

Describing uses of additives in plastic material for articles and estimating related exposure Practical Guide for Industry

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1. Background

About 20 % of all registered substances under REACH will become part of an article during their lifecycle. About 50 % of these substances are reported to be hazardous by industry, and therefore require a safety assessment, if produced or imported in amounts of 10 tonnes per year or more. Of the materials used to produce articles and buildings, plastics play a prominent role¹.

Paragraph 0.3 of REACH Annex I states that “the chemical safety assessment shall consider the use of the substance on its own (including any major impurities and additives), in a mixture and in an article, as defined by the identified uses. The assessment shall consider all stages of the lifecycle of the substance resulting from the manufacture and identified uses”. Therefore, if a substance that fulfils the criteria specified in Article 14(4)² becomes part of an article, the conditions of safe use during the service life of the article and waste operations have to be determined, together with the corresponding estimation of release and exposure. This requirement applies to substances registered in amounts of 10 tonnes per year or more.

Based on this assessment, registrants determine which information in terms of safe handling and exposure controls needs to be communicated with the extended safety data sheets down the supply chain. Such information may, for example, include a maximum safe concentration in certain types of plastic material³ or articles, uses advised against in certain article types, advice to apply barrier-layers to prevent leaching or measures to control exposure when cutting or machining certain plastic materials. However, based on the assessment, registrants can also conclude that no particular measures are needed to control the release of the substance.

The aim of this document is to provide some guiding principles for the chemical safety assessment, addressing substances in or on article matrices. It also includes some short practical advice on:

- how to describe the use as a plastic additive in the registration dossier; and
- how to get started with an exposure assessment for plastic materials.

The document is largely based on the outcome of the “Plastic additives initiative”⁴ (PLASI), a joint ECHA and industry-sector project, and in particular on the findings documented in “Supplementary Information on Scope and Methods”⁵.

¹ Preliminary analysis of REACH registration database (Article 10 registrations), based on search functions available at ECHA website. 7 % of all registered are reported to end-up in plastic articles, with about 40% of these reported to be hazardous. In this calculation, substances self-classified for long-term systemic health effects, skin sensitisation and chronic aquatic toxicity have been taken into account.

² For substances manufactured or imported in quantities of 10 tonnes per year or more (Article 14(1)) that fulfil the criteria for certain hazard classes or categories, or are considered as persistent, bio-accumulative and toxic (PBT) or very persistent and very bio-accumulative (vPvB), the chemical safety assessment has to include additional steps: a) an exposure assessment including the generation of an exposure scenario and b) a risk characterisation for all identified hazards (Article 14(4) of REACH).

³ Plastic material means any mixture or article made of a particular type of plastic (LDPE, PVC, etc.). The material includes all additives, but its form may vary (granules, sheets, films before final forming, or finally shaped material in the article). Worker exposure has to be assessed wherever workers are in contact (with master-batches, compounds (mixtures), semi-finished or finished articles), while the consumer exposure assessment refers to finished articles only.

⁴ <https://echa.europa.eu/plastic-additives-initiative>

⁵ https://echa.europa.eu/documents/10162/13630/plastic_additives_supplementary_en.pdf/79bea2d6-8e45-f38c-a318-7d7e812890a1

This practical guide specifically addresses exposure (human and environment) to substances in plastic articles when used by consumers. The methods described can also be applied to the use of articles by workers, if the conditions are similar.

This guide does not cover:

- Compounding of plastic material and production of articles (and the related occupational exposure).
- Installation and maintenance of articles or complex objects by workers, for example, installing floorings and other virgin materials (potentially releasing substances at a higher rate than during the 'normal' service-life) or maintaining electronic appliances.
- Operations with plastic waste (dismantling of articles and processing plastic waste fractions).
- Communication obligations regarding substances of very high concern in articles.
- Exposure from micro-plastics (e.g. formed by abrasion/degradation of articles contained in consumer products).

While this guide specifically addresses additives in plastic articles, some of the advice can be applied to any substance in any article type, for example, additives in rubber or textiles.

2. Reporting uses of additives in plastics

When registering a substance, manufacturers and importers have to describe the anticipated uses in a brief, general manner. Following ECHA Guidance R.12, the uses need to be described in Section 3.5 of the IUCLID dossier in a complete and consistent way, irrespective of the tonnage band or hazard classification.

2.1 Rules for describing uses

A number of basic rules apply when describing the uses of a plastic additive in a REACH registration dossier.

- Always distinguish between the lifecycle stages: manufacturing of the additive, production of compounds⁶ and master-batches⁷ (formulation), conversion into shaped plastic articles (use at industrial site), and service-life in the article (which may include assembling with other articles into complex products). This means that for a plastic additive manufactured and used in the EU/EEA, the use description must usually include at least one use-record in each of the four relevant tables in Section 3.5 of IUCLID. Uses outside of the EU/EEA do not need to be described in the registration dossier.
- When characterising the article service-life of an additive in plastic materials, the foreseeable releases to workers (professional and/or at industrial sites), to consumers and to the environment need to be taken into account. Processing of articles by workers

⁶ Compounding consists of preparing plastic formulations by mixing and/or blending polymers and additives in a molten state.

⁷ A master-batch is a concentrated mixture of pigments and/or additives encapsulated during a heat process into a carrier resin, which is then cooled and cut into a granular shape. Master-batches allow the processor to colour (or equip with other additives) raw polymer safely and economically during the production of plastic materials and articles.

(and the expected release pattern to the environment) and consumer uses (and the expected release pattern to the environment) need to be distinguished. Depending on the expected release potential under the anticipated conditions of use, further differentiation among worker and consumer uses may be needed. It may, for example, be sensible to systematically differentiate the following uses:

- Uses where the additive is foreseeably released from the (intact) article matrix (e.g. slip promoters, plastic matrices with a high erosion potential, such as shoe soles; plastic matrices remaining in the environment after use, for example, in agriculture; plastic material processed by workers under high temperature or dust-forming conditions).
- Long-lived articles in outdoor use (due to the higher expected release).
- Large surface indoor articles (due to potential impact on indoor air quality).
- Articles with intense dermal or oral contact (e.g. food contact materials, toys, handles, gloves, upholstery).
- Each of these uses can be characterised through a number of use descriptor categories and free-text narratives. For further explanation and examples, consult the attachment to this document.

2.2 Technical function

The technical function of the additive is another crucial piece of information. It characterises what the substance or mixture is intended to do, and may already trigger exposure considerations.

The function of the additive may be delivered at polymer production, at the compounding stage, during conversion or during the use of the article material. The service life needs to be described and assessed in all cases where the substance is present in the final material matrix, independent of whether the substance still has a function during the service life or not.

The technical function may be associated with a chemical reaction in the material matrix, during which the substance may be partly or fully turned into reaction products. These products may become part of the polymer matrix (e.g. cross-linkers, coupling agents, hardeners, curing agents) or stay as a "free" reaction product in the matrix (e.g. some anti-oxidants and heat stabilisers).

At the same time, a fraction of unreacted substance may still be contained in the matrix. In these cases, reporting a use at service life and the assessment requirements depends on the residual concentration of the parent substance and the hazardousness of the reaction product.

Only if the residual concentration is low and remains low during the use of the material (see cut-offs mentioned in Section 3.2), and any "free" reaction product can be characterised as non-hazardous, can the life-cycle of the registered substance be regarded as terminated, and no further reporting and assessment is needed.

The attachment to this document provides an overview on the main functions of plastic additives, many of them can be directly found in the dropdown list for the corresponding field in IUCLID 3.5, others would need to be specified under the entry "other".

The exposure considerations triggered by the technical functions include, for example:

- Substances acting as slip promoters or anti-statics are meant to move towards the plastic surface and are therefore characterised by a high potential for exposure.
- Substances acting as coupling agents or cross-linkers (technical function “others”) are meant to be reacted into the polymer matrix and, as such, are less likely to be released unless used under (highly) abrasive conditions. The same applies e.g. to flame-retardants polymerised into the matrix.
- Substances acting as plasticisers or flame-retardants are – due to their function – by default expected to be present in higher concentration bands⁸. Exceptions may exist, for example where the polymer itself has already flame-retarding properties.

The technical function of the substance also predetermines the choice for the right Environmental Release Category (ERC) for industrial use of the additive. For additives in plastic (including those reacting on use), ERC 5 (inclusion into/onto matrix) and ERC 6d (process regulators in polymerisation) are applicable.

2.3 Tonnage breakdown

ECHA also advises to break down the overall tonnage registered for a substance into different types of plastic materials/articles, as this may form the basis for the environmental exposure assessment.

The differentiation of the tonnage per use at service life stage would be particularly relevant for those articles used indoor and those used outdoor (e.g. roof covers), since they are characterised by a different default release factor.

If no information is available for registrants, worst-case assumptions can be made, as suggested in the Chapter 2 of the attachment.

2.4 Use maps

Use maps⁹ developed by EuPC (European Plastic Converters) so far describe uses of plastic additives for formulation (master-batches) and industrial end use (conversion). This may be a suitable starting point when extending the use map to the article service life stage.

Another relevant input to such a use map is the 2019 supplement to the OECD Emission Scenario Document on plastic additives¹⁰. One of the outcomes of the PLASI project was EuPC's commitment to consider when and how to extend the existing use map.

⁸ Low (high) concentrations in plastics does not mean *per se* low (high) release potential. Also other chemical properties (e.g. molecular weight, vapour pressure, partition n-octanol water, etc.), the type of matrix (e.g. soft PVC vs rigid PVC) and use conditions need to be taken into account.

⁹ <https://echa.europa.eu/csr-es-roadmap/use-maps/use-maps-library>

¹⁰ [http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=ENV/JM/MONO\(2019\)10&doclanguage=en](http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=ENV/JM/MONO(2019)10&doclanguage=en)

3. Exposure assessment

The exposure considerations provided below only refer to the service life of plastics. Releases from i) plastics remaining in the environment after the end of service life (litter, particles from erosion, long-lived articles such as cables/pipes not removed when taking out of service); and ii) waste operations are not yet addressed in this document. This may be added at a later stage.

The Tier 1 (conservative) assessment approach targets plastic-(mono)-materials in the form of “simple” articles. The combination of material layers potentially reducing the release, or the release from complex objects, may come into play when safe use cannot be demonstrated for the simple matrix. If so, the multilayer description has to be reflected in the exposure scenario. If this requires knowledge beyond the information available to registrants of the additive, the article producer may need to carry out a downstream user chemical safety report and notify the corresponding use description to ECHA (see Article 38 (2)(a)).

3.1 Chemistry during service life

As a starting point, the assessor needs to understand the chemistry of the additive during polymer processing and service life, i.e. its composition and intended or unintended reaction processes. Such an understanding is required to identify the risk driving constituents and/or reaction products in terms of release or exposure behaviour (driven by molecular weight, vapour pressure and solubility in the contact medium) and hazard characteristics.

The assessor should include information on the chemistry of the additive and the related approach for exposure assessment and risk characterisation into IUCLID Section 1.10, which is then reported in Section 1.3 of the chemical safety report.

3.2 Qualitative argumentation that expected release is negligible

In some cases, the quantitative (exposure) assessment is not needed. This usually applies when the substance is contained in the plastic matrix in a concentration below the limits identified in Article 14(2) of REACH, in particular when the concentration is lower than:

- the cut-off value referred to in Article 11, Paragraph 3 of CLP (<0.1-10 % depending on the hazard classification of the substance).
- 0.1 % weight by weight (w/w), if the substance meets the criteria in Annex XIII to REACH (substance is PBT/vPvB) or is an endocrine disruptor (ED).

In other cases, the quantitative exposure estimation might be replaced by qualitative argumentation supporting “negligible release/exposure”. The type of evidence that can be used is:

- The substance is characterised by a very high molecular weight, very low solubility in water, high octanol water partition coefficient and low vapour pressure (and no reaction generating smaller molecules). Having such properties, a substance hardly diffuses through the plastic matrix, and partitioning to skin, saliva, or water, and release to indoor air is unlikely¹¹.

¹¹ Benchmarks for supporting a qualitative argumentation (see appendix)

- The substance is reacted into the polymer chain, as coupling, terminating or cross-linking agents. If such a claim is made, suitable evidence needs to be provided, for example, analytical evidence (such as measured residual amounts of a non-reacted substance, or results from release tests), demonstration of the covalent bonding mechanism and the rate constants of reaction (i.e. showing completeness of the reaction and its irreversibility).

It should be noted that Tier 1 exposure modelling is usually preferable compared to qualitative considerations. Registrants may find it easier to carry out a quantitative assessment than convincing authorities that such an assessment is not needed. However, Tier 1 exposure estimations (ECETOC TRA consumers 3.1 and/ CEM model, see Chapter 2 of the attachment) are quite conservative for substances with a high octanol water partition coefficient and high molecular weight. Therefore, qualitative argumentation might be acceptable in those cases.

The above argumentation for “negligible release/exposure” does not hold for additives that are meant to move to the surface (slip promoters, anti-statics), or to work as a plasticiser. Also, if significant leaching promotion (e.g. mouthing of articles by children), abrasion (i.e. visible material losses as, for example, from shoe soles or tarpaulins) or volatilisation due to high temperature occurs during use, the above arguments may not be relevant anymore.

In any case, even if qualitative argumentation on negligible release/exposure is provided instead of quantitative exposure estimates, the registration dossier must still contain information on the total tonnage of the substance entering into articles (see also REACH Annex VI, Point 3.4).

3.3 Tier I exposure assessment

Tier I models enable assessors to show in a generic way whether articles made from materials containing the substance are likely to be safe to use. These models are simple to use and provide a conservative exposure estimation. Such assessments do not aim to estimate exposure related to specific articles in their specific use-contacts.

Exposure can be estimated with relatively few parameters (e.g. molecular weight, vapour pressure, concentration of the substance in the matrix) using worst-case assumptions (e.g. large surface plastic articles for human health and outdoor articles for environment), if the type of article in which the substance ends up is not known¹².

In the attachment, we describe Tier I models covering consumer and environmental exposure for substances in plastic articles, and the default assessment if the plastic article type is not known.

3.4 Tier II exposure assessment

If Tier I models fail to show safe use, higher tier estimates might be used instead. Models

¹² Tier I assessment methods and tools are described in ECHA Guidance: Guidance R.15 on consumers exposure, especially in chapter R15.4 (ECETOC TRA), https://echa.europa.eu/documents/10162/13632/information_requirements_r15_en.pdf
- Guidance R.16 on environmental exposure, especially in chapter R16.2.2.1 (tonnage information) and R16.2.3.1 (ERC default release estimation), https://echa.europa.eu/documents/10162/13632/information_requirements_r16_en.pdf

covering consumer and environmental exposure, which particularly address substances in plastic articles, are described in the attachment, together with possible further refinements based on measured data.

For inhalation exposure estimation tools, the required input data are readily available. For dermal, oral contact and the environment, a sufficiently simple and reliable modelling approach is so far lacking, and some workarounds are required. In particular, for dermal contact, there is further development needed to obtain measured data with sufficient reliability.

Attachment

1. Use description elements

According to ECHA Guidance R.12¹³, the following use descriptor categories for article service life stage are available. Explanations on the scope of these categories is available in Guidance R.12.

Descriptor list for Environmental Release Categories

- ERC 10a: Widespread use of articles with low release (outdoor)
- ERC 10b: Widespread use of articles with high or intended release (outdoor)
- ERC 11a: Widespread use of articles with low release (indoor)
- ERC 11b: Widespread use of articles with high or intended release (indoor)
- ERC 12a: Processing of articles at industrial sites with low release
- ERC 12b: Processing of articles at industrial sites with high release
- ERC 12c: Use of articles at industrial sites with low release

Advice: Unless the additive is used in plastic material i) particularly subject to erosion during use or ii) where the additive is released from the matrix as part of its function (slip promoters or scents), you may define a use according to ERC 10a or 11a as a starting point. Industrial processing of article matrices may play a particular role as the source of release of additives when surfaces undergo maintenance, or complex articles are dismantled. If this is relevant, define a use according to ERC 12a or 12b.

Descriptor list for Article Categories

- AC13: Plastic article¹⁴;
- AC13a: Plastic articles: Large surface area articles
- AC13b: Plastic articles: Toys intended for children's use (and child-dedicated articles)
- AC13c: Plastic articles: Packaging (excluding food packaging)
- AC13d: Plastic articles: Articles intended for food contact
- AC13e: Plastic articles: Furniture & furnishings, including furniture coverings
- AC13f: Plastic articles: Articles with intense direct dermal contact during normal use
- AC13g: other plastic articles

Advice: If no further information is available or a generic Tier I assessment is sufficient (see Paragraph 3.1 and 3.2) to show safe use for consumers, apply AC13 as a generic descriptor. If a refined assessment is required, and information is available on specific uses, more specific article categories could be assigned. Note: Even when showing safe use does not require specification of article types, it may nevertheless be useful to illustrate the use of the substance with typical article types, to support authorities in understanding what is practically done with the substance.

¹³ https://echa.europa.eu/documents/10162/13632/information_requirements_r12_en.pdf

¹⁴ These are the generic descriptors. More specific and exposure-oriented ones are mentioned later in the attachment.

Additive function

Additive function	Category available in Guidance R.12 and IUCLID dropdown
Antioxidants	X
Antistatic agents	X
Blowing agents	X
Colourants (dyes)	X
Colourants (pigments)	X
Coupling agents	Specify under "other"
Curing agents	Specify under "other"
Fillers	X
Flame retardant	X
Plasticisers	X
Polymeric impact modifiers	Specify under "other"
Slip promoters	Specify under "other"
Lubricants*	X
Stabiliser (UV/light)	X
Stabiliser (heat/thermo)	X
Stabilising agent (other)	X
Viscosity aids	X

* Further differentiation on whether external or internal lubricant is desirable. Internal lubricants remaining in the article during service life as an additive are of particular interest.

Overview on the functions of plastic additives (OECD 2019)¹⁵

Additive classification	Additive sub-classification	Description
Additives for processability	Plasticizers	Plasticizers improve the fluidity of plastics during processing and flexibility at room temperature. Used extensively in polyvinyl chloride (PVC) molding.
	Lubricants	Lubricants help prevent the adhesion of plastics to the surface of metal molds and to each other, improve the fluidity of plastics, and reduce friction during melting and molding plastics.
	Blowing agents	Blowing agents, used in foam molding, decompose through heat and compression to produce carbon dioxide, water, nitrogen, and other gases.
Surface protector/ modifier	Antistatic agents	Antistatic agents prevent static electrification of electrical insulators. Classified into coating agents and blending agents. Surfactants are used.
	Antifriction agents	Antifriction agents reduce the surface friction coefficient.
	Adhesion-improving agents	Adhesion-improving agents improve the adhesiveness of the surface of plastics.
	Anti-fog additives	Hydrophobic surfaces permit condensation, leading to loss of translucency. Surfactants prevent fogging.
Material protectants	Antioxidants	Some plastics produce radicals in response to heat and/or light. Antioxidants prevent oxidation and deterioration caused by heat during processing.
	Light stabilizers	Light stabilizers prevent oxidation caused by light during the service life of a plastic product.
	Ultraviolet-absorbing agents	UV-absorbing agents prevent the breakage of molecular bonds by UV light and the generation of radicals.
	Thermo-stabilizers	Thermo-stabilizers inhibit discoloration caused by the HCl produced from vinyl chloride resin because of heat during processing.
Physical-chemical property improvers	Flame retardants	Added to combustible plastics.
	Fillers/reinforcement materials	Various fibers and powders improve the strength of plastics.
Functionalization agents	Coloring agents	Organic or inorganic pigments add color and make plastics light resistant.

¹⁵[http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=ENV/JM/MONO\(2019\)10&doclanguage=en](http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=ENV/JM/MONO(2019)10&doclanguage=en)

Advice: Assign one or more functions to the additive, depending on its market. If the function type is not available in the IUCLID dropdown list, create a specific entry under “other”.

Article service life name

For each entry in Section 3.5.6 of the IUCLID dossier, a name has to be created. The name should be sufficiently generic to cover all the article types¹⁶ (for consumer exposure assessment) or worker activity categories (PROC for worker exposure assessment) reported under it.

Differentiation into two or more uses may be relevant if these uses are associated with a significantly different release potential (in particular for the environment). As such, for a proper assessment, the tonnage fraction of the additive relevant for these use types needs to be determined.

Contributing activity names

If no further specification is to be made for the contributing activity, the name can be identical with the standard category name, for example:

- widespread use of articles with low release (indoor) (ERC 11a);
- large surface materials (AC 13a).

If particular hazards through the dermal exposure route are to be addressed, it may be useful to differentiate the large surface materials according to intensity of skin contact, for example: i) flooring material and ii) wall-covering material.

¹⁶ Please note: for systematic reasons, article types specified under a use are called “consumer contributing activity”. A “contributing activity” refers to an article category, and can specify sub-categories under the article category if relevant (i.e. two or more “contributing activities” referring to the same article category).

2. Exposure assessment

Tier I assessment

Inhalation

ECETOC TRA consumer version 3.1¹⁷ (and its implementation in Chesar¹⁸) provides a suitable model addressing inhalation exposure¹⁹.

A few input parameters are needed to perform the exposure assessment:

- Molecular weight (g/mol) and vapour pressure (Pa) of the substance.
- Concentration of the substance in plastic matrix²⁰.
- If the article type is not known, choose the following TRA article subcategory: Plastic larger articles (e.g. plastic chair, PVC-flooring, lawn mower, PC), corresponding to AC13a Plastic: large surface area articles: this is the most suitable choice to obtain a conservative estimation for indoor air.

The exposure estimation performed by ECETOC TRA considers as an input: the amount in the panel (8 kg of panel for AC13a), the room size (20 m³, standard room), dilution due to air exchange (0.6 exchange per hour) and the exposure duration (8 hours for residence in a room where the panel has been applied).

The vapour pressure plays an important role in the TRA: At $V_p < 0.1$ Pa (like most plastic additives) only 0.1% of the substance in the panel is considered to be released. Note: The released substance may not necessarily stay in air but could accumulate in house-dust and lead to exposure from there. However, it is assumed that related risks for that route would be identified by the assessment for the other routes described later in this attachment.

Dermal/oral

The dermal and oral exposure model implemented in ECETOC TRA Consumer 3.1 is based on the thickness of the layer (mixture or article) of 0.01 cm, from which the substance can migrate to skin or saliva upon direct contact, within the timeframe of an exposure event. For some article scenarios, the thickness of the (uniform) layer has been set as 0.001 cm in TRA 3.1 to account for the reduced mobility of substances in the article matrix.

There is little documentation available for the TRA comparing the modelled transfer to skin with measured data, and hence it could be questioned whether the estimated exposure is sufficiently conservative. For example, by using another model, Delmaar et al. (2013) showed that for 10 article types, the TRA estimates were lower than the predictions obtained with a simplified mechanistic infinite diffusion-based model (i.e. no material-skin transfer resistance)²¹ as, for

¹⁷ <http://www.ecetoc.org/tools/targeted-risk-assessment-tra/>, see Chapter R15.4.2 of Guidance R.15.

¹⁸ <https://chesar.echa.europa.eu/>

¹⁹ https://echa.europa.eu/documents/10162/13632/information_requirements_r15_en.pdf

²⁰ Default concentrations for (plastic) article type are given in ECETOC TRA consumer v 3.1 tool. More specific default (maximum) concentrations of additives (per technical function) in plastic articles are proposed by EuPC in their *Plastic Industries Supply Chain Exposure Scenario Tool*: <https://www.polymercomplyeurope.eu/pce-services/pestool-service> and www.pestool.eu.

²¹ First tier modelling of consumer dermal exposure to substances in consumer articles under REACH: a quantitative evaluation of the ECETOC TRA for consumers tool, J.E. Delmaar, B.G.H. Bokkers, W. ter Burg, J.G.M. van Engelen, Regulatory Toxicology and Pharmacology, 2013

example, used in the CEM²² model developed by the US EPA. Therefore, for screening purposes, we suggest using also the CEM²³ model. A few input parameters are needed to perform the exposure estimation:

- Molecular weight of the substance (g/mol), which is needed to estimate the diffusion coefficient (see later in this attachment).
- Matrix type (also needed to estimate the diffusion coefficient).
- Concentration of the substance in the plastic matrix.
- Number of events over the day, duration of the contact²⁴, surface in contact with the article and body weight (these are available for different plastic articles through the CEM documentation²⁵).

The diffusion coefficient of additives in the plastic matrix can be estimated from the specific equations set in the Technical Guidance²⁶ for plastic materials in contact with food. There are equations available for specific plastic matrices; if it is not possible to determine the specific matrices in which the additive ends up, the diffusion coefficient should be estimated for high diffusivity materials (LDPE for generic additives, soft PVC for plasticisers).

If the specific use of articles is unknown, the worst case might be selected for a generic assessment. For dermal exposure, this corresponds to an adult lying down on a plastic surface (can be a sofa with a plastic cover), with half body surface (8 750 cm²) exposed for eight hours (ECETOC). For oral exposure, this corresponds to an exposed area of 10 cm² (article mouthed) for one hour a day by a child. Please note that under these assumptions, the dermal exposure estimate is always more conservative than oral.

The CEM model/method provides a very conservative dermal (oral) exposure estimation, based on infinite diffusion (not limited by the contact medium) and overestimated coefficients, if defaults are used, especially for semi-volatile organic compounds (SVOCs). ECETOC TRA might give more suitable Tier I estimates, but clarification is needed whether this holds across all substances or whether the applicability domain of the TRA is more limited in terms of substance properties²⁷.

Environment

Environmental exposure from articles is considered to result from widespread use; this means that the tonnage for a specific use of article is spread over the EU/EEA and the amount ending up in a standard town of 10 000 inhabitants is used for local exposure assessment. The main elements needed to perform a Tier I assessment are²⁸:

²² Consumer Exposure Model (CEM) version 2.0 – User Guide, OPPT, USEPA, Risk Assessment Division, 2016.

²³ Consumer Exposure Model (CEM) version 2.0 – User Guide, OPPT, USEPA, Risk Assessment Division, 2016.

²⁴ See equation 99 in the Consumer Exposure Model (CEM) version 2.0, where the exposure is “diluted” over the time of averaging (years). Please note, that averaging exposure concentrations from single, infrequent events with times of no exposure is not supported by the ECHA Guidance R.15 on consumer exposure.

²⁵ Consumer Exposure Model (CEM) version 2.0 – Appendices, OPPT, USEPA, Risk Assessment Division, 2016, see table B5 and B6.

²⁶ Practical guidelines on the application of migration modelling for the estimation of specific migration – JRC Technical Report In support of Regulation (EU) No 10/2011 on plastic food contact materials (2015).

²⁷ ECETOC Consumer TRA steering team is working on a manuscript aiming to demonstrate the conservative nature of the tool. The approach for modelling dermal/oral exposure to substances in articles is also under discussion (comment by ECETOC to ECHA regarding Draft Practical Guide, 9/2019).

²⁸ https://echa.europa.eu/documents/10162/13632/information_requirements_r16_en.pdf

- The tonnage for use in a plastic article. A factor of 5.5×10^{-7} is applied to the total EU tonnage for that use to estimate the daily amount used in a standard town (local tonnage). It means that, if the total tonnage for the use in the article is, for example, 1000 tonnes per year, the amount in a standard town will be 0.55 kg/d (low amount due to dilution over the EU/EEA).
- Verification that the assumption on equal distribution across EU/EEA matches reality. Otherwise, the assumed amount for a 10 000 inhabitant town needs to be increased.
- The release rate can then be calculated from the local amount and the release factors; default release factors are given for the use of articles with low release indoors (ERC 11a, 0.05% release factor to water) and long-lived outdoors (ERC 10a, 3.2% of release factor to water). The ERC 10a and 11a are the most appropriate release factors for plastic articles: these factors are independent of substance properties (should reflect the worse-case).
- In such a way, release rates for other article types can be calculated as well. The release rates for the different article types need to be summed up.
- Releases are then processed by the fate and transport model (EUSES) to estimate exposure concentrations (so called PECs).
- Chesar provides a guided framework to perform the environmental exposure assessment.

If the use of the article is unknown, outdoor use (covered by ERC 10a) needs to be selected, since it corresponds to the worst-case default release factor.

A low fraction at local scale (due to dispersion across whole of the EU/EEA) and relatively low default release factors imply that a Tier I assessment is, in most cases, sufficient for demonstrating safe use of plastic articles in terms of the environment.

Only for a combination of high tonnages for use in plastic articles and relatively low PNECs, might there be a need for refinement of the Tier I assessment. Note: For PBT and vPvB substances, releases to the environment have to be minimised, and thus quantitative risk characterisation is not applicable. Nevertheless, a complete chemical safety report must not only describe the measures to minimise releases and quantify the residual releases, but should also provide a comparison of the predicted local environmental concentrations in water and soil with the related PNECs.

Tier II assessment

Inhalation

Inhalation exposure can also be estimated using more complex models, such as the Emission model²⁹, implemented in the Consexpo tool³⁰. The model requires quite a number of input parameters:

- Diffusion coefficient (D), partition coefficient (K) and transport velocity (hm) depend on the combination of basic substance properties and matrix type; equations to estimate these coefficients are discussed in "Plastic Additives Initiative" documents³¹;

²⁹ Emission of chemical substances from solid matrices – a method for consumer exposure assessment, Report 320104011/2010, J.E. Delmaar.

³⁰ Web access: <https://login-ext.rivm.nl/nidp/idff/sso?id=85&sid=0&option=credential&sid=0&target=https://esp-ext.rivm.nl/LAGBroker?%22http://consexpweb.nl/%22>

³¹ https://echa.europa.eu/documents/10162/13630/plastic_additives_supplementary_en.pdf/79bea2d6-8e45-f38c-a318-7d7e812890a1; see attachment, Paragraphs 1.1 (diffusion), 1.2.3 (partition) and 1.2.4 (transport velocity).

- Concentration of the substance in the matrix; and
- Panel (surface, thickness) and room (volume, air rate exchange, defaults are 20 m³ and 0.6 exchanges/hour) characteristics³².

The model requires expertise in exposure assessment. It enables the estimation of more realistic indoor air concentrations compared to the Tier I approach. It might not be appropriate for (high) abrasive action on the plastic matrix, since it only addresses the vapour (passive) exchange between the matrix and indoor air.

Dermal/oral

There are a number of models and analytical solutions available addressing the migration from plastics to a contact medium³³. They take both diffusion within the plastic matrix and partitioning from the plastic matrix to the contact medium into account. They are built for risk assessment in the area of food contact materials, but might be also useful to estimate dermal (oral) exposure as well.

The main input parameters needed are the diffusion coefficient and partition coefficient from plastic to skin or saliva. The diffusion coefficient can be estimated as reported in the Technical Guidance²⁶ for plastic materials. Partition coefficient can be estimated from basic substance properties (K_{ow}), matrix type and type of food simulants (e.g. different percentage of ethanol/water)³⁴. How food “simulants” can be used to approximate the skin and saliva medium, and the related limitations, are discussed in the Plastic Additives Initiative documentation⁵.

Environment

Tier II assessment for environment would imply a refinement of the default release factors (those based on ERC), most likely based on measurements of releases and/or sewage treatment plant (STP) effluent concentration survey; these data might be collected by sector organisation and reflected in Specific Environmental Release Categories (SpERCs) covering the use of plastic articles. Such SpERCs are not (yet) available (as for use in any article). It would be beneficial if the plastic manufacturing and conversion sector would initiate the development of SpERCs covering the article service life, starting from the documentation already available³⁵.

For advanced modelling, specific models are under development which enable emission estimations into water³⁶ for specific article types.

Measurements

If the default migration factors of the available modelling tools do not enable safe use to be demonstrated, measured data from migration/leaching tests could be used. Downstream users might perform such tests (e.g. article producers) according to different legislation (e.g.

³² These defaults are suggested by the Emission Model and are consistent to those used in ECETOC TRA Consumers v 3.1; slightly different values are foreseen in chamber tests under the Construction Products Regulation 305/2011, namely 0.5 air exchange rate per hour and a volume of 30 m³.

³³ JRC document (see footnote 13) Chapter 2 and Annex 9.

³⁴ Correlation of partition coefficients K_{Polymer/Food} and K_{Octanol/Water} for potential migrants in food contact polymers, Asako Ozaki, Anita Gruner, Angela Störmer, Rainer Brandsch, Roland Franz, Poster presentation at the Fourth International Symposium on Food Packaging, 19-21 November 2008, Prague.

³⁵ For example, the new OECD ESD for plastic additives:

[http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=ENV/JM/MONO\(2019\)10&doclanguage=en](http://www.oecd.org/officialdocuments/publicdisplaydocumentpdf/?cote=ENV/JM/MONO(2019)10&doclanguage=en)

³⁶ FaBES *Simaqua* and *Migrapipe* as well as custom advanced modelling jobs, see for instance estimate of lead leaching from selected PVC construction products (as part of the Lead in PVC restriction dossier; Fraunhofer IVV Freising (<https://www.ivv.fraunhofer.de/en.html>), or MDCTEC: <https://mdctec-systems.de/en/our-solutions/akts-smi>)

Construction Products Regulation – CPR) or upon specific requests and make the outcome available to registrants who need to perform the chemical safety assessment. Different kinds of chamber tests and migration tests in defined conditions can be used to experimentally assess the releases from the articles:

- “Chamber test” which simulates the indoor air concentration arising from the releases of a certain substance from a construction product under typical real-life conditions. Long-term emissions are determined 28-days after installation of the product in the test chamber, and if necessary, short-term emissions are determined at three days³⁷.
- Migration tests to water, artificial sweat and saliva³⁸ for estimating oral and/or dermal (external) exposure, e.g. tests that measure the flux of a chemical from an article surface to the saliva during mouthing (e.g. $\mu\text{g}/\text{cm}^2/\text{h}$), or the amount per mass of matrix released under certain conditions ($\mu\text{g}/\text{g}$). The test simulates exposure from the article by taking into account the conditions of use (temperature, agitation simulating the active or passive contact, frequency and duration). The value can be used in the risk assessment to estimate the dose that is released during the mouthing event or during a skin contact, when the exposed surface area and duration of the contact is known. It may also be possible to use the methods/knowledge from testing food contact material with food simulants to derive estimates for migration to skin or saliva. However, some research is needed here to explore and demonstrate applicability.
- Directly measuring absorption of additives into the body through the skin (internal exposure) is more difficult and much less standardised; ex vivo skin permeation tests are possible (e.g. Franz cell chamber assay) to directly estimate the migration of additives in polymer matrices through the skin. Examples of such experiments are reported in the literature³⁹. This results in information on internal exposure.
- Testing methods for releases from outdoor articles to the environment are under development, in particular for construction products. The CEN/TS 16637-2:2014 test may be suitable to test leaching from outdoor surfaces in contact with water. For further information, see overview publication by Bandow et al, 2018⁴⁰.

³⁷ As defined in EN16516.

³⁸ Migration to artificial sweat was used to simulate the releases from rubber granules to skin e.g. RIVM report 2017-0016, <https://www.rivm.nl/bibliotheek/rapporten/2017-0016.pdf>; JRC report about migration of PAHs from plastic and rubber articles includes different experiments to simulate dermal exposure, <https://publications.jrc.ec.europa.eu/repository/bitstream/JRC111476/kjna29282enn.pdf>; migration rate to artificial saliva to estimate oral exposure is described in a Danish report: <https://www2.mst.dk/Udgiv/publications/2016/08/978-87-93529-01-4.pdf>

³⁹ Skin permeation of polycyclic aromatic hydrocarbons: a solvent based *in vitro* approach to assess dermal exposure against benzo(a)pyrene and dibenzopyrenes, N. M.Bartsch, J. Heidler, B. Vieth, C. Hutzler, A. Luch, Journal of Occupational and Environmental Hygiene, 2016

Chemical stabilization of polymers: Implications for dermal exposure to additives, N. Bartsch, M. Girard, L. Schneider, V. Van De Weijgert, A. Wilde, O. Kappenstein, B. Vieth, C. Hutzler & A. Luch, Journal of Environmental Science and Health, Part A, 2018.

⁴⁰ Evaluation of the impact of construction products on the environment by leaching of possibly hazardous substances; Bandow et al. Environ Sci Eur (2018) 30:14; <https://enveurope.springeropen.com/track/pdf/10.1186/s12302-018-0144-2>

Appendix

Indicative benchmarks supporting qualitative argumentation

Indicative benchmarks supporting qualitative argumentation on low potential for release and/or exposure. The benchmarks need to be fulfilled simultaneously. They should not be used in isolation from other contextual information, and may undergo changes in future, with increasing knowledge on the release behaviour of substances from article matrices.

Molecular weight: >700 g/mol and Log K_{ow} >9.

References: According to the TGD for Risk Assessment of New and Existing Substances (EC, 2003), certain classes of substances with a molecular mass greater than 700 are unlikely to bio-accumulate significantly (regardless of the log K_{ow} -value). At the level of log K_{ow} = 9 the bio-magnification factor is set to a minimum value of 1 (R16 ECHA Guidance). According to the Guidance Document on Dermal Absorption (EC, 2004), dermal absorption could be assumed to be <10 % based on physicochemical properties, in particular if MW > 500 g/mol and log K_{ow} > 4.5.

Note: When using the log K_{ow} as an argument, make sure that the value is sufficiently reliable. In particular where a substance shows a very low solubility in both, water and octanol, the log K_{ow} may lack reliability and relevance. When using the molecular weight as an argument, keep in mind that the mobility of a substance in a polymer matrix may also depend on its structure, the loading and on the presence of other additives.

Water solubility: 0.01 mg/l.

Reference: Indicative value used in the Plastic Additive Initiative to determine a group of inorganics and organic pigments reported to have a very low water solubility:
<https://echa.europa.eu/plastic-additives-initiative>

Note: When using low water solubility as an argument, keep in mind that the water solubility depends on ph-conditions in the polymer matrix and the water in contact.

Vapour pressure: 10⁻⁴ Pa

Reference: The upper bound for the lowest release band to indoor air set in Tier I model (ECETOC TRA consumer) is 0.1 Pa.

Note: When using the vapour pressure as an argument, keep in mind that the vapour pressure depends on the temperature the polymer matrix is exposed to.

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