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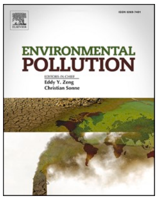

Ecotoxicity effect factors for plastic additives on the aquatic environment: a new approach for life cycle impact assessment☆

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ABSTRACT

All plastic contains additives. Once in the environment, these will start to leach out and will expose and harm aquatic biota, causing potentially lethal and sub-lethal toxic effects. Even though life cycle assessment covers the toxic impacts of several thousands of chemicals, models to assess the toxic impacts of plastic additives are only emerging. We gathered 461 data points from the literature (266 for freshwater and 195 for marine ecosystems) for 75 species belonging to 9 different phyla. The endpoints effective concentration and lethal concentration, no observed effects concentrations and lowest observed effect concentration tested in acute and chronic exposure, were harmonized into chronic values by applying extrapolation factors. The collected data points covered 75 main plastic additives. This allowed us to calculate 25 Effect factors, 19 for single chemicals and four for overarching categories (alkylphenols, benzophenones, brominated flame retardants and phosphates. In addition, we calculated an aggregated effect factor for chemicals that did not fit in any of the previous groups, as well as a Generic effect factor including 404 gathered data points. The estimated potentially affected fraction (PAF) for the single additives varied between 20.69 PAF$\cdot$m$^3\cdot$kg^{-1} for diethyl phthalate and 11081.85 PAF$\cdot$m$^3\cdot$kg^{-1} for 4-Nonylphenol. The factors can in future be combined with fate and exposure factors to derive a characterization factor for toxicity caused by additives in aquatic species. This is an important advancement for the assessment of the impacts of plastic debris on aquatic species, thus providing information for decision-makers, as well as guiding policies for the use of additives, ultimately aiming to make the plastic value chain more sustainable.

1. Introduction

All plastic products contain additives aiming to enhance the mechanical, chemical, and physical properties of the products (Callister and Rethwisch, 2009). The additives are chemical substances integrated during manufacturing and provide different functions (Wiesinger et al., 2021). For example, stabilizers prevent deterioration of the plastic, discolouration and molecular weight change (Wypych and Wypych, 2020), and plasticizers improve the flexibility of the material (Callister and Rethwisch, 2009). Stabilizers, flame retardants, plasticizers, fillers and colourants are the most common polymer additives (Kühn et al., 2020).

More than 2500 additives were identified in the global market (Wiesinger et al., 2021). These chemicals have attracted attention due to the growing amount of plastic debris released into the ocean with consequential leaching of these additives and potential impacts on the biota (Markic et al., 2020). The additives are not chemically bound to the polymers and can leach to the aquatic ecosystem (Bridson et al., 2023; Viljoen et al., 2023). They have been detected in the aquatic ecosystem, as well as in different organisms that were exposed to these chemicals (Luo et al., 2022; Tanaka et al., 2020). In the ecosystem the exposure of species to additives takes place via ingestion of microplastics or additives bioaccumulated in prey species, as well as inhalation and dermal uptake from the ambient water (Koelmans et al., 2014; Takada, 2019). This exposure causes a range of potentially adverse effects, such as growth inhibition of microalgae (Tato et al., 2018), reductions of fertilization and reproduction in mussel species (Rolton et al., 2022), as well as increased mortality of fish species (Moreman et al., 2017). Some

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additives are already restricted in some countries due to their potential for endocrine-disrupting properties (Conti et al., 2021).

Aiming to assess damages associated with the life cycle of products or processes there is the methodology called Life Cycle Assessment (LCA) accredited by the International Organization for Standardization (ISO) (ISO, 2006), quantifying multiple impacts in each life cycle phase, from raw material acquisition to final disposal (i.e., cradle-to-grave). One part of LCA is the so-called life cycle impact assessment (LCIA) (Hauschild and Huijbregts, 2015). Within LCIA a range of impact models (e.g., for climate change, land use or toxicity) are used, indicating the potential consequences for the environment per unit of emission (e.g., 1 kg of CO_2 or 1 kg of toxic substance released) (Hauschild and Huijbregts, 2015). Within the toxicity category, LCIA includes effects caused by hazardous substances on both ecosystem quality and human health (Casagrande, 2018; Rosenbaum et al., 2008; Woods et al., 2021).

LCIA indicators, in general, are expressed as characterization factors (CF) per unit of environmental intervention, in this case, the intervention is the additives in the aquatic biota. The CF includes a fate factor (FF), an exposure factor (XF) and an effect factor (EF), which represent, respectively, the substance emissions to and distribution in the ecosystem, interactions of the chemicals with the aquatic biota, and the effects resulting from this interaction (Rosenbaum et al., 2008).

Despite growing attention in the public space, the impacts of plastic pollution are rarely covered. Models to cover the range of impacts that plastic debris can cause are in their infancy and include the physical effects of micro- and macroplastic (Boulay et al., 2021; Høiberg et al., 2022; Lavoie et al., 2021; Woods et al., 2019) and a first approach for EFs from additives in aquatic ecosystems (Tang et al. (2022). This approach calculated EFs for ecotoxicological effects caused by six chemical additives acting as stabilizers, plasticizers, antioxidants or biocides in the aquatic ecosystem. We aim to expand the number of covered additives and thus contribute to the advancement of LCIA by refining and expanding the sets of effect factors previously available.

2. Methodology

We followed the modelling procedure outlined by USEtox (Rosenbaum et al., 2008), the consensus model for toxic impacts within the LCA community, which includes both data collection (step 1) and the calculation of effect factors (step 2).

2.1. Data collection and compilation

Ecotoxicity tests quantify the magnitude of the adverse effects of chemical agents on different species of living organisms (Klaassen, 2008). In the LCIA context, the calculation of EFs is based on the dose-response factors for groups of species. We, therefore, searched for ecotoxicity data provided by tests which exposed aquatic species to plastic additives and reported the dose-response factor.

To search for data we conducted a literature review on Google Scholar, Scopus, and Web of Science and US EPA ecotox knowledgebase by using a combination of different keywords, namely "additive* AND "toxicity" AND "plastic". In a second phase of the literature review we narrowed our research using the functions and the names of substances, such as "plasticizers" AND "toxicity" AND "plastic"; "flame retardants" AND "toxicity" AND "plastic" aiming to increase the number of precise data points for those additives already included.

The chemical toxicity reported as a dose-response factor is commonly indicated as EC50, the effective concentration at which 50% of a population shows an effect (e.g. growth inhibition, reproduction failure), LC50 (lethal concentration for 50% of a population), Lowest Observed Effect Concentration (LOEC) and Non Observable Effect Concentration (NOEC). Dose-response factors can also be indicated for the concentration at which 20% and 10% of the population is affected, EC20, LC20, EC10 and LC10, respectively.

We collected 366 new data points, in addition, to the 95 data points previously provided by Tang et al. (2022). The data collected includes the name of the additives, species tested, assessed toxicological endpoint, exposure duration, units of the values, and the reported dose-response factor (see Table S1 in Supplementary Information 2 (SI2)). PubChem® (2023) and ECHA, 2023 provided further information on chemicals, such as the Chemical Abstracts Service (CAS) registry number, the unique identifier of the chemical substance, their major functions as a plastic additive, molecular weight, and their main chemical category.

2.2. Data analysis and processing

Ecotoxicity effect factors in LCIA are species-generic. Since data is not available for each species and each ecosystem, the species that do have data available are acting as proxies for other species, i.e., the impact calculated based on a selected set of species is assumed to be the effect on the entire ecosystem quality.

We classified the species tested into their phyla and trophic levels, such as *i*) primary producers, *ii*) primary consumers, *iii*) secondary consumers and *iv*) decomposers. We checked the number of data points gathered for each additive corresponding to different trophic levels, dose-response factors and exposure duration. Additives tested in more than three trophic levels were used to calculate single EFs, the others were aggregated into groups from the same chemical category (e.g. benzophenones, phosphates, phthalates, alkylphenols and brominated flame retardants) to calculate an EF. Synonyms with the same CAS number, such as Dibutyl phthalate and -n-butyl phthalate were also grouped.

Studies report a diversity of dose-response factors representing the ECx, LCx, median inhibition concentration (ICx), LOEC and NOEC. These indicators are representative of the tested endpoints, such as reduced mobility, reduced growth or reproduction rate, mutations, behavioural changes, and changes in biomass or photosynthesis rate and mortality. To expand the available data basis we used all dose-response factors. That means we integrated data points for acute and chronic exposure, lethal and sublethal effects, as well as the combination of potential ecotoxicity on species from marine and freshwater.

For the integration of different data points and harmonization into chronic exposure duration and EC50, we applied the extrapolation factors calculated by Aurisano et al. (2019), shown in Table S5, SI2. In this harmonization process, we converted the acute exposure which causes mortality (LC50) into chronic EC50. In addition, endpoints represented by LOEC were merged and expressed as EC10-equivalents (EC10eq); one study reported the concentration-effect as the Lowest Observed Adverse Effect Level (LOAEL) which is equivalent to LOEC. Finally, for the EF calculation, we omitted 55 endpoints related to acute exposure of primary producers with no extrapolation factor available.

As a result of data harmonization, the species-specific data points were expressed as chronic EC50, which represents the concentration of the additives at which 50% of the species displays an effect (e.g. embryo growth, reproduction, mortality) due to chronic exposure (Rosenbaum et al., 2008).

2.3. Effect factors calculation

Aquatic ecotoxicity effect factors were calculated by applying the average equation provided by USEtox (Rosenbaum et al., 2008), shown in Eq. (1).

$$EF_{\text{ecotox}} = 0,5 / HC50_{\text{chronic EC50}} \tag{1}$$

EF_{ecotox} is an aquatic ecotoxicological effect factor, expressed as a potentially affected fraction of species (PAF) integrated over volume per unit mass of a chemical emitted (PAF m^3. kg^{-1}). The hazardous concentration of additives for 50% of the species (i.e. HC50) was calculated by the geometric mean of the gathered and harmonized chronic EC50 data points. Estimation of HC50, as well as the EFs for ecotoxicity, has to be representative of at least three trophic levels aiming to meet the USETox requirement (Rosenbaum et al., 2008). We calculated EFs for single additives that meet this requirement and also calculated EFs for overarching categories of additives.

The generic EF was calculated using all data points for all additives. For this, we determined the geometric mean of the species-specific chronic EC50 which was used to determine the generic geometric mean HC50 for the whole ecosystem.

The determination of our EFs was compared to those previously calculated by Tang et al. (202) by qualitative indexes. The EFs were classified into: (N) new – calculated only by this study; (S) substantially new - recalculated applying more than 50% of new data points; (M) marginally new - recalculated with less than 50% additional data points compared to Tang et al. (2022); (T) remained the same EF reported by Tang et al. (2022).

Furthermore, we determined the Species Sensitivity Distribution (SSD), showing the different levels of sensitivity of the species exposed to the chemicals (Del Signore, 2015). Aiming to show the most and least sensitive species, we performed analyses for different additives characterized by at least five species (Payet, 2004), using the R-4.3.0 software and the *ssdtools* package based on the data points of the chronic EC50 log-normal distribution (Thorley and Schwarz, 2018).

2.4. Statistical analysis

We applied the 95% confidence interval (CI) for the determination of the lower and upper limits of uncertainty associated with the geometric mean of HC50s and with the determined EFs. Furthermore, We identified in our database potential factors contributing to uncertainties in our results. Some factors are associated with differences in the test conditions such as types of exposure (acute and chronic), the endpoint tested, the dose-response factor, as well as the sensitivity of the different species exposed to the chemicals. In addition to this, the harmonization process of all gathered data points into chronic EC50 can potentially add a level of uncertainty to the results. For this reason, an uncertainty analysis was performed based on the AMI (Assessment of the Mean Impact) (Payet, 2004).

It is common in LCIA to mix endpoints, which from the biological point of view can add a level of uncertainty. This is because when the studies are performed in the same conditions (e.g. exposure, chemical and species) the lethal and sublethal effects are caused by different concentrations. Owing to this fact, we recalculated the EFs applying only sublethal effects for single additives meeting the requirements of at least three trophic levels to analyse whether this mix influences our results.

3. Results

3.1. Database of ecotoxicity of additives

The database (Table S1, SI2) encompasses 75 additives categorized as alkylphenols, benzophenones, bisphenols, brominated flame retardants (BFRS), chlorinated phenols, citrate esters, phosphates, phthalate, and polycyclic aromatic hydrocarbons (PAHs) and “other” (Table S2, SI1). Additives are commonly applied for more than one function. According to the data collected, the ecotoxicological tests focused on four main functions: (*i*) plasticizers (44%), (*ii*) stabilizers (21%), (*iii*) flame retardants (19%) and (*iv*) pesticides (16%).

The toxicity of these additives was tested in 75 aquatic species of nine different phyla: Proteobacteria, Ochrophyta, Haptophyta, Chlorophyta, Cnidaria, Mollusca, Arthropoda, Echinodermata and Chordata. Among all the gathered 461 ecotoxicity data points, 266 belong to freshwater species and 195 to marine species. The most tested trophic level is primary consumers (55%), followed by secondary consumers with 24%, primary producers (20%) and finally decomposers (2%) (see Fig. 1).

The number of data points gathered for each chemical tested in each phylum, the type of exposure and the dose-response factors are described in detail in Table S3, SI2.

In terms of types of exposure, overall, acute tests represent the majority of the studies, 85%, and chronic tests 15% (see Fig. 2A). Also, studies most commonly reported toxicity as EC50 and LC50 (77%) in all four different trophic levels, see Fig. 2B.

The harmonization process of data points into chronic EC50 is displayed in Table S4, SI2. In general, 404 of the data points were extrapolated, while 57 data points were omitted. The data points omitted were those for primary producers because of a lack of extrapolation factors for acute NOEC, LOEC, EC10 and LC10 to this trophic level. We omitted these factors instead of applying extrapolation factors

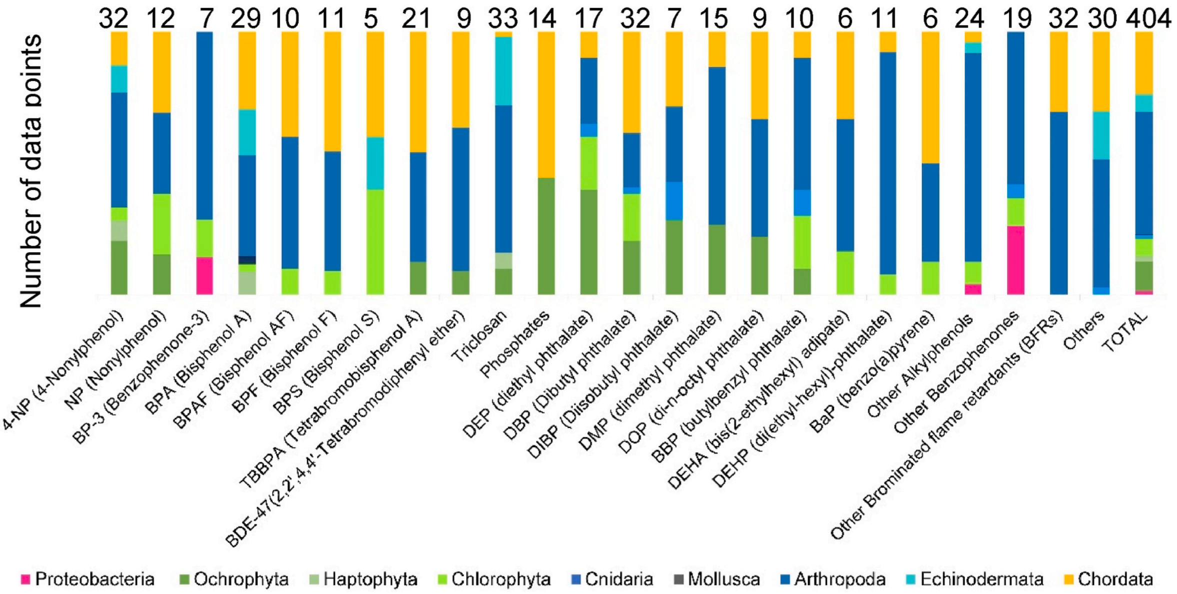

Fig. 1. Number of data points on the ecotoxicity caused by each single additive and groups of additives as well as the total tested in 9 different phyla: Proteobacteria, Ochrophyta, Haptophyta, Chlorophyta, Cnidaria, Mollusca, Arthropoda, Echinodermata and Chordata. Shades of different colours represent the data availability for each trophic level: pink: decomposers; shades of green: primary producers; shades of blue: primary consumers; yellow: secondary consumers. (For interpretation of the references to colour in this figure legend, the reader is referred to the Web version of this article.)

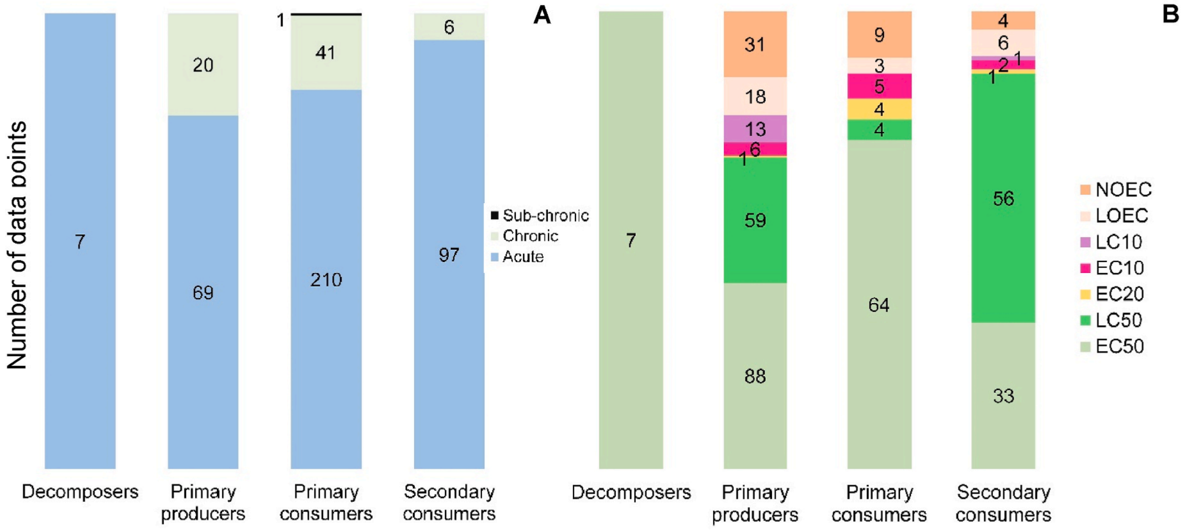

Fig. 2. Number of data points collected in studies according to the test conditions applied to the different trophic levels of species (Decomposers, primary producers, primary and secondary consumers) **(A)** acute and chronic exposure **(B)** Dose-response factors EC50, LC50, EC20, EC10, LC10, LOEC/LOAEL and NOEC.

from other methods/sources aiming to derive consistent and reliable data points for the calculation of HC50 and EF calculation.

3.2. *Effect factors*

Our collected data support the calculation of 25 EFs, encompassing 75 chemicals and synonyms, for example, dibutyl phthalate and di-n-butyl phthalate; DOP (dioctyl phthalate) and DOP (di-n-octyl phthalate) (see Table 1). The calculation process and results of HC50, and EF as well as the uncertainties associated with the results are presented in Table S6 in SI2 for the single and grouped additives. The Generic EF calculation process is in Table S7 in SI2.

In general, among the determined EF, there are 19 which express the ecotoxicity associated with individual substances, four EF are for substances grouped such as other alkylphenols, benzophenones, brominated flame retardants, phosphate, and one for additives grouped as others as well as the Generic EF. Compared with the ones previously determined by Tang et al. (2022), there are 17 EFs which are new, five are substantially new; two are marginally new and one remained the same as reported by these authors. The comparison of values, as well as the number of data points applied for the calculation, can be seen in more detail in Table S8 in SI2.

The EFs for single substances vary between 20.69 PAF·m^3·kg^{-1} for diethyl phthalate to 11081,85 PAF·m^3·kg^{-1} for 4-Nonylphenol. The second highest EF is for Triclosan, followed by BDE-47. A comparison between the EFs related to the main groups of chemicals shows that flame retardants have the highest EF (42314.83 PAF·m^3·kg^{-1}) and Benzophenones have the lowest (47.57 PAF·m^3·kg^{-1}).

Table 1

Results of HC50$_{\text{chronic EC50}}$ [kg·m^{-3}] and EF [PAF·m^3·kg^{-1}] from this research compared to those calculated by Tang et al. (2022) and the USEtox_3.0beta (2020) database for freshwater species.

Category	Additives	This study		Tang et al. (2022)		USEtox_3.0beta (2020)	
		HC50	EF	HC50	EF	HC50	EF
Alkylphenols	4-NP $^{(N)}$	4.51E-05	11081.85	n/a	n/a	n/a	n/a
	NP $^{(M)}$	3.52E-04	1419.57	3.51E-03	142.49	n/a	n/a
	other Alkylphenols$^{(N)}$	2.54E-04	1969.63	n/a	n/a	n/a	n/a
Benzophenone	BP-3 $^{(N)}$	2.90E-03	172.35	n/a	n/a	n/a	n/a
	Others Benzophenones$^{(N)}$	1.05E-02	47.57	n/a	n/a	n/a	n/a
Bisphenol	BPA $^{(S)}$	1.42E-03	351.84	8.82E-03	56.71	n/a	n/a
	BPAF $^{(T)}$	1.48E-03	338.05	1.48E-03	338.05	n/a	n/a
	BPF $^{(M)}$	1.66E-02	30.18	1.53E-02	32.78	n/a	n/a
	BPS $^{(N)}$	8.80E-03	56.81	n/a	n/a	n/a	n/a
	TBBPA $^{(N)}$	6.57E-04	760.86	n/a	n/a	n/a	n/a
Brominated flame retardant	BDE-47 $^{(N)}$	1.71E-04	2929.45	n/a	n/a	n/a	n/a
	other BFRs$^{(N)}$	1.18E-05	42314.83	n/a	n/a	n/a	n/a
Phenol	Triclosan $^{(S)}$	7.66E-05	6529.99	1.57E-04	3188.80	1.78E-04	2809.17
Phosphates		3.92E-03	127.64	n/a	n/a	n/a	n/a
Phthalate	DEP $^{(N)}$	2.42E-02	20.69	n/a	n/a	n/a	n/a
	DBP $^{(S)}$	2.24E-03	222.88	4.36E-03	114.70	n/a	n/a
	DOP $^{(N)}$	2.02E-03	246.95	n/a	n/a	2.23E-02	22.46
	DMP $^{(N)}$	3.59E-03	139.15	n/a	n/a	n/a	
	DIBP $^{(N)}$	4.72E-03	105.96	n/a	n/a	1.31E-03	382.48
	BBP $^{(N)}$	1.23E-03	406.32	n/a	n/a	n/a	n/a
	DEHA$^{(N)}$	3.14E-03	159.45	n/a	n/a	n/a	n/a
	DEHP$^{(N)}$	3.04E-04	1643.36	n/a	n/a	n/a	n/a
Polycyclic aromatic hydrocarbon	BaP $^{(N)}$	1.85E-04	2703.81	n/a	n/a	n/a	n/a
	others $^{(S)}$	4.16E-04	1201.02	n/a	n/a	n/a	n/a
	Generic EF$^{(S)}$	4.96E-04	1007.38	1.54E-03	324.61	n/a	n/a

Note: (N): New EF; (S): Substantial new; (M): Marginally new; (T): Tang et al. (2022) explained in detail in section 2.3.

SSDs to individual additives were calculated for 4-NP, NP, BPA, TBBPA, Triclosan, DBP, DEP, DIBP, DMP, DOP and BBP, as well as for the generic EF (for data, see Table S9 and Table S10). The results of substance specific SSDs are shown in Fig. S4 to Fig. S14 in SI1, while the generic one is shown in Fig. 3.

Furthermore, the factors were recalculated to analyse the uncertainty due to the mix of lethal and sublethal effects for the single additives such as 4-NP, NP, BP-3, BPA, BPAF, BPF, BPS, TBBPA, BDE-47, BaP, other Alkylphenols as well as for Generic EF are presented in Table S11 and Table S12 in SI2, respectively.

In general, 63 data points reported as mortality were omitted from recalculation. This analysis showed that, in general, mortality does not influence much on the results, see Table S13 in SI2. Most of the recalculated factors remained in the same order of magnitude. For instance, Nonylphenol went from 1419.57 PAF·m^3·kg^{-1} to 1215.43 PAF·m^3·kg^{-1}. An exception of drastic variation was noticed for two phthalates, the EF for 4-NP dropped from 11081.85 PAF·m^3·kg^{-1} to 5445.55 PAF·m^3·kg^{-1} and for BaP it highly raised from 2703.81 PAF·m^3·kg^{-1} to 7344.17 PAF·m^3·kg^{-1}.

4. Discussion

4.1. Fitting the new effect factors approaches into LCIA

25 EFs have good enough data to be classified as recommended according to USEtox 2.0 which demands that the ecotoxicity must have been tested in at least three trophic levels. For other brominated retardants, the EFs are only indicative as they encompass two different trophic levels instead of three in the toxicity data (Fantke et al., 2018). The new approaches integrated into LCIA in terms of the EFs for single substances allow input of individual substances in the inventory phase and impact assessment of their single contribution to toxicity. As a result, this facilitates the comparison of levels of ecotoxicity between substances and compares competitive products for the same function (Rosenbaum, 2015). For the EFs calculated for groups of substances, they can be useful for unspecified additives which are also covered by the generic EF. Both substances grouped and the generic EF can be applied to model the toxicity in cases of “unspecified/unidentified and/or unknown substances” known as NIAS (non-intentionally added

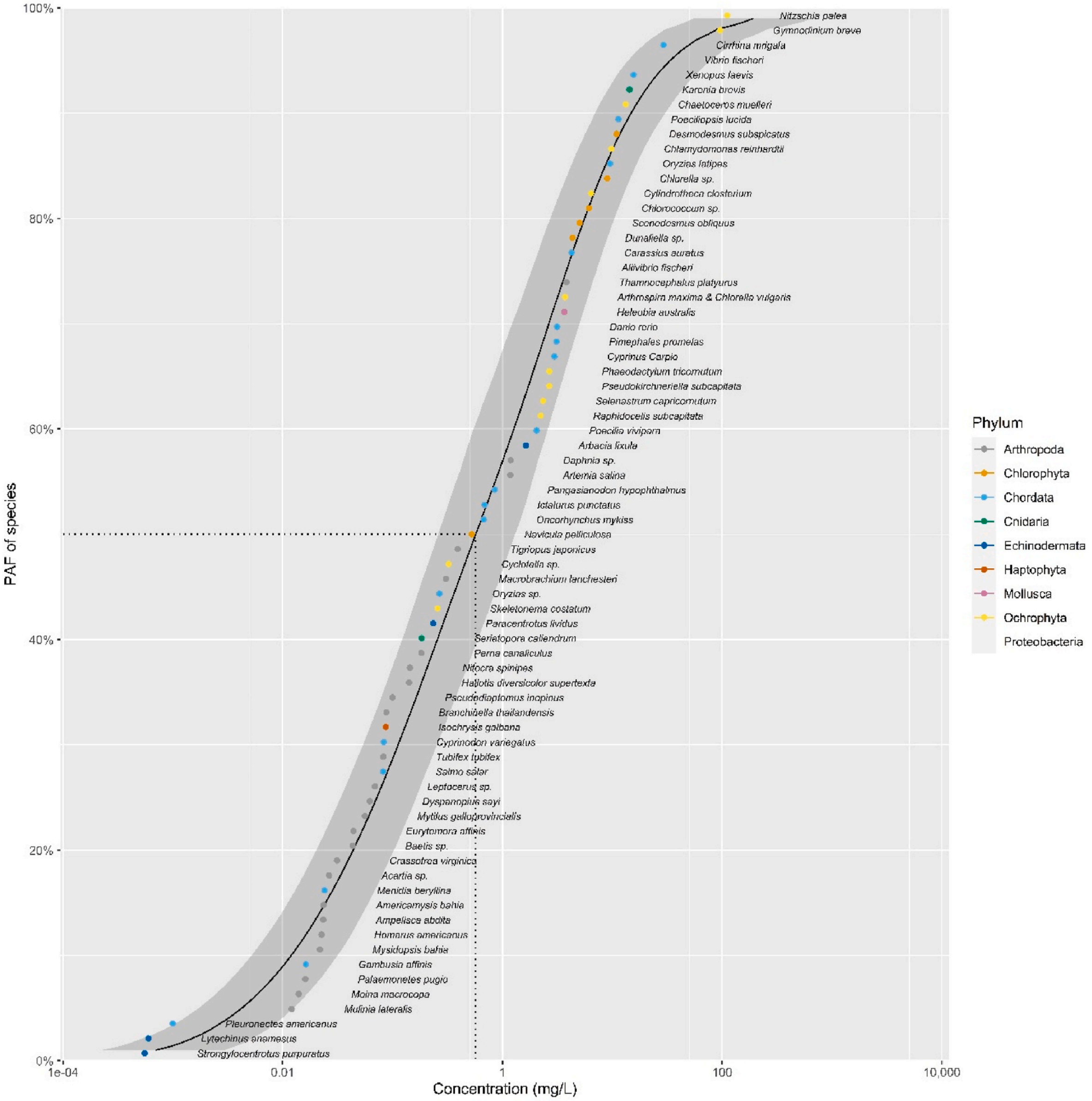

Fig. 3. Species sensitivity distribution (SSD) for the generic EF integrating the ecotoxicity dose-response for all the tested chemicals on 75 aquatic species of 9 phyla. Each dot represents the reported values of species-specific EC50 due to chronic exposure to the additives.

substances) (UNEP, 2023).

These options of EF applications maximise effectiveness depending on the substances analysed by the model. The combination of different factors covers a broader range of substances and enables the assessment of the impact of additives in general. The LCIA models increase precision and reliability while covering more substances, as well as applying more data on ecotoxicity effects on aquatic species. However, improvements are essential as currently the risk of not having factors to assess potentially toxic products for the aquatic ecosystem is the main uncertainty. Then, the application of ecotoxicity caused by additives considering their uncertainties allows the assessment as far as known (Fantke et al., 2018).

4.2. Uncertainties associated with the results

Available literature data for calculating ecotoxicological EFs for additives tested in more than three trophic levels in aquatic species are limited. Owing to this fact, to determine the EFs we integrated data reporting different test conditions, which can add a level of uncertainty to the results. Uncertainty is related to the data integration on the concentration of additives leading to lethal and sublethal effects on species, and extrapolation of acute and chronic exposure and different dose-response factors. In terms of the harmonization process despite the Owsianiak et al. (2023) recommendation to switch from using EC50 and HC50s to HC20 based on chronic EC20 equivalent, 77% of our collected data points indicate the concentration of the substances affecting 50% of the individuals. Other concentration-effect factors represented summed 23% (3% each for EC10 and LC10, 1% for EC20 1%, LOEC 6% and NOEC 10%). As a result, we extrapolated all data points collected into chronic EC50 aiming to maintain the level of reliability.

The concentration of additives leading to lethal and sublethal effects, from a biological perspective, could overestimate or underestimate the values of HC50 and EF, for species tested at the same conditions (e.g. exposure period and chemical). In addition to this, while sub-lethal effects (e.g., cell and embryo growth, reproduction, malformation and others) may be reversible, lethal effects are not. For this reason, we analysed the uncertainty related to a mix of lethal and sublethal effects and showed that in general, this mix of effects does not influence the finalresults (Table S14, SI2).

In the results, the highest variations were reported by 4-Nonylphenol (4-NP) and BaP (benzo(a)pyrene). The recalculated EF for 4-NP dropped from 11081.85 $\mathrm{PAF \cdot m^3 \cdot kg^{-1}}$ (mix of lethal and sublethal effects) to 5445.55 $\mathrm{PAF \cdot m^3 \cdot kg^{-1}}$ (only sublethal effects) and the EF for BaP has grown from 2703.81 $\mathrm{PAF \cdot m^3 \cdot kg^{-1}}$ to 7344.17 $\mathrm{PAF \cdot m^3 \cdot kg^{-1}}$. The variation is probably related to the decrease in several data points and the level of sensitivity of the species to the chemicals. The calculation of the hazardous concentration of chemicals for 50% of the species encompasses different levels of sensitivity of species and our results showed that the integration of lethal and sublethal effects is not a major issue related to the uncertainty on the EFs. In general lower trophic level species are more sensitive and most of our data points are composed of primary consumers (58%) from the phyla Cnidaria, Mollusca, Arthropoda and Echinodermata. The sensitivity of the species to the chemicals can also be associated with the life stage of the tested species, but the life stage was not reported in all the papers we gathered data and this information was not taken into consideration for the calculation of HC50s and EFs.

Based on the uncertainty analysis, we recommend the EFs consider all data points to be integrated into LCIA. Even when applying the harmonization factors, the number of data points has high importance for the reliability of the results and a calculation of EFs as much representative as possible to the ecosystem. Furthermore, in this study, the integration of lethal and sublethal data points allowed to have data for the calculation of 19 EFs for single additives covering at least three trophic levels, while applying only sublethal effects the data met the requirement to the calculation of only 10 EFs.

Analysis of the 95% CI ranges showed that the main factors contributing to the variation of the lower and upper limit ranges are mostly the number of data points, as well as the difference between minimum and maximum chronic EC50s/species (Δ), see Table S14 in SI2. Among the factors contributing to the uncertainty of the results, the number of data points seems to be most important, as long as the generic EF has a high Δ for chronic EC50/species (110.95 $\mathrm{mg\ L^{-1}}$) and still a low range of confidence interval due to the high number of data points (404). In contrast, the highest range of 95% CI is for BaP (from 1.45 to 5057821.52 $\mathrm{PAF \cdot m^3 \cdot kg^{-1}}$) with only 6 data points and at the same time a low Δ for chronic EC50 per species = 6,09 $\mathrm{mg\ L^{-1}}$).

Overall, our results are in line with the previous studies which estimated EFs reported by Tang et al. (2022) and for freshwater in the USEtox_3.0beta (2020), see Table S9, SI2. Compared to Tang et al. (2022) the BPA (Bisphenol A), NP (Nonylphenol) and Generic EF were the EFs which changed one order of magnitude. A comparison between our EFs and those reported by USEtox shows a difference for DOP (di-n-octyl phthalate) which changed one order of magnitude. A difference can also be seen for Tricloclan comparing the EFs reported by this study, USEtox and Tang et al. (2022), but all the values are in the same order of magnitude. These variations in the values can be explained by the variation in several data points applied for the calculation of the EFs as well as the sensitivity of the species.

4.3. Limitations and recommendations for future research

In the literature review, we found data on toxicity in aquatic species (from freshwater and marine ecosystems) exposed to 75 additives applied in the plastic industry. This is a small number compared to the large number of substances reported as additives applied in the plastic industry and exposed to aquatic species (Aurisano et al., 2021; UNEP, 2023; Wiesinger et al., 2021). Most of our data are related to plasticizers, stabilizers, flame retardants and pesticides. More data on ecotoxicity caused by additives as well as colourants and substances which promote the biodegradation of polymers are still lacking to provide new EFs. Our results also show that most of the ecotoxicity tests conducted are acute exposure. A higher number of lab tests, mainly related to chronic exposure are required to represent the ecotoxicity of a larger number of additives on both marine and freshwater species.

Furthermore, the plastic industry applies a mixture of substances to achieve the required properties in the products. This, in addition to the NIAS (non-intentionally added substances) may range from thousands of potentially emitted chemicals to the aquatic ecosystem. In the general context of pollution, aquatic systems are highly vulnerable due to accumulation and persistence of mixed chemicals (Pfister and Raptis, 2014; Qin et al., 2015). Data on the effects on the organisms due to the interaction between these substances are still lacking in the literature and is not encompassed by this study. This means that the assessment of the effects on biota due to exposure to several different substances should be improved for future assessment of multi-substance PAF (msPAF) (Larsen and Hauschild, 2007).

The presented EFs represent the exposure of single chemicals directly to species. Substances acting as a mixture in the organisms or the biomagnification of substances are not considered. There is a potential for some additives to biomagnify via trophic transfer through the food web, and to accumulate in higher-trophic-level organisms, including humans (Lynch et al., 2023; Saley et al., 2019). Although in this study, neither the effects caused by a mixture of substances nor biomagnification are considered, we recommend considering these factors in future research.

In general, the new EF calculated by this study, as well as the EFs reported by Tang et al. (2022) and those already integrated into the USEtox, supply factors for ecotoxicity according to the framework designed by the MarILCA working group. However, we still have limitations on the calculation of the fate and exposure factors to determine a characterization factor. For the determination of the fate factor the physicochemical properties of the chemicals have to be taken into consideration (Henderson et al., 2011; Kwon et al., 2017). This is because the leaching of the additives and the exposure of chemicals to biota depend on these properties. The solubility and hydrophobicity, for example, will influence amount of additive released into the water (Andrade et al., 2021). The model of the fate and exposure factor will also depend on the properties of the polymers and the environmental conditions (Aminot et al., 2020; Suhrhoff and Scholz-Böttcher, 2016).

When determining new approach on LCIA it is of importance flow of chemicals which match from the life cycle inventory (LCI) to the LCIA methods (Sanyé-Mengual et al., 2022). Nevertheless, as the advances on this topic are dependent on data available in the literature, mismatches might be found when developing ecotoxicity indicators for plastic additives further. In this case, the Generic EF will always be an alternative representing the ecotoxicity of additives in general, as well as when modelling NIAS substances.

5. Conclusion

The new approach developed by this study contributes to modelling EFs for a large number of additives. Despite the uncertainties associated with the results, this is an important advancement in the derivation of the characterisation factor for aquatic ecotoxicity of additives in life cycle impact assessment. The interpretation on LCA results provides information of the environmental charge of additives released from plastic pollution in the analysis of the plastics life cycle. Advances on this topic contribute to the plastic life cycle assessment which can identify the toxicity associated with the additives as well as estimate their chemical footprint.

Author statement

Naiara Casagrande: Literature search, Data analysis, Writing-review and editing the original draft. Carla Silva: Literature search, Methodology, Writing, review & editing. Francesca Verones: Conceptualization, Methodology, Writing – maps, review & editing. Paula Sobral: Conceptualization, Methodology, Writing – review & editing. Graça Martinho: Conceptualization, Review and revision to the text.

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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.

Data availability

I have shared the link to my data at the SI1 and SI2

Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.envpol.2023.122935.

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