to collect relevant data on the toxicity effect of plastic additives on aquatic species. Information was acquired from the search engines ScienceDirect, Google Scholar, and Web of Science. Relevant publications were identified from peer-reviewed journals using groups of keywords combining “plastic additives,” “plastic chemicals” with “ecotoxicity,” “toxicity,” “impact,” or “effect.” Moreover, articles mentioned in these publications were further analyzed if they provided useful test results. Data were collected applying the following selection criteria:

- Ecotoxicity tests conducted in recent years (2016–2021)
- Ecotoxicity tests with detailed information on experimental conditions
- Ecotoxicity tests with quantitative results such as EC50s and NOECs
- Ecotoxicity tests focusing on one specific plastic additive

Recent ecotoxicological studies were considered if they provide detailed information on the experimental context and quantitative outcomes for the EF calculation. However, many existing studies assessed the combined effect of additives and polymers or focused on leachates containing various chemicals. These studies were not considered because their results are not suitable for this additive-specific EF development. Moreover, when a study contained information on multiple additives, species, or test endpoints, each combination was considered as a separate input value. All extracted data points were compiled into a separate Excel file, and a further data quality assessment was carried out during the EF calculation. Consequently, some effect data were eliminated, and the EFs for certain additives were considered as unsatisfactory outcomes (see “Sect. 4.2” for details).

3.2 Data analysis and processing

The collected data points were classified according to the additive, species, test endpoint, and exposure duration. The exposure type of each input value was identified based on the USEtox approach, and the identification was distinguished between vertebrates, invertebrates, and algae (Table 1).

As the main goal of this study is to assess the ecotoxicity of additives in line with the approach applied for virgin MNP particles in Lavoie et al. (2021), the USEtox approach was adopted as the basis for the EF development. The underlying data for “USEtox recommended” characterization factors must cover at least three trophic levels, normally represented by algae, crustaceans, and fish (Fantke et al. 2017). According to this requirement, sufficient ecotoxicity data are available for eight additives in the database (Table 2). The CAS Registry Number and major function of each additive, as well as information on compatible polymers sourced from Wiesinger et al. (2021), are also provided in the table for easier orientation.

In the USEtox approach, an acute-to-chronic ratio is used to extrapolate chronic values from acute data. Similarly, two types of extrapolation factors were applied in this study, converting acute EC50s to chronic EC50s, chronic NOECs to chronic EC50s, respectively (Table 3). These were extracted from a recent study, which provided a set of robust extrapolation factors for different species groups (Aurisano et al. 2019). The extrapolation factors for fish were applied for amphibians, and sub-chronic values were considered chronic. After the extrapolation of data, all EC50 values were converted into a standard unit of mg/L. For reported values expressed in molar concentration (μM), the

| Group    | Acute     | Sub-chronic | Chronic  |
|----------|-----------|-------------|----------|
| Vertebrates | <7 days   | ≥7 days; <32 days | ≥32 days |
| Invertebrates | <7 days   | ≥7 days; <21 days | ≥21 days |
| Algae     | <3 days   | -           | ≥3 days  |

Table 1 Criteria for the classification of ecotoxicological tests as acute, sub-chronic, or chronic (Fantke et al. 2017)
3.3 Effect factor calculation

The USEtox approach was adopted for the EF calculation as follows (Eqs. 1 and 2):

$$EF = \frac{0.5}{\frac{HC50_{EC50}}{EC50}}$$

(1)

$$\log_{10}HC50_{EC50} = \frac{1}{n} \times \sum_{i=1}^{n} \log_{10} \left( \frac{EC_{50,i}}{1000} \right)$$

(2)

with

- $EF$: Ecotoxicological effect factors for aquatic ecosystems [PAF·m³·kg⁻¹]
- $HC50_{EC50}$: Geometric mean of chronic EC50s [kg·m⁻³]
- $EC_{50,i}$: Concentration at which 50% of the test organisms of species $i$ are affected [mg·L⁻¹]

When a species is represented by more than one data point, the $EC_{50,i}$ value for that species equals the geometric mean of all available EC50s. Apart from the additive-specific EFs, a generic EF was derived based on all data points without exclusion of any value. The idea behind this EF is to gain an insight into the environmental significance of plastic additives. In addition, an SSD was generated for this EF to provide information on the species and phyla represented in the compiled data. Regarding additive-specific EFs, SSDs were generated solely for bisphenol A and dibutyl phthalate due to the limited number of species (no more than five) represented for other additives. The “ssdtools” package in R, proposed by Thorley and Schwarz (2018), was applied to plot the SSDs based on a log-normal distribution. In addition, uncertainty is given with the 95% confidence interval (CI) of each EF, and the 95% CI calculation was done on $HC50_{EC50}$ values using the R package “DescTools”.

4 Results and discussion

4.1 Compiled data

Data for the EF development were obtained from 23 peer-reviewed journal articles. Our database covers 27 additives in total and contains detailed information on the experimental condition of each data point (see Table S1 in Online Resource). In summary, a total of 95 data points were extracted from ecotoxicity tests on 21 aquatic species (14 freshwater and 7 marine) (Fig. 1).

4.2 Effect factors

The SSD for the generic EF is presented here for quick visualization of the gathered data (Fig. 2). The generic EF is represented by 21 species from 9 phyla. For those species represented by several input values, the converted EC50s may have a wide range. The dots representing each species in Fig. 2 refer to the corresponding $EC_{50,i}$ values. Additive-specific EFs were initially calculated for eight additives, but 4-nonylphenol and benzophenone-1 were excluded because of poor data quality from a statistical perspective. There is a huge disparity in the $EC_{50,i}$ values for 4-nonylphenol (see Table S4 in Online Resource), and the EF for benzophenone-1 has an excessively wide 95% CI range (see Table S5 in Online Resource). Of all additives
considered (Table 4), triclosan has the highest EF with over 3000 PAF·m³·kg⁻¹. This result is in line with the study of Beiras et al. (2020), which defines triclosan as a “very toxic” functional additive. In contrast, EFs for bisphenol A and bisphenol F are under 100 PAF·m³·kg⁻¹, suggesting comparably lower levels of ecotoxicity effect on biota. Such ranking can eventually help the plastics industry in the choice of additives that are least harmful or innocuous to aquatic life. For instance, it would be better to reduce the use of triclosan in the plastics industry by finding less toxic alternatives.
As mentioned above, Lavoie et al. (2021) derived the BEST EF (72.90 PAF·m³·kg⁻¹) and the ALL EF (82.28 PAF·m³·kg⁻¹) to quantify the toxicity impact of MNPs on aquatic biota from a holistic viewpoint. Likewise, a generic EF was generated in this study (about 320 PAF·m³·kg⁻¹) (see Table S6 in Online Resource). Direct comparison of EFs derived in different studies is not appropriate due to the differences in research focus, data sources, and extrapolation factors used. However, since plastic additives were not considered in Lavoie et al. (2021), the generic EF developed in this preliminary work suggests that additives can be more toxic than pure polymers and thus deserve serious consideration within the impact assessment of marine MNPs.

### 4.3 Limitations of the approach

This study is a first attempt to quantify the toxicity impact of plastic additives in the marine environment, for which a systematic assessment is currently missing in the LCIA toolbox. However, the proposed EF approach is still at an early stage, and there are several factors that have to be considered alongside the results. Firstly, due to a general lack of effect data, ecotoxicity data for freshwater species were also included to calculate the EFs. Secondly, as shown in Fig. 1, the majority of the compiled data are acute values which need to be extrapolated, and the calculation of 95% CIs did not consider the proportion of extrapolated values. Finally, as the compiled data come from diverse sources, uncertainty can arise from differences in toxicity test methods, exposure concentrations, etc.

To close the gap in the underlying data of this EF development, future ecotoxicological studies are needed to provide data for more marine species as well as for other commonly used plastic additives. Chronic toxicity data are particularly in demand, so that the calculated EFs can rely less on extrapolated values. More consistent, standardized chronic data could also enable the dots representing each species to fit better in the SSDs generated for the generic EF and for individual additives.

Regarding the calculation of the generic EF, an important limitation lies in the fact that the mass of additives released into the marine compartment was not included, which is essential for a better understanding of the environmental significance of these pollutants. This aspect was not considered herein owing to a lack of relevant information, especially from industrial data sources. Further research might explore how to assign weight factors to different additives by investigating their amount and leaching behavior. It is also worth noting that the additive-specific EFs, calculated based on the USEtox approach, can be used for comparative purposes but not for describing absolute toxicity risks.

### 4.4 Suggestions for the way forward

The outcome of this study contributes to the impact assessment of marine MNPs. The impact of virgin polymers has been addressed by Lavoie et al. (2021), and this study goes one step further by including the impact of plastic additives. Future studies should attempt to quantify the impact of marine MNPs as a vector for environmental contaminants as well as for invasive species. To complete the impact characterization of MNPs, we also need fate factors and exposure factors for polymers and associated chemicals. In this respect, Saling et al. (2020) proposed a fate model focusing on the fragmentation and degradation process of microplastics in the marine environment. The USEtox model contains fate and eco-exposure factors for five of the eight additives investigated here (4-nonylphenol, bisphenol A, dibutyl phthalate, nonylphenol, and triclosan), quantifying their dispersion in various environmental compartments (air, soil, freshwater, and marine) and their dissolved fraction in freshwater respectively. At present, some researchers from MarILCA are working on the development of fate and exposure factors for MNPs.

One major challenge identified for further research is the interactive effect between polymers and additives. This phenomenon has been proven by recent studies. Li et al. (2020) observed antagonistic toxicity effects between polystyrene microplastics and dibutyl phthalate on the marine copepod *T. japonicus* for both acute and chronic reproduction tests. Conversely, polyethylene fragments and benzophenone-3 exhibited synergistic effects on both lethal and sublethal toxicity to the freshwater crustacean *D. magna* (Na et al. 2021). As regards the pollutants adsorbed from the environment, Bellas and Gil (2020) demonstrated that the presence

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**Table 4** Calculated effect factors (EFs) with 95% CI ranges and associated HC50s

| Additive     | HC50_{EC50} [kg·m⁻³] | EF [PAF·m³·kg⁻¹] | 95% CI ranges  |
|--------------|----------------------|------------------|----------------|
| Bisphenol A  | 8.82E-03             | 56.71            | (22.17–145.06) |
| Bisphenol AF | 1.48E-03             | 338.05           | (73.49–1555.04)|
| Bisphenol F  | 1.53E-02             | 32.78            | (7.36–145.97)  |
| Dibutyl phthalate | 4.36E-03     | 114.70           | (27.95–470.70) |
| Nonylphenol  | 3.51E-03             | 142.49           | (13.94–1456.74)|
| Triclosan    | 1.57E-04             | 3188.80          | (687.02–14,800.75)|
| The generic EF | 1.54E-03        | 324.61           | (100.83–1045.05)|

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of polyethylene microplastics increased the toxicity of chlorpyrifos to the marine copepod *A. tonsa*. Similarly, the presence of polystyrene particles led to increasing toxicity of triphenyltin chloride to the freshwater algae *C. pyrenoidosa* (Yi et al. 2019). The mechanisms of such interactions are differing and still less understood. Comprehensive analysis and cautious interpretation are essential in defining the combined ecotoxicity of polymers and associated chemicals, since there are often discrepancies between calculated and measured values when it comes to the ecotoxicity of mixtures (Gade et al. 2012).

The harmonization of different assessment methods is of vital importance to ensure their comparability and soundness. Toxicity effects of MNPs on biota are affected by various parameters such as particle size, particle shape, and polymer type (Miloloža et al. 2021). Regarding this issue, Koelmans et al. (2020) made a great start by developing rescaling methods to improve the alignment of approaches adopted in microplastic research, correcting for differences in particle size range, concentration unit, and threshold effect data used in SSDs. To avoid potential double-counting of marine plastic impacts in LCIA, it is necessary to have a meaningful combination of methods that focus on different size classes (e.g., macro, micro, and nano), particle shapes (e.g., pellets, beads, and films), and impact pathways (e.g., entanglement, ingestion, and ecotoxicity). Further discussion is needed about whether such an all-embracing impact assessment is necessary and sensible. In other words, consensus building processes among model developers, LCA practitioners and other stakeholders can be foreseen. Although decisions may vary among different products or processes, achieving an optimum balance between complexity and simplicity would be beneficial.

5 Conclusions

Marine plastic is now a global issue of great concern, yet its environmental impacts are not adequately addressed in LCA. In recent years, attempts have been made to quantify several specific impacts such as marine littering, entanglement in macroplastics, and ingestion of microplastics. However, there is still a lack of quantification methods regarding the toxicity of plastic-related chemicals to marine biota. To fill this gap, the proposed EF approach brings together recent ecotoxicity data to develop EFs for plastic additives. Based on the USEtox methodology, EFs were derived for six commonly used additives. While triclosan shows extremely high toxicity to aquatic species, bisphenol A and bisphenol F are considered less toxic. The generic EF shows that the effect of additives is likely to be significant in the impact assessment of marine MNPs and should thus be included. This EF can be used together with the BEST EF proposed by Lavoie et al. (2021) and a future ecotoxicity EF considering plastic particles as a vector for other adsorbed contaminants. Further ecotoxicity data are expected to expand the coverage of plastic additives and marine species for this EF approach. The interactive effect between polymers and additives remains to be further explored. Additionally, collaborative research efforts are required for a comprehensive impact characterization of marine plastic and its integration into the LCA framework.

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Data availability The datasets generated and analyzed during the current study are available in the Supplementary Information.

Declarations

Competing interests The authors declare no competing interests.

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