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Additive inclusion in plastic life cycle assessments, part II

Review of additive inventory data trends and availability

H. Logan^{1,2}  | S. DeMeester² | T. F. Astrup¹  | A. Damgaard¹ 

¹Department of Environmental and Resource Engineering, Technical University of Denmark, Lyngby, Denmark

²Department of Green Chemistry and Technology, University of Ghent, Ghent, Belgium

Correspondence

Heather Logan, Department of Environmental and Resource Engineering, Technical University of Denmark, Bygningstorvet, Building 115, 2800 Kgs. Lyngby, Denmark. Email: healo@env.dtu.dk

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Abstract

Plastic additives are as essential as polymers to the production and performance of plastic materials. Additive content can vary in composition and functionality depending on the product, producer, application, and production method. Such variation may be a barrier to achieving high-quality recycling and planning for plastic circular economy futures. Yet, as found in Part I, although there is increasing awareness of the importance of additives in plastics, they are often poorly disclosed or only briefly discussed in life cycle assessments (LCAs). In part II, we focus on the inclusion of additives in plastic processes in the database most used in plastic LCAs to date (Ecoinvent) and find that additives have historically been omitted from plastic granulate data and in production processes in the evaluated database. Thus, many practitioners will need to separately include additives in their models of plastic life cycles. To support practitioners in this endeavor, we then assess the availability of the 13,587 additives identified in the recent UN Chemicals in Plastics Report across the three major LCI databases (CarbonMinds, Ecoinvent, and LCA for Experts [GaBi]). We find that databases currently cover only 1,209 of these additives. Moreover, we assert that transparency regarding additive inclusion in plastics datasets, availability of additive datasets, and additive data completeness are major barriers to additive inclusion in plastic LCAs. Thus, we recommend focusing on the development of additive datasets, and we provide a tool for the identification of additive dataset availability and data gaps to improve the quality of plastic LCAs.

KEYWORDS

additives, circular economy, industrial ecology, LCA, plastics, sustainable transitions

1 | INTRODUCTION

Additives provide the multifunctionality that renders plastics desirable (Gu et al., 2016; Hahladakis et al., 2018). The combination of additives and polymers is further refined by conversion processes that make plastics suitable for many functionalities. As of 2023, over 13,000 additives were estimated to be available for use in plastic within the European Union (EU) (UNEP, 2023). The mass-based contribution of these additives in plastics ranges from 0.01% to 70% depending on the polymer, application, additive function, industry, and producer (Aurisano, Weber et al., 2021; OECD,

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2009; Wiesinger et al., 2021). Yet, when considering the sustainability of plastics, additives are often forgotten leaving all the focus on the polymer itself (i.e., polyethylene terephthalate [PET], polyethylene [PE], polypropylene [PP], etc.).

For example, life cycle assessments (LCAs) commonly omit additives when assessing the impact of a plastic life cycle (van Oers et al., 2012; Logan et al., 2024, part I). Additive exclusion in LCA was first identified over a decade ago (van Oers et al., 2012) and most likely occurs due to knowledge gaps, black boxes in databases, and intellectual property barriers (Bishop et al., 2021; NIST 2022), as well as poor regulation and monitoring of plastic additives (Aurisano, Weber et al., 2021; Wiesinger et al., 2021). This is further compounded by the lack of chemical data in LCA databases (Bauer et al., 2022; Edelen et al., 2017). Coupled together, these challenges have created a critical gap in the role and environmental impacts of additives in the life cycles of plastics and are a barrier to circular plastic transition planning using LCA.

Additive omissions pose a concern when LCA is used to help identify and plan for using safe and circular chemicals in plastics (Aurisano, Weber et al., 2021; UNEP, 2023). Negating additive flows in circular plastics fails to capture the risks and environmental impacts additives may have in recycled plastic materials. Recent studies into additive impacts on children's toys (Aurisano, Huang et al., 2021; 2022; Guzzonato et al., 2017) and food packaging (Andra et al., 2012; Groh et al., 2019; Guzzonato et al., 2017) highlight the importance of capturing these flows in LCAs. Furthermore, using mined materials (e.g., titanium dioxide [TiO₂] and other metals) as additives means that when additives are omitted from LCAs, some studies may underrepresent the mineral resource and environmental impacts of plastic materials, such as polyvinyl chloride (PVC) (Turner & Filella, 2021).

Thus, this article examines how well additives are considered in plastics dataset and major life cycle inventory (LCI) databases today. This exploration builds upon the work of Logan et al. (2024, part I), which established that additive exclusion occurs in both discourses about plastic impacts and within the data included in individual LCA articles. Part II tests the hypothesis that poor transparency of additive inclusion and additive data gaps within existing data sources are major barriers to including additives in plastic LCAs. These barriers are then addressed by providing insight into additive inclusion in existing plastics datasets and a tool to help practitioners identify which additive datasets are available to include in future plastic studies.

To achieve this, we have vetted plastic granulate datasets and plastic production processes (polymer manufacturing, compounding, and conversion) within the selected databases to verify if and how additives are included in the available datasets. We then compare UNEP (2023) list of known additives in the EU to the current chemical processes available in major LCA databases. These outcomes are made available in Supporting Information (S1). These results are then translated into a tool in (S2) to help LCA practitioners identify which additives are available to include in plastic LCAs today and identify opportunities for targeted data development. This work concludes with guidance aimed at improving additive data coverage within plastic LCAs.

2 | METHODS

2.1 | Additive terminology

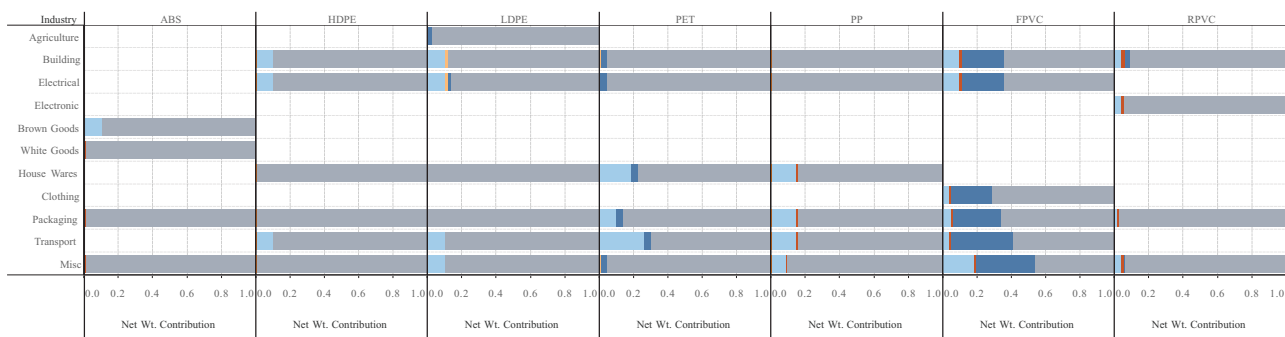
As there are many different approaches to terminology and naming of processes included in plastic production or additive functionality, this article utilizes the terminology and functional classifications utilized by the OECD documents on plastic additives (OECD, 2009, 2014, 2019). Plastic production generally comprises four steps, namely, monomer production, polymer manufacturing, compounding, and conversion, with additives commonly introduced during the latter two stages. Typically, polymers and additives are combined during compounding to enhance performance during conversion or to offer a particular function during the use-life of the final product (OECD, 2009; UNEP, 2023). Conversion utilizes the compounded polymer and, often, additional select additives to produce finished plastic products (OECD, 2009; UNEP, 2023).

Typically, additives are categorized and referenced by their functionality rather than a specific chemical name, for example, stabilizers, flame retardants, and plasticizers (Bart, 2005; Zweifel, 2001). The OECD groups these functions into five main classifications: additives for processability, surface protectors and modifiers, material protectants, physical-chemical property improvers, and functionalization agents (OECD, 2019). Throughout this manuscript, we refer to these classifications rather than to independent functions, as an additive can exhibit multiple functions within a given polymer mix, production method, or application.

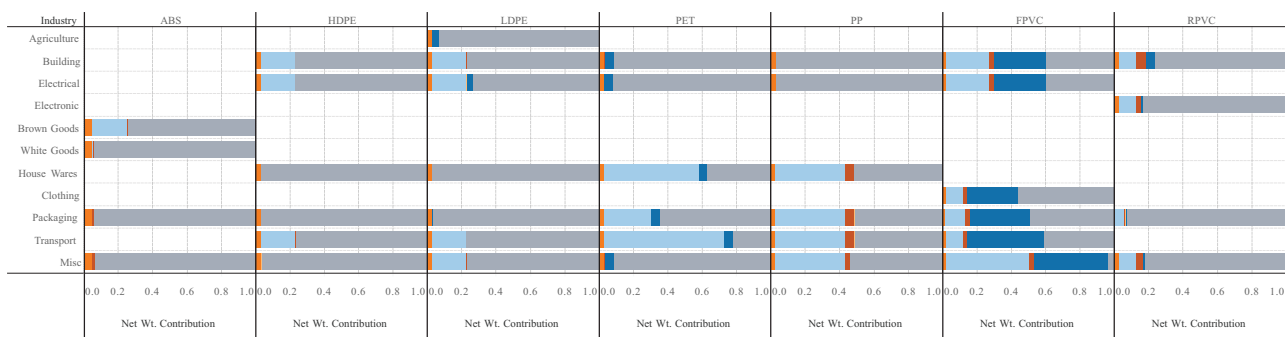
2.2 | Additive contributions to plastic composition

In previous additive research, the OECD established possible max loading rates for individual additives per polymer type, application, and industry (OECD, 2009, 2014). These contents were calculated per intended function, thus providing expected concentration rates across several plastic production and application scenarios. To illustrate the uncertainty in these rates, we have converted them into ranges and grouped the functions to reflect the OECD's (2019) classification approach in Figure 1. These bars do not indicate a recipe for the given polymer and application; rather, they communicate the maximum and minimum loading ranges of additives per desired function in a given application and polymer. They are presented in a single bar for ease of illustration. Detailed information on these ranges is available in the Supporting Information S3 per both the OECD (2019) classification and subclassification approaches.

Low Range Contribution of Additives to Plastics (OECD2009) per OECDClassification (2019) by Polymer and Industry (OECD2009)



High Range Contribution of Additives to Plastics (OECD2009) per OECDClassification (2019) by Polymer and Industry (OECD2009)



*Note these bars are illustrative of potential additive contributions to net weight if an additive is present in the chosen polymer and classification. The representation of all classifications is illustrative and does not represent an average recipe. For further details on the ranges per classification, polymer, and industry refer to S3 of this article.

Measure Names

- Functionalization Agents
- Physical Chemical Improvers
- Material Protectants
- Surface Protectors /Modifiers
- Additives For Processability
- Polymer

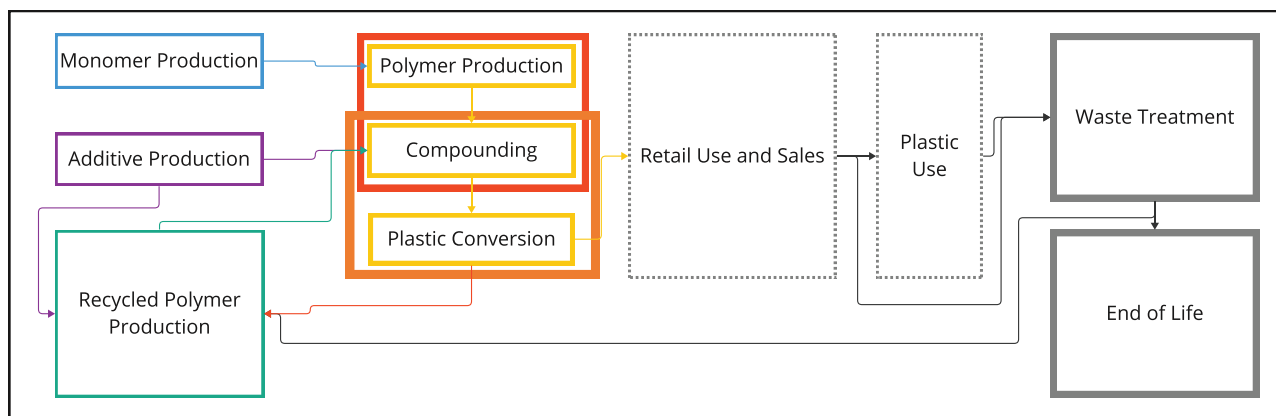
FIGURE 1 Low to high additive content range baselines for plastics by polymer and industry and has been modified from OECD (2009). These bars illustrate the high and low loading rates of additives per polymer in select applications. The bars are stacked for ease of illustration and represent individual contribution per function, not to imply recipes. ABS, acrylonitrile butadiene styrene; HDPE, high density polyethylene; LDPE, low density polyethylene; PET, polyethylene terephthalate; PP, polypropylene; FPVC, flexible polyvinyl chloride; RPVC, rigid polyvinyl chloride. A table view of these ranges both by OECD (2019) classification, and subclassification (2019) is available in Supporting Information S1.

As illustrated in Figure 1, high-density polyethylene (HDPE), low-density polyethylene (LDPE), PET, and PP have the highest capacity usage of physical-chemical property improvers when they are present, while flexible PVC (FPVC) utilizes higher concentrations of physical-chemical property improvers and additives for processability when present (OECD, 2009, 2014, 2019). Additionally, FPVC often utilizes higher concentrations of additives than rigid PVC (RPVC). Of the plastic types assessed in this study, 66% of plastics can contain a max concentration of between 8% and 17% additives by net weight, and about 10% can contain between 37% and 72% additives by net weight (OECD, 2009). Such variability in composition highlights that appropriate accounting for plastic additives is case-dependent.

2.3 | Determining additive inclusion in production processes in LCI databases

In part I, we identified Ecoinvent as the LCI database most used in academic LCA articles on plastics (90% of the 93 articles reviewed by Logan et al., 2024, part I). LCA for Experts (formally GaBi) was the second most used software and database source in the remaining articles. Due to licensing constraints, we can only assess the availability of additive data from LCA for Experts' publicly available 2023 data overview. Similarly, CarbonMinds (2022) is a database released after the scope of the literature review presented in Logan et al. (2024, part I). As this database specifically focuses on providing data for chemical production, we include a review of additive availability in this database. Due to the brief nature of the modeling methodologies provided publicly by LCA for Experts (Baitz et al., 2012; Kupher et al., 2020) and CarbonMinds (Stellner et al., 2022), we cannot assess additive inclusion in polymer production processes. Therefore, our critical review of polymer and plastic process sets primarily focuses on Ecoinvent.

Ecoinvent datasets document their modeling methodology for plastics in guidance documents for v1.0-3.0 (Hischier, 2004, 2007). To review the polymer compounding and conversion processes for acrylonitrile butadiene styrene (ABS), HDPE, LDPE, linear low-density polyethylene (LLDPE),



Plastic Data Coverage Key

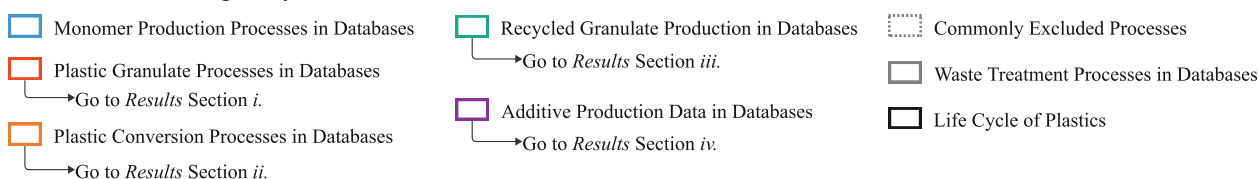


FIGURE 2 Additives within the life cycle of circular plastics, including ecosphere and technosphere transfers. Each border color is explained in the key at the bottom of the figure. The flows of materials in each process set are depicted by arrows. The correlating section in the results exploring additive inclusion and data availability per process type is communicated in the key to the right. *As only mechanical recycling pathways are considered in Part I, the illustrated life cycle does not consider monomer recycling processes.

PE, PET, PP, and PVC, we utilize the modeling methodologies provided by Ecoinvent (Althaus et al., 2004, 2007; Hischier, 2004, 2007; Steubing et al., 2016; Weidema et al., 2013; Wernet et al., 2016) to identify how and which additives are included in granulate production per polymer type in Ecoinvent v3.0, v3.6, and v3.9.1.

The methodology documents for Ecoinvent v1.0–3.9.1 primarily cite PlasticsEurope EcoProfiles as sources of polymer production data (Boustead, 1993, 1994, 1995, 1997, 2005; CPME, 2017; PlasticsEurope, 2015, 2016a, 2016b). To account for the absence of similarly detailed documentation in subsequent updates to Ecoinvent v3.0, Ecoinvent change reports have been used to assess if plastic processes have changed to include additives, as well as to assess if additive data have been subsequently adjusted within these datasets.

In Ecoinvent methodology reports for v 1.0-2.2, the chapter on “Packaging and Graphical Papers” stresses that due to the vertical aggregation methodology adopted by PlasticsEurope, it is impossible to separate individual processes throughout the production value chain when seeking to determine individual process contributions to any final impacts (Hischier, 2004; 2007). There are many types of aggregation used in dataset modeling (Kuczenski et al., 2017; Zhang et al., 2021); however, vertical aggregation is the aggregation of processes (i.e., combining production steps) and even data (i.e., combining unique chemicals into a single generic chemical production process) into a black box where it is impossible to separate individual impacts of the combined processes and data within the dataset (Kuczenski et al., 2017). Thus, clear reporting for individual process contributions and emissions is not available. Figure 2 illustrates a simplified life cycle for recycled or circular plastic materials and identifies the processes currently included in Ecoinvent databases.

As illustrated in Figure 2, the key steps in plastic production where additives are added are vertically aggregated, as illustrated by the red and orange overlapping boxes in which additives are used. This therefore makes it difficult to separate additives from other chemicals used for the maintenance or operation of machinery included in granulate production processes. Therefore, plastic granulate production data were only checked for possible additive presence.

To check conversion processes, OECD additive emission scenarios were used to assess if additive inclusion in the data reflected the average additive content baseline ranges (Figure 1) per conversion process. This was done to assess any gaps between documentation, the modeling method, and the expected ranges of additive composition in existing plastic production. Ecoinvent v2.2 through v3.6 were reviewed as Ecoinvent up to v3.6 were the most common databases in the literature reviewed in part I.

Due to the interlinkages between LCA for Experts, Ecoinvent, and PlasticsEurope (Bauer et al., 2022), similar vertical aggregation challenges are expected in the plastic production, resin, compounded polymer, and plastic part datasets. LCA for Experts, however, offers plastic granulate datasets “without additives” (Baitz et al., 2012; Kupfer et al., 2020). Due to the broad nature of the modeling methodology provided publicly by CarbonMinds, the inclusion of additive data within polymer processes is not assessed in this study.

2.4 | Assessing additive data availability and coverage

To select the additives for our review, we utilized the list of additives from UNEP (2023). This list combines Aurisano, Weber et al. (2021) and Weisinger et al. (2021) reports, individually listing all chemical abstract service registration numbers (CAS RNs) for the chemicals contained in these reports (38,531 CAS RNs). We have also included the function, polymer application, industry application, tonnage, and regulation status as reported by Aurisano, Weber et al. (2021) and Weisinger et al. (2021) per chemical (13,587 additives). This list is provided in the Supporting Information S2, as reported by Aurisano, Weber et al. (2021), UNEP (2023), and Wiesinger et al. (2021).

We then reviewed these CAS RNs against the CAS RNs reported for the datasets available from major LCA databases. We focused first on Ecoinvent v3.6 as this was the most common in the literature reviewed in part I. While insight into past practices can inform decision-making about future models, information about additive inclusion in datasets that will be used going forward is essential to improving modeling in plastic LCAs. As such, we also reviewed Ecoinvent v3.9.1, LCA for Experts 2023, and CarbonMinds 22 dataset lists in our CAS RN matching.

For Ecoinvent v3.6, CAS RNs were not provided. Thus, to identify applicable CAS RNs, we used name matching of the Ecoinvent v3.6 APOS data to Ecoinvent v3.9.1 APOS and reviewed change reports to ensure we captured data that had been removed between updates. This entire data review process has been illustrated in Figure 3. While we have only checked the APOS system in Ecoinvent v3.6, the Cut-off, APOS, EN 15804, and consequential databases have been reviewed in Ecoinvent v3.9.1. For further reading on the differences between these databases, refer to the Ecoinvent website (Ecoinvent, 2023).

We utilized CAS RNs to distinguish additive datasets because there are many naming and metadata discrepancies between databases (Edelen et al., 2017). To help address this, we have checked the multiple CAS RNs for single chemicals by using the list provided in UNEP (2023), which gives us the best chance of identifying additives with LCI data available despite differences in naming across the different databases. Additionally, not all processes have linked CAS RNs, so there may be additives included in the databases that we could not match in this review. For example, LCA for Experts labels some processes from their *Plastics Extension Database* as plastic additives. However, CAS RNs were not provided for these data, and therefore, they were omitted from the matching process.

The full CAS list (UNEP, 2023) and data matching outcomes (Ecoinvent v3.6; Ecoinvent v3.9.1; CarbonMinds 22; LCA for Experts 2023), as well as linked functions, applications, tonnage, and regulatory status (Aurisano, Weber et al., 2021; Wiesinger et al., 2021), are available in the supplemental information (S3). Additionally, we have categorized the additives based on known functions in line with the OECD, 2019 classification and subclassification approaches. This information is stored in a searchable Excel and only contains additives with available LCI datasets. The tool can be found in the supplemental information (S2). This is intended as a reference tool for LCA practitioners looking to include additives in plastic LCAs.

3 | RESULTS AND DISCUSSION

In the following section, we investigate additive availability in LCA databases. First, we review additive inclusion in plastic processes in Ecoinvent v2.2, v3.6, and v3.9.1. Part 1 reviews Ecoinvent v2.2, v3.6, and v3.9.1. The review of Ecoinvent v2.2 and v3.6 informs practitioners on the additive presence and gaps in prior LCAs, while the review of v3.9.1 provides insights for future studies. Then, we perform an analysis of available additive processes in Ecoinvent v3.6 and v3.9.1, Carbon Minds 22 and LCA for Experts 23. This is done using CAS RN matching. Ecoinvent v3.6 is reviewed to provide an overview of additive choices in previous studies while Ecoinvent v3.9.1, CarbonMinds 22, and LCA for Experts 23 are reviewed to provide an overview of options for future studies.

3.1 | Additives in plastic process

The review of modeling methodologies for plastics datasets revealed that the production of plastics is often split into three stages instead of the traditional four-step approach. Thus, in the plastics datasets in Ecoinvent, the three stages available to include in plastic production are monomer production, polymer production (combines polymer production and compounding into output plastic granulates), and plastic conversion (compounding of input plastic granulates and transformation processes) (Hischier, 2004, 2007). Given this structure, additives should be included in both polymer production and plastic conversion processes.

However, due to vertical aggregation, it is often difficult to discern if generic chemical processes represent the additives in the plastic or are representative of chemicals utilized for other functions (such as machine maintenance) within the process. This modeling approach seems to have been adapted to account for data reporting in the original PlasticsEurope (then APME) data used to create plastics datasets as early as Ecoinvent v2.2 (Hischier et al., 2004, 2007).

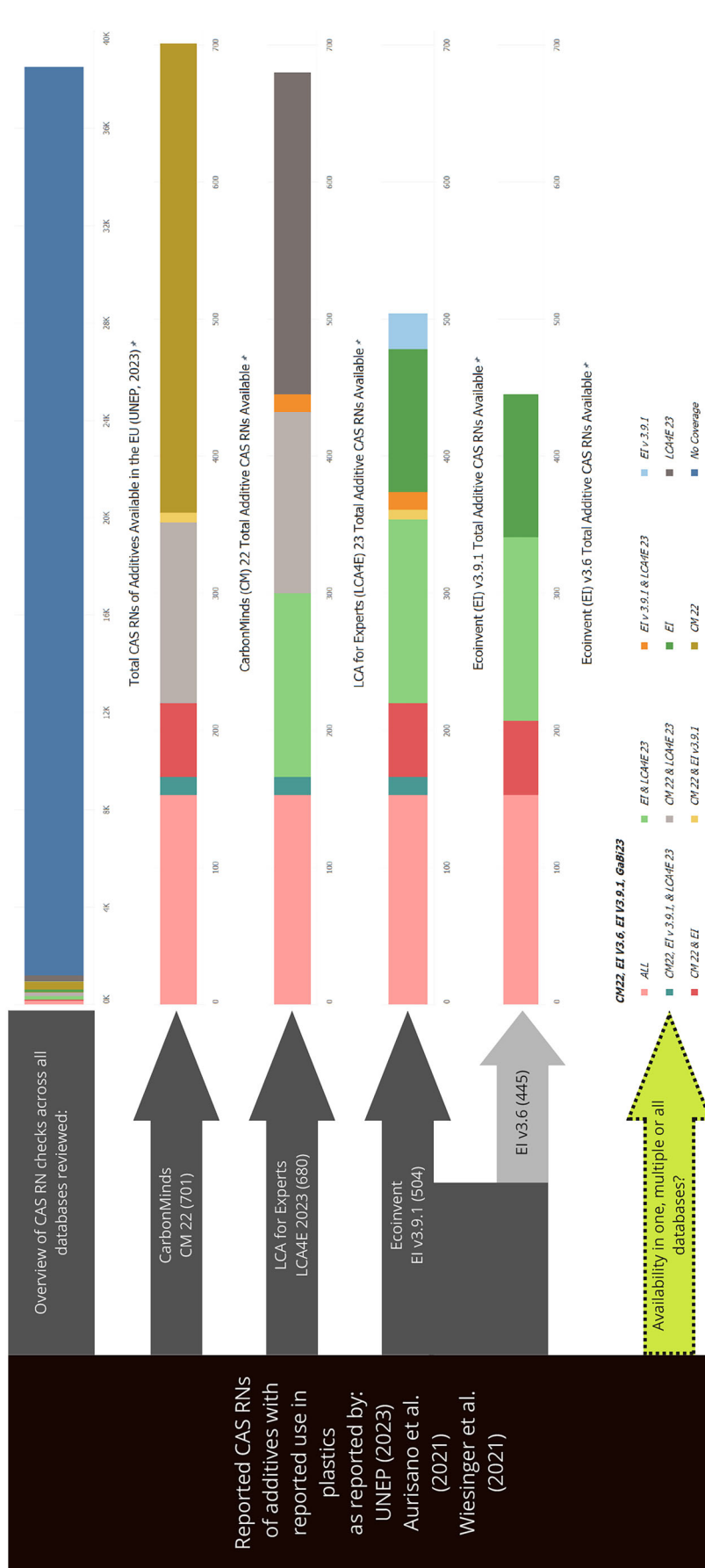


FIGURE 3 Additive data coverage check methodology and outcomes 38,531 chemical abstract service registration numbers (CAS RNs) of additives (UNEP, 2023) were checked against the CarbonMinds 22 (CM), Ecoinvent v3.6 (EI3.6), Ecoinvent v3.9.1 (EI 3.9.1), and life cycle assessment (LCA) for Experts 2023 (LCA for Experts) databases. The outcomes of the full review (top bar) as well as each database review (lower three bars) can be found in the bar graphs on the right. The colors for each bar indicate if the additives found were available in one or more databases and the key can be found along the bottom of the graph. The complete dataset for this figure can be found in Supporting Information S4.

The databases also offer granulate recycling processes, which include remanufacturing steps through plastic production, as such additives are also expected in these datasets. In each sub-section, we present an overview of additive inclusion and vertical aggregation in Ecoinvent v2.2, v3.6, and v3.9.1 based on our review of the methodology and processes.

3.2 | Additives in plastic production process

In our review of the methodology documents for Ecoinvent v2.2, we find that although polymer production data consist of the necessary steps for producing a specified polymer and some compounding (Hischier, 2004; 2007), plastic conversion focuses solely on converting a polymer into a finished plastic product, often omitting additives (Boustead, 1993, 1994, 1997, 2005; Hischier, 2004, 2007). Additionally, these documents state that additives are outside of the scope of modeling for most plastic granulates, although some additives may be nominally included for specific polymers (Hischier, 2004, 2007). A review of the documentation reveals that nominal additives may include bauxite, sodium chloride, clay, iron ore, limestone, sand, and phosphate in LDPE, HDPE, PET, PVC, and PP (Boustead, 1994); and barytes, bentonite, calcium sulfate, dolomite, fluorspar, gravel, iron, limestone, magnesium, nitrogen, potassium chloride, sand, shale, and sodium chloride for ABS (Boustead, 1997). However, as illustrated in Table 1, due to the vertical aggregation, these flows are only reported as elementary flows; therefore, it is not clear if these chemicals and raw materials are included as additives or for other purposes within the processes.

In Ecoinvent v3.6, plastic production processes are updated with data from the PlasticsEurope EcoProfiles. In this change, the vertical aggregation approach was updated from elementary flows to process inputs; however, all additives and chemicals were updated to “generic data” from Ecoinvent (CPME, 2017; Plastics Europe & ECVM, 2015; PlasticsEurope, 2015, 2016a, 2016b, 2016c). Upon review of the datasets, we assume this term refers to “organic, chemical” and “inorganic, chemical” datasets, which act as a “catch-all” for chemicals that are not currently modeled explicitly in the database. While this change made it easier to separate chemical impacts from polymers, all chemicals used in the production process are grouped with any additives in another form of vertical aggregation. Thus, as documented in Table 1, it is still not possible to separate additive impacts from polymer impacts in these studies or verify if the inclusions are representative due to the aggregation approach for chemicals in the datasets.

In Ecoinvent v3.9.1, the vertical aggregation has been addressed through improved transparency for some granulate production process sets, which now include targeted catalysts, stabilizers, or colorants. These changes are reflected in the last two columns of Table 1. However, all process sets still utilize “organic, chemical” and “inorganic, chemical” as a catch-all for chemicals used in the process and may therefore include additives. Furthermore, polymer production steps are still combined with compounding steps to create the polymer granulate datasets listed in Table 1.

This continued aggregation makes it challenging to accurately substitute generic chemicals data for more representative additives without utilizing advanced LCI data manipulation techniques. While such techniques would allow a practitioner to remove vertically aggregated chemicals outright, the practitioner would then need full insight into the chemicals used in each process, per polymer type. Such insight is not always achievable as insight into additive use is not always transparent (refer to Section 2.2) and additives data may not be available in the selected LCA databases (refer to Section 3.2).

3.3 | Additives in plastic production process

When assessing plastics conversion processes in Ecoinvent, we found that additives are generally not included or are not transparently identified. However, this omission allows LCA practitioners to include additives—provided appropriate data can be obtained.

In Ecoinvent v2.2, plastic conversion processes are generated by averaging the inputs and outputs of associated products in the Boustead (1997) and Habersatter et al. (1998) reports. The procedures included in Ecoinvent v2.2, v3.6, and v 3.9.1 are recorded in Table 2. In v3.6 and v3.9.1, extrusion and thermoforming are updated with data from Quantis (2015); however, none of the added methods (“extrusion of plastic sheets,” “thermoforming, inline,” and “extrusion, co-extrusion of plastic sheets”) include additives (Quantis, 2015). Only “injection molding” conversion processes state additives are included; that is, lubricants, solvents, stabilizers, pigments, and fillers are included (Hischier, 2004; 2007).

In these datasets, additive inclusions are averaged from reporting from Boustead (1997) and Habersatter et al. (1998) across various eligible polymer types (Hischier, 2004, 2007), thus the additives included in these datasets are more representative for some polymers and applications than others. This means that the additives included may not be applicable to the production of each polymer eligible for use in this conversion process. When reviewing the injection molding processes, these additives correspond to lubricating oil; solvent, organic, chemical, organic; titanium dioxide; kaolin; and lime. Note that lubricants, solvents, and stabilizers use “generic data” instead of a specific additive dataset. An overview of additive presence in plastic conversion processes is presented in Table 2.

Apart from the impact of producing additives, conversion processes can also have emissions. When assessing the flow of additives in compounding and conversion, the OECD (2009) refers to open, closed, and partially open production methods during plastic compounding and polymer

TABLE 1 Additive inclusion and aggregation status in Ecoinvent data by polymer type.

Polymer	Ecoinvent v2.2 Additives included	Ecoinvent v2.2 Vertically aggregated?	Ecoinvent v3.6 Additives included	Ecoinvent v3.6 Vertically aggregated?	Ecoinvent v3.9.1 Additives included	Ecoinvent v3.9.1 Vertically aggregated?
Plastic granulate, unspecified	NA	NA	"Generic" Ecoinvent data	Yes	Same as v3.6	Same as v3.6
ABS	Potentially	Yes	"Generic" Ecoinvent data	Yes	Same as v3.6	Same as v3.6
LLDPE	Potentially	Yes	"Generic" Ecoinvent data	Yes	Generic chemicals (organic and inorganic), solvents, catalysts	No
LDPE	Potentially	Yes	"Generic" Ecoinvent data	Yes	Generic chemicals (organic and inorganic), solvents	No
HDPE	Potentially	Yes	"Generic" Ecoinvent data	Yes	Generic chemicals (organic and inorganic), solvents, colorants, catalysts	No
PE	NA	NA	NA	NA	NA	NA
PET, amorphous	Potentially	Yes	"Generic" Ecoinvent data	Yes	Generic chemicals (organic)	No
PET, bottle grade	Potentially	Yes	"Generic" Ecoinvent data	Yes	Generic chemicals (organic and inorganic), plasticizers, stabilizers, solvents, catalysts	No
PP	Potentially	Yes	"Generic" Ecoinvent data	Yes	Generic chemicals (organic and inorganic), solvents	No
PVC emulsion	Potentially	Yes	"Generic" Ecoinvent data	Yes	Generic chemicals (organic)	No
PVC bulk	Potentially	Yes	Not available	Not available	Generic chemicals (organic)	No
PVC suspension	Potentially	Yes	"Generic" Ecoinvent data	Yes	Generic chemicals (organic)	No

Note: NA indicates a process is not available in that dataset. Potentially indicates that additives were included in the referenced literature but not in the methodological literature for the dataset and due to vertical aggregation, the additive presence cannot be derived from process contributions.

Abbreviations: ABS, acrylonitrile butadiene styrene; LLDPE, linear-low density polyethylene; LDPE, low-density polyethylene; HDPE, high-density polyethylene; PE, polyethylene; PET, polyethylene terephthalate; PP, polypropylene; PVC, polyvinyl chloride.

conversion. The terms open, closed, and partially open refer to the risk of increased additive losses into the air or surrounding environment during a given production type and are essential for estimating the expected loss rate of additives during production.

These processes are divided as follows: closed processes include injection molding, extrusion, blow molding, compression molding, and foaming; partially open processes include film extrusion and sheet extrusion; and open processes include thermosetting, calendaring, fabric coating, thermoforming, and casting (OECD, 2009). During our screening of the conversion processes, no emissions to air are considered related to open production or closed production that also might have emissions during degassing or cooling stages.

3.4 | Additive inclusion in recycling datasets in Ecoinvent

All recycling processes included in Ecoinvent v3.6 and v3.9.1 include extrusion but exclude additives. In all versions, individual additives are not explicitly included as either an input from the technosphere, as an output, or as continuing in the new product in recycling processes. The outcomes

TABLE 2 Additive inclusion in plastic conversion datasets in Ecoinvent.

Conversion process	Process type	Plastic products	Eligible polymers	Additives incl. Ecoinvent v2.2	Additives incl. Ecoinvent v3.6	Additives incl. Ecoinvent v3.9.1
Extrusion	Partially open	Films	PE, PP; PVC	No	No	No
	Closed	Pipes	PE; PVC	No	No	No
Extrusion of plastic sheets and thermoforming, inline	Partially open	Plastic sheets	Various	NA	No	No
Extrusion, co-extrusion of plastic sheets	Partially open	Plastic sheets	Various	NA	No	No
Injection molding	Closed	Various	Various	Yes (lubricant, solvent, stabilizer, pigment, filler)	Yes (lubricant, solvent, stabilizer, pigment, filler)	Yes (lubricant, solvent, stabilizer, pigment, filler)
Blow molding	Closed	Bottles	PET; PE	No	No	No
Stretch blow molding	Closed	Various	PVC; PP; PET	No	No	No
Calendaring (updated to calendaring, rigid sheets in v3.0)	Open	Sheet	PVC	No	No	No
Thermoforming, with calendaring	Open	Various	Various	No	No	No
Foaming or expanding	Closed	Foamed parts	E(PS)	No	No	No

Note: This table conveys the conversion process, production type, typical products, and eligible polymers in the Ecoinvent databases. NA indicates that a process is not available within the dataset. Eligible polymers are derived from the Ecoinvent dataset documentation. Plastic products and process types are classified using OECD (2009).

Abbreviations: PE, polyethylene; PP, polypropylene; PVC, polyvinyl chloride.

of this review are presented in Table 3. The omission of additives from recycling processes is concerning as additives are crucial to plastic recycling as they protect the polymer during reprocessing and improve the properties of the recycled granulate (Gu et al., 2016). However, additives in recycling also include persistent, partially degraded, unintended additives already prevalent in the recycled material (Hahladakis et al., 2018). Thus, the omission of additives from these datasets is a substantial gap in assessing the impacts of plastic recycling as both virgin inputs and effects from additive losses, degradation, and unintended additives are not accounted for.

4 | ADDITIVES INCLUDED IN MAJOR LCI DATABASES

Our analysis of plastic additive availability, which compared the additive lists from UNEP (2023) against the Ecoinvent v3.6, Ecoinvent v3.9.1, CarbonMinds 22, and LCA for Experts 2023 process lists, found 1213 CAS RNs for plastic additives (1209 unique additives), which have matching LCI data available. This equates to 9% of all additives, and 3% of all CAS RNs checked have matching LCI data. The results by CAS RN per database are illustrated in Figure 4 and are as follows: Ecoinvent v3.6 APOS (445), Ecoinvent v3.9.1_APOS (504), CarbonMinds 22 (701), and LCA for Experts 2023 (680).

Using the additive compatibilities per polymer recorded by Aurisano, Weber et al. (2021) and Wiesinger et al. (2021), we matched the 1209 additives with their reported functions and applications in ABS, LDPE, HDPE, PET, PP, polystyrene (PS), polyurethane (PUR), and PVC. These polymers were selected as they were the most common polymers studied in part I. Figure 4 illustrates the functionality and applicability of additives across the four databases overall and per polymer to provide a general understanding of the repressiveness of additive coverage available today. Please note that more chemicals used as additives may be available in the databases, but their use as additives may not be included in this review as additive use and functions in plastics are under-reported (UNEP, 2023).

As additives can have multiple or different functions within an individual application or polymer, a single additive may be counted in multiple function classifications. As recommended in part I of this study, a detailed breakdown of additives per functionality following the OECD Additive Sub-Classifications (2019) can be found in the Supporting Information S2. As illustrated in Figure 4, our analysis found that additives included in databases are most often additives for processability (792), functionalization agents (527), and/or physical-chemical improvers (527).

TABLE 3 Additive inclusion in plastic recycling datasets in Ecoinvent.

Recycling process	Products	Eligible polymers	Additives in Ecoinvent v2.2?	Additives in Ecoinvent v3.6?	Additives in Ecoinvent v3.9.1?
Plastic granulate production, unspecified, recycled, formal sector	Generic plastic granulate recycled	MISC (ABS, PP HIPS, PC)	NA	No	No
Plastic granulate production, unspecified, recycled, informal sector	Generic plastic granulate recycled	MISC (ABS, PP HIPS, PC)	NA	No	No
Polyethylene production, high density, granulate, recycled	HDPE granulate	HDPE	NA	No	No
Polyethylene terephthalate production, granulate, amorphous, recycled	PET granulate	PET	NA	No	No
Polyethylene terephthalate production, granulate, bottle grade, recycled	PET granulate	PET	NA	No	No
Plastic flake, consumer electronics, for recycling	NA	Mix	NA	No	No

Note: This table depicts the recycling processes in Ecoinvent, the database to which they apply, OECD production type, typical products, and eligible polymers within the Ecoinvent databases. NA indicates that a process is not available in that dataset.

Abbreviations: ABS, acrylonitrile butadiene styrene; HIPS, high-impact polystyrene; HDPE, high-density polyethylene; MISC, miscellaneous; PC, polycarbonate; PET, polyethylene terephthalate, PP, polypropylene.

By comparing the functionality of additives included in Ecoinvent (Figure 4) to the functionality of those in the baseline ranges (Figure 1), we observe that additives for processability are overrepresented in the available data. This is likely due to the multifunctional role of additives outside of the plastics industry, meaning that chemicals used to ease the production of many materials may be more likely to be reported. We also find that physical-chemical improvers and functionalization agents were the most common additives in plastics and are the second and third most present functionalities within the data.

The list of 1209 additives, their available data, and functions has been compiled into a tool for practitioners in the Supporting Information S2, to advance plastic LCA modeling by improving transparency around additive impacts. Practitioners can utilize this tool to determine which database has the most representative processes available for the plastic assessed. Paired with the ranges in Figure 1 and Supporting Information S3, practitioners may also use the tool in (S2) to begin creating scenarios when they are unable to obtain disclosures from plastics industry stakeholders.

For example, practitioners can run preliminary perturbation analysis using the high and low ranges (Figure 1) for additives via a selection of additives in each relative category (Figure 4) using their preferred database and the information in the tool (S2). The sensitivity of each additive and the ranges within the plastic application could then be correlated with the data quality of the chosen datasets and used to identify the most sensitive or important parameters to target for improved data disclosures from industry stakeholders.

It is important to note that just because an additive process is available does not mean that the full impact of the additive can be measured across all life cycle impact assessment (LCIA) methods and their characterization factors. In this review, due to data accessibility and differences in end user license agreements, we do not disclose the completeness or process coverage of all datasets found in this review. However, practitioners should keep in mind that discrepancies in naming and metadata may affect how the impact of an additive is calculated during the matching of elementary flows to characterization factors for different LCIA impact methods (Edelen et al., 2017; Laurent et al., 2020). This means that even though data may be available in each database, it may not always be possible to fully quantify the impact of a plastic additive throughout its life cycle. Completeness and matching will also vary depending on the database, software, and LCIA method used, so practitioners should keep this in mind when selecting data for additive inclusions in plastic LCAs.

5 | CONCLUSIONS AND RECOMMENDATIONS

This research reveals that poor additive data availability and the lack of additive inclusions in plastic production processes in LCA databases, coupled with the lack of reporting of additive impacts highlighted in part I (Logan et al., 2024), confirm that LCAs of plastics are indeed missing accurate accounting for additives. However, accounting for additives ensures plastics data are representative and are essential for comparative or

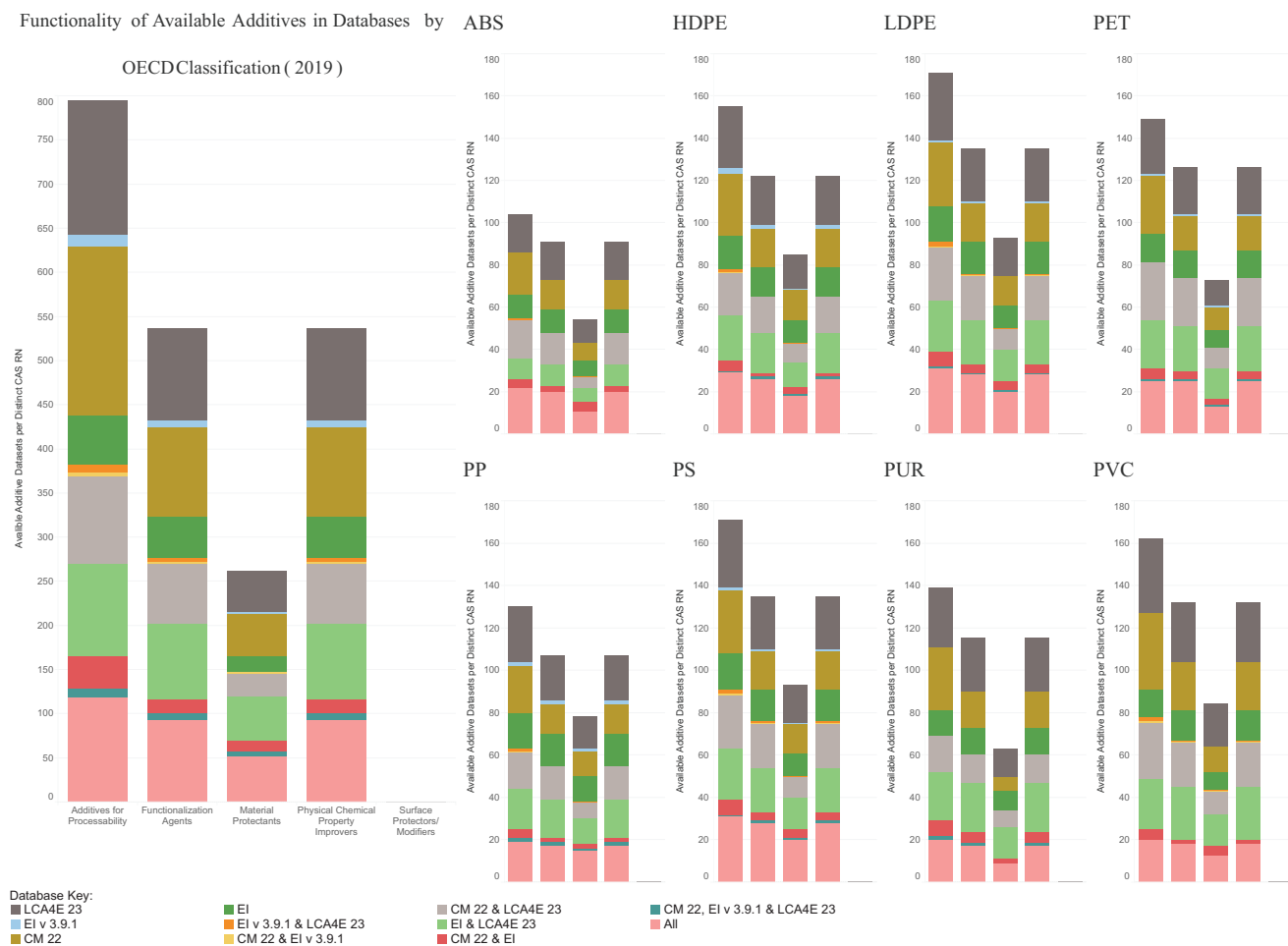


FIGURE 4 Functionality of additives included in databases per polymer. This figure presents the total number of additives available in each database and their applicability to each polymer per OECD (2019). The applicability per polymer is broken down on the right side of the figure as individual graphs per polymer. To show if the applicable additives are available across one, multiple, or all databases, we have color coded each bar, the key for these colors is available at the bottom of the figure. EI indicates availability in both EI3.6 and EI3.9.1. The data used in this calculation can be found as a table in Supporting Information S2.

multiple-loop studies. Thus, including additives not only helps in assessing the environmental hotspots of plastics, but can increase our understanding of interactions between additives and plastics in recycling and circular studies.

While we find that vertical aggregation in past databases may have often led to accidental omissions of additives, we also find that the challenges of vertical aggregation are diminishing as new and updated databases become available. By identifying which additives are available across the databases available today, this work provides LCA practitioners with a starting point from which to improve the accounting of additives in plastics. Therefore, the authors recommend that additives should be included in all plastic LCAs going forward, even those where additives contribute less than 10% to the net weight of the material.

Although the underrepresentation of chemicals within LCA databases is still a known limitation of LCAs and process coverage of chemicals is a challenge in ensuring accurate impact assessments (Edelen et al., 2017; GLAM 2022), improving accounting for additives in plastic LCAs will help raise awareness of these data gaps. While this work has provided a tool in (S2) for practitioners to begin identifying and including additives, the low data availability indicates that practitioners will also need to utilize primary data from stakeholders going forward. As such, our final recommendation is for improved transparency and collaboration between plastic producers, LCA practitioners, and LCA database creators to improve additive data availability in LCA databases and plastic LCAs going forward.

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CONFLICT OF INTEREST STATEMENT

The authors declare no conflict of interest.

DATA AVAILABILITY STATEMENT

The data that support the findings of this study are available in the supporting information of this article.

ORCID

H. Logan  <https://orcid.org/0000-0002-7156-0174>

T. F. Astrup  <https://orcid.org/0000-0002-2853-1001>

A. Damgaard  <https://orcid.org/0000-0002-0452-1220>

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SUPPORTING INFORMATION

Additional supporting information can be found online in the Supporting Information section at the end of this article.

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