

UBA R+D Project FKZ 204 67 456 / 02

OECD Matrix Project

Branch- and product-related emission estimation tool for manufacturers, importers, and downstream users within the REACH-system

Supplement M4

Manual for Emission Estimation of Plastic Additives

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This publication is part of the OECD Matrix Project (“Branch- and product-related emission estimation tool for manufacturers, importers, and downstream users within the REACH-system”, UBA R+D Project FKZ 204 67 456).

The results of the OECD Matrix Project are documented in a summary report with six supplements.

The **summary report** contains the main results of the OECD Matrix Project

The additional reports (**supplement M1 – M6**) refer in detail to specific parts of the OECD Matrix Project:

Supplement M1: Developing the Target Funnel [Results of project part A]

Supplement M2: Developing the ESD Matrix [Results of project part B1]

Supplement M3: The ESD Matrix

Supplement M4: Manual for Emission Estimation, Plastic Additives (Project Part B2)

Supplement M5: IT System Manual (Part I); IT Design Document (Part II) (Project Part B2)

Supplement M6: Document Emission Estimation Photochemicals (Project Part B2)

The summary report and the supplements are available as a zip-file. Please contact us.

R+D Project FKZ 204 67 456/02

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Manual for environmental emission estimation of plastic additives

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1 Introduction to chemical safety assessment under REACH

1.1 Overall framework of the chemical safety assessment under REACH¹

For all substances produced / imported in amounts > 10 t/a per manufacturer/importer (M/I), a chemical safety assessment is to be carried out and documented as part of the registration dossier. The aim of the chemical safety assessment (CSA) is to determine the conditions, under which a substance can be safely manufactured and handled for all identified uses². The first part of the assessment relates to the hazards of a substance. For all dangerous substances³ the chemical safety assessment must contain an exposure assessment and a risk characterisation. Safe handling during the life cycle of a substance is regarded as ensured, if the exposure of humans or the environment remain under the level at which adverse effects are expected (PNEC⁴ / DNEL⁵).

In the CSA, the description of the safe conditions of use is called exposure scenario (ES). The development of an ES is an iterative process and involves three main steps, starting from a so called 'tentative exposure scenario', which is a first description of the conditions of use. Several exposure scenarios may have to be described for one substance, depending on how many different uses are identified. For each of the substance's life cycle steps the processes and/or the types and uses of articles into which the substance may be incorporated (service life) are to be identified. For each of the lifecycle stages, the substance amounts used, duration and frequency of substance handling as well as the application type and efficiency of risk reduction measures (emission control devices, e.g. waste gas treatment) are to be specified in the exposure scenarios.

The second step of the exposure assessment is the exposure estimation for the described exposure scenarios. The exposure estimation entails three elements:

1. Emission estimation: determines emissions from products and processes during all relevant life cycle stages into the human environment (workplace, living environment etc.) and to the natural environment (water, air, soil, and solid waste) based on the information in the exposure scenario including the implementation of risk management measures (RMMs);

¹ REACH: Proposal for a Regulation of the European Parliament and of the Council concerning the Registration, Evaluation, and Authorisation of Chemicals, 29 October 2003.

² Identified use: The discussion on how an identified use is described under REACH is ongoing at EU level.

³ Classification and labelling in accordance with the criteria of the EU Directive 67/548

⁴ PNEC = Predicted no effect concentration: concentration below which no effects are expected to occur in the environment. This value is to be derived for different environmental compartments by the manufacturers or importers of dangerous substances from ecotoxicological information.

⁵ DNEL = Derived no effect level: dose or concentration below which no adverse effects to human health are expected. This value is to be derived from different exposure pathways and different effects by the manufacturer or importer of dangerous substances from toxicological information.

2. Chemical fate and pathways: modelling and prediction of environmental behaviour of substances in the environment, considering degradation, transformation, reaction processes as well as the distribution of a substance between compartments;
3. Estimation of exposure levels of humans and different environmental compartments: calculation or measurement of substance concentrations in the natural and human environment.

In a subsequent step of the CSA, a risk characterisation is performed comparing the exposure levels with the derived no effect levels (DNEL or PNEC).

If the risk characterisation shows that the risks are adequately controlled, the chemical safety assessment is finalised and the 'tentative ES' becomes a 'final ES'. Otherwise, the ES has to be refined (e.g. by changing the operational conditions of use or using stricter risk management measures) and the exposure assessment is to be recalculated.

The final assessment is documented in the chemical safety report (CSR), which is part of the registration dossier of dangerous substances produced/imported in amounts > 10 t/a. The final ES (or the relevant part thereof) is to be communicated to the downstream users as annex to the safety data sheet (SDS).

This manual and the IT-tool focus on the first step of the environmental exposure estimation: the estimation of substance emissions from the technosphere or the articles produced into the environment.

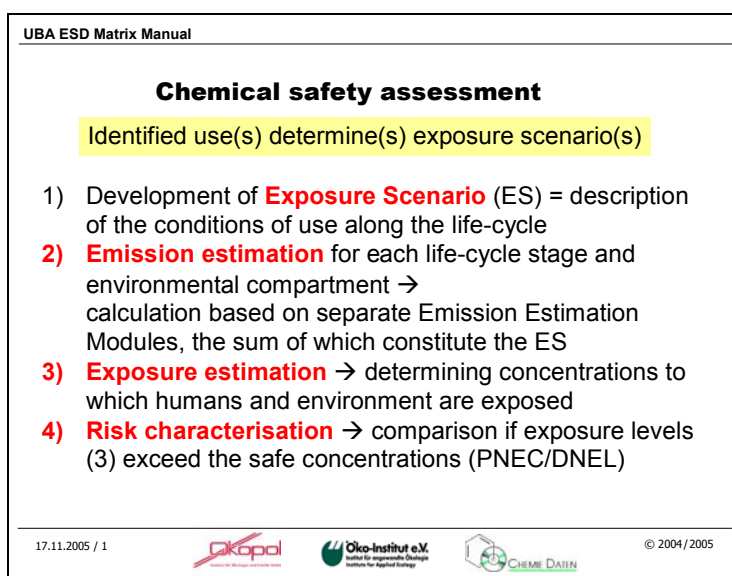


Figure 1.1: Steps of the environmental exposure assessment under REACH

1.2 Environmental emission estimation as key element of environmental exposure estimation

The estimation of emissions from products and processes into the environment is the key element of the environmental safety assessment as all subsequent steps are based these.

Emission estimation means to quantitatively estimate the releases of a substance from a specific life cycle stage into the receiving environmental compartments (water, air, soil) and (solid) waste. It is estimated as emission rate in mass per time. The life cycle stages to be considered are:

- production,
- formulation,
- industrial use,
- professional use (skilled trades),
- private and consumer use,
- service life of article/product,
- recovery, and
- waste disposal.

1.3 Important concepts in chemical safety assessment under REACH

Guidance for the chemical safety assessment (CSA) under REACH is not yet available as discussion at EU level is still ongoing. Nevertheless, basic rules can be deduced from the REACH proposal (2003):

1) Every manufacturer / importer (M/I) has got the responsibility that his own production volume of a substance is used and handled in a safe way by himself and his downstream users (DU).

Therefore, M/I has to assess the safety along the whole life cycle of the substance and to inform the actors downstream of how to use it. For environmental assessments, the used amount is one important parameter to be taken account of.

To estimate the used amount by a customer, the concept of the 'fraction of main source' is applied. The 'fraction of main source' describes the share of the production/import volume of M/I which is used by the biggest client. It describes a point source (e.g. installation or sewage treatment plant) and is used for estimating local emissions.

For regional emissions it is assumed that the production volume ends up in different types of products. The amounts contained in products are emitted diffusely to the environment.

2) Every user of a substance (DU) is responsible to ensure that risks are adequately controlled in his own use

All downstream users have to ensure that they comply with the exposure scenarios communicated to them. This implies that the downstream user has to compare the own company practice (processes, used amounts, risk reduction measures etc.) with the conditions described in the ES.

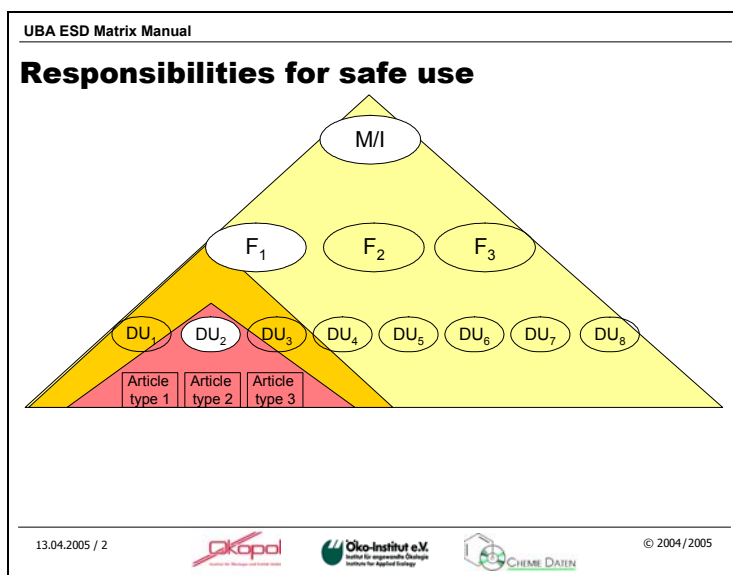


Figure 1.2: Responsibility to ensure safe use of a substance.
The triangles represent the coverage in an exposure scenario.

3) In the assessment, the scale of emissions is to be taken into account.

Emissions from production, formulation, industrial use, professional use, and partly from waste disposal are local emissions: substances are emitted from distinct points and are assessed at local scale. Emissions from consumer use and service life are usually⁶ assessed at regional level, because the use of chemicals and articles by consumers is wide dispersed.

The assessment scale determines 'the dimension of the environment' which is receiving a given emission. Thus, the scale is important for modelling exposure levels and for the risk characterisation. In the existing EU technical guidance document the parameters of a "standard" local and regional environment have been defined.

4) For emissions from articles, steady state is assumed

Substance emissions during service life are usually assessed at regional level. Therefore, M/I has to estimate, which share of his production volume is emitted during the service life of articles and has to sum up the single fractions resulting in a regional emission rate per environmental compartment.

⁶ Exceptions are indoor uses of articles and formulations where emissions to water are regarded local because they are emitted to the environment through the sewage treatment plant. This is not part of the IT-tool.

Steady state means that the total emission from articles remains constant over time, because the substance amount being disposed of via articles equals that being newly placed on the market. Figure 1.3 shows exemplary emission curves from one article type with a lifetime of 5 years. The black line at the top is the sum of all emissions from articles during their service life (e.g. in year 5, the sum of the purple, bright blue, yellow, pink, and dark blue line).

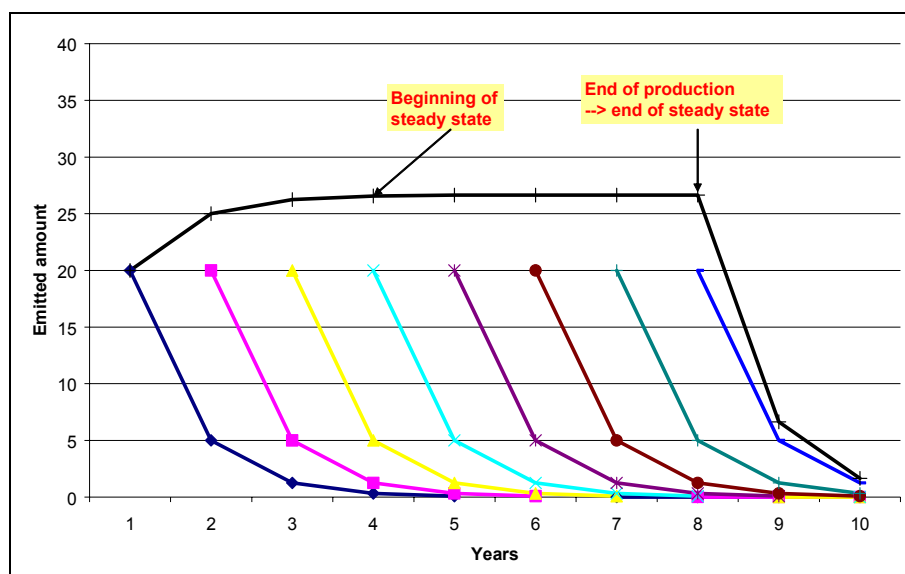


Figure 1.3: Steady state of emissions during service life

1.4 Open questions of aggregation

Under REACH, each manufacturer/importer (M/I) is responsible that risks are adequately controlled for the entire lifecycle (own production, handling and use by all downstream users, during service life and disposal). The downstream users have to check if their use(s) is covered by the communicated ES.

In order to cover cumulative risks resulting from the fact that there are several actors handling a substance two questions arise:

1.4.1 Accumulation of amounts at DU level

If a downstream user (DU) assesses the use of his substance is safe, all sources and amounts should be taken into account to determine local risks. This would mean to sum up all substance amounts used, whether as pure substance or contained in preparations regardless by whom they were supplied. The total substance emission should be compared to the values of no concern (PNEC).

However, this approach is currently not supported by REACH. The downstream user is not to assess cumulative risks at his installation. Therefore, difficulties related to summing up substance amounts in different products (e.g. how to identify concentrations in preparations or to determine in which way the exposure scenario for a preparation corresponds to the safety of single components) are not discussed here.

1.4.2 Accumulation of amounts from different manufacturers

Usually substances are produced / imported by different M/I. If M/I assesses safety only accounting for the own substance volume, he disregards other M/I's contributing to the overall risk. For example, in modelling local environmental concentrations, according to the REACH proposal it can be disregarded that the sewage may also be used by other companies which discharge the same substance. Two options could be taken to consider other emission sources in estimation:

1) Each actor ensures that his emissions remain under the safe level. This means e.g. that at the point of discharge the substance concentration in the company wastewater is so low that no effects in the environment are expected to occur (below PNEC). The regional background concentration of the substance needs not be taken into account.

2) The regional background concentration⁷ is added to the predicted local concentrations. The background concentration integrates all pollution sources which contribute to environmental concentrations of a substance (the current EU TGD approach).

Which approach will be chosen at EU level is not clear at the moment. In the frame of this project, the addition of background concentrations to local emissions is supported.

2 Introduction to the manual and the IT-tool

In the REACH Implementation Projects (RIPs) guidance documents and tools will be developed to support the implementation of REACH. In the RIP 3.2 guidance for elaborating a chemical safety assessment will be developed. The manual and IT-tool at hand support the emission estimation to be done in the chemical safety assessment.

2.1 Target group

The target group of the manual and IT-tool are:

- o manufacturers and importers having to assess exposure under REACH,
- o formulators and other actors using (= downstream users) substances and/or preparations and wanting to check their conditions of use against the exposure scenario communicated to them in the annex of the SDS,
- o formulators and other actors using substances and/or preparations performing a downstream user CSA.

2.2 Aim of the manual

The aim of the manual is to:

- o explain how to use the emission estimation tool for plastic additives,
- o make the calculation routines of the IT-tool transparent and understandable,
- o give background information for the assessment where needed or helpful.

⁷ The method for modelling background concentrations has been described in the EU TGD on Risk Assessment (2003). In principle it is assumed that one tenth of the total EU production volume of a substance is emitted. This amount is received by a "standard regional environment", resulting in regional predicted environmental concentrations for the different environmental compartments.

2.3 Scope of the manual and the IT-tool

The overall scope of the guidance (manual plus IT-tool) is environmental emission estimation occurring at all relevant life cycle stages of plastic additives in thermoplastics⁸. The manual and IT-tool applies to different types of additives, but the PEC derivation and risk characterisation for the water compartment are not directly applicable for metals and complex mixtures of substances. The same applies to substances for which the log Pow is not a reliable predictor for the partitioning behaviour between water and sediments (e.g. ionic substances or surfactants).

Emissions to air, water, soil, and solid waste are distinguished. Thus, the results of the estimation are daily emission rates to the local environment (e.g. $E_{\text{local_air}}$; [kg.d⁻¹]) and annual emission rates to the regional environment (e.g. $E_{\text{regional_water}}$; [t.a⁻¹])

An environmental fate model is not part of the guidance and IT-tool. The result of the emission estimation should be used in existing environmental fate models to derive predicted environmental concentrations (PECs; e.g. SimpleTreat model for STP, EUSES etc.).

Nevertheless, to facilitate testing the tool and demonstrating the refinement need of an exposure assessment a simple module accounting for the municipal sewage treatment plant (STP) and the dilution in the receiving surface water is added. This module estimates a PEC in the surface water. Figure 2.1 visualises the scope of the emission estimation tool, the arrow points to the estimation result.

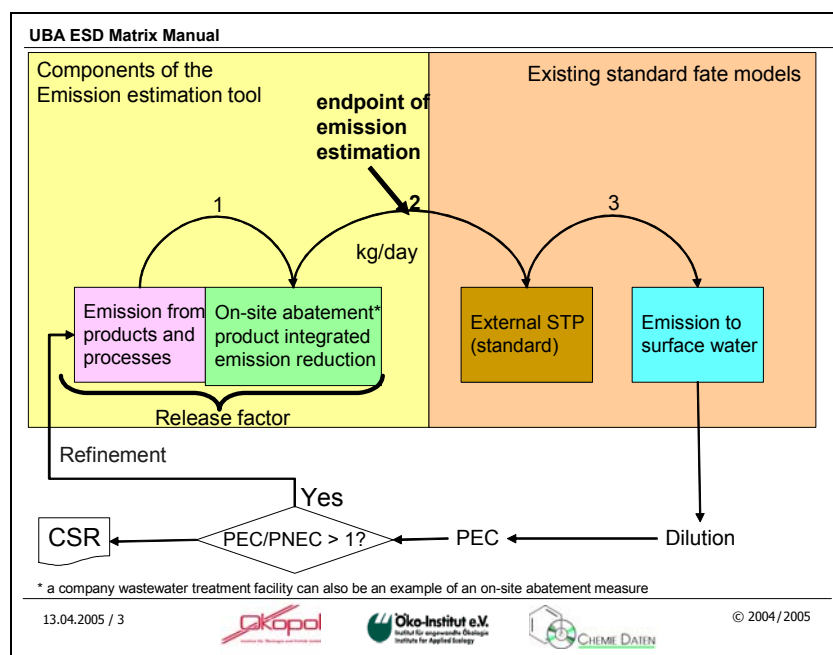


Figure 2.1: Scope of the emission estimation tool

⁸ The tool does not contain specific emission factors for thermosetting plastics.

2.4 Important terms used in the manual

Emission driver (ED) = parameter significantly influencing the amount of a substance emitted to the environment. The term is used at conceptual level.

(Emission) parameter (EP) = input category of the tool, corresponding to the emission drivers. The parameters are: Quantity of a substance (Q), days of release (T), fraction of main source (f), scale of release (local/regional), and the emission factor (F). The parameters may be composed of further values (e.g. the used amount is derived from the production volume x fraction applied by main client).

Emission (rate) to the environment (E) = result of the emission estimation = amount of a substance emitted to the environment. The dimension is [kg per day]. The emission is usually further qualified regarding its pathway (index = air, water, soil).

Emission factor (F) = numeric value describing which share of the substance amount used in a product or process is emitted. It consists of the fraction emitted from a product or process and the efficacy of risk management measures applied. The factor is specific for each life cycle stage and for each environmental compartment (indices for emission pathways are: air, water, soil, waste and indices for the emission sources are: prod (production), form (formulation), conv (conversions/industrial use), service (service life) and disp (disposal), respectively).

Emission estimation module (EEM) = smallest calculation unit of the emission estimation, delivering the emitted amount of a substance from a product or process of a given life cycle stage.

3 Overview of manual structure

The manual is divided into an introduction to the estimation method (Chapter 4 to 6) and specific chapters on the "production", "formulation", "industrial use (= here conversion)", "service life", and "waste disposal" of plastic additives in thermoplastics (Chapter 7). The methods and default values used in the calculation are taken from the OECD Emission Scenario Document on Plastic Additives (OECD ESD, 2004)⁹ and the EU Technical Guidance Document on Risk Assessment (EU TGD, 2003)¹⁰.

Chapter 7 describes the different life cycle stages and the equations to estimate emissions. The parameters used are explained and internationally agreed default values (reasonable worst case) are given. The use of default values has two advantages: For low-risk uses of a substance, an estimation with default values should result in "adequate control of the risk". Thus no detailed data collection is needed. Secondly, default values can be used in case specific data is not available.

⁹ OECD Series on Emission Scenario Documents (ESDs), Number 3: Emission Scenario Document on Plastic Additives, Document Number ENV/JM/MONO(2004)8, June 2004.

¹⁰ Technical Guidance Document in support of Commission Directive 93/67/EEC on risk assessment of new notified substances, Commission Regulation (EC) No 1488/94 on Risk Assessment for existing substances, and Directive 98/8/EC of the European Parliament and of the Council concerning the placing of biocidal products on the market. 2003.

Depending on the knowledge of the conditions of use either the proposed default values can be used or, where possible and relevant, the safety assessor may overwrite the default values and insert his own, more specific values. Own information should be validated and describe the emission situation correctly.

Own information used instead of defaults may be measured data (e.g. waste gas concentration), information from downstream users (e.g. used amounts) or from producers of abatement technology (e.g. efficacy of air filters). Own information can be used, when the estimation with defaults results in a risk and a refinement of the safety assessment is necessary. Refinement options of the emission assessment are explained in the manual. Table 2.1 gives an overview of life cycle steps and information necessary for the estimation.

Table 3.1: Lifecycle and input parameters for estimating emissions of plastic additives

	P Production See 7.1	F Formulation See 7.2	IU Industrial Use See 7.3	PU Professional Use	CU Consumer Use	SL Service Life 7.4	W Waste 7.6
amount per year	production volume	fraction of volume used for the process(es) assessed		not relevant for plastic additives	not relevant for plastic additives	fraction of total amount	fraction in waste
release days	production days		days of operation			article lifetime	days of operation
release scale ¹¹	local	Local	local			regional / local ¹²	local / regional ¹³
loss from process	Specific emission factors, depending on substance properties, processes and products as well as conditions of use / service life. Detailed discussion: see relevant sub-chapters.						

4 Understanding the underlying equation

The emission estimation is based on one equation, which is applicable for all lifecycle steps.

$$E \text{ [kg/d]} = \frac{Q[t/a] * F * 1000}{T[d/a]}$$

Equ. 1: Basic formula for the emission estimation

E [kg/d] = emission rate to the environment. To be specified for the environmental compartment/waste and the emission scale (e.g. $E_{\text{local,air}}$)

Q [t/a] = substance amount used in the lifecycle step under assessment

F = emission factor from a specific activity of the lifecycle step. To be specified for each process and environmental compartment/waste (e.g. $F_{\text{form,air}}$)

T [d/a] = release days; the amount of days on which release of the substance occurs. To be specified for each process.

¹¹ The release scale is set as default value for each lifecycle stage as shown in the table but can be changed by the safety assessor if required

¹² No local scenario can be estimated for the service life stage by the tool as yet.

¹³ No regional scenario can be estimated for the waste life stage by the tool as yet.

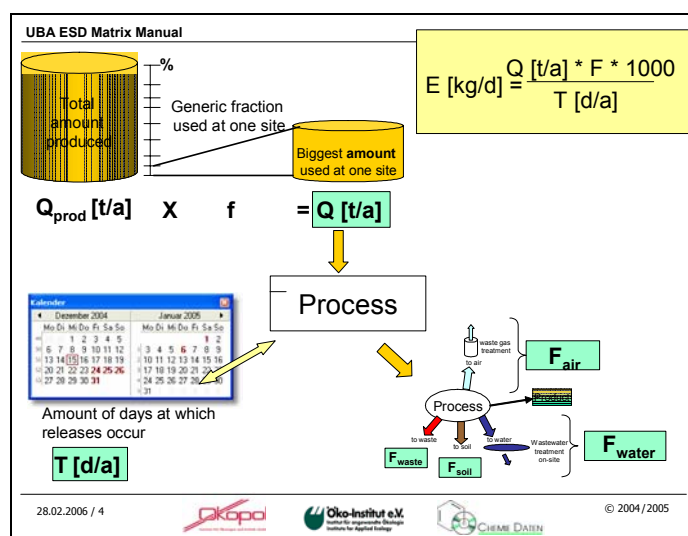


Figure 4.1: Parameters and factors (turquoise) to estimate substance emissions from production, formulation, use and disposal

M/I calculating local emissions of their downstream users (DU), assume their biggest client (compare also Chapter 1.2). This biggest client is determined using Equation 2. The production/import volume is multiplied with the “fraction of main source”.

$$Q[t/a] = Q_{own}[t/a] * f$$

Equ. 2: Derivation of amount used at main source

Q [t/a] = used amount by biggest client

Q_{own} [t/a] = total volume of substance for which the assessment is made

f = factor for the main emission source = the biggest client

If a DU estimates emissions from his processes, he calculates with the own use volume¹⁴. If the DU assesses emissions from uses further downstream, his use volume is to be applied for the total amount (Q of Equ. 2)¹⁵.

The emission factor (F) describes the fraction of the total amount Q which is emitted to the environment/waste. For each compartment/waste, the factor is different, depending on the substance properties, types of products/processes and risk management measures applied.

Default emission factors are specific to the emission pathway. Air emissions from evaporation during formulation may condensate in the mixing vessel. The condensation film in the vessel's lid may be removed during cleaning operations. Hence, the final emission pathway is wastewater and not air.

¹⁴ In the IT-tool, the own use volume can be entered in the beginning of the program.

¹⁵ When a downstream user is assessor, he can hardly make use of the pick-lists with default values for the biggest client (fraction of main source) as these relate to the substance volume of M/I in the chain. This is usually not known to the DU. Due to resource constraints and lack of an existing methodological solution, this issue could not be resolved in the current project. However, the DU may still make an input based on his own information in the IT-tool.

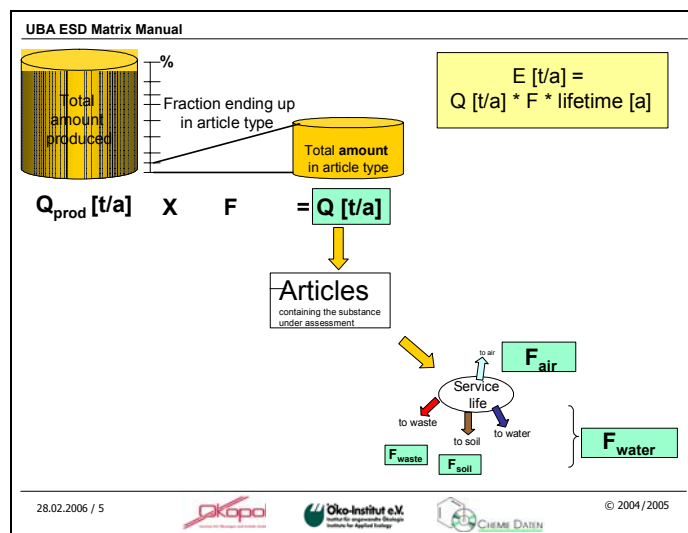


Figure 4.2: Parameters and factors (turquoise) for estimating emissions from service life

Emissions to waste are not considered in assessing the service life, as the entire article and the additives contained are used as input to the lifecycle stage “waste disposal”. For reasons of simplification in this manual and the IT-tool, the industrial wastes containing the substance and occurring during production, formulation and conversion are not further assessed¹⁶. The following figure shows the concept of how the waste stage should be processed, also including disposal of processing wastes (which could be covered in an extended version of the IT tool).

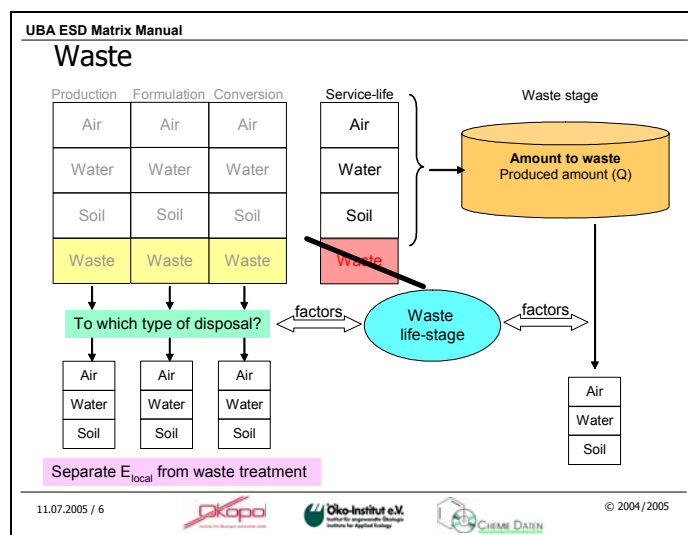


Figure 4.3: Conceptual approach for the waste stage

¹⁶ The substance amounts lost to waste can be assessed separately by inserting the amounts ‘emitted to waste’ of the respective life cycle stages into the module for the waste life stage.

4.1 Iterations in the assessment

The IT-tool and this manual aim to provide an emission estimation method, which is resource efficient and valid under REACH. The approach is to start with information, which is readily available to the safety assessor, namely information on the substance properties¹⁷, the marketed amount per year, the uses of a substance¹⁸ and the default values proposed here. For each lifecycle stage¹⁹ three iterations are foreseen which enable a tiered assessment, where each iteration becomes more detailed. Moving from iteration to the next is triggered if the PEC/PNEC comparison results in a value exceeding 1 for the water compartment.

The following figures show the iterations for the assessment of the production, formulation and conversion lifecycle step²⁰ of plastic additives supported by the manual and IT-tool. Parameters shaded in orange indicate parameters or values newly introduced in the respective iteration. Parameters belonging to the modelling of a predicted environmental concentration are shaded in green (dilution, emission factor from STP).

The aim of the first iteration is to sort out all substances and their uses, which are uncritical, even if no abatement is applied. It is assumed that the entire production volume is used in one single application. Conservative emission factors are used and no treatment is accounted for. The factors cannot be changed by the user of the tool. The calculation is done 'automatically' by the IT-tool.

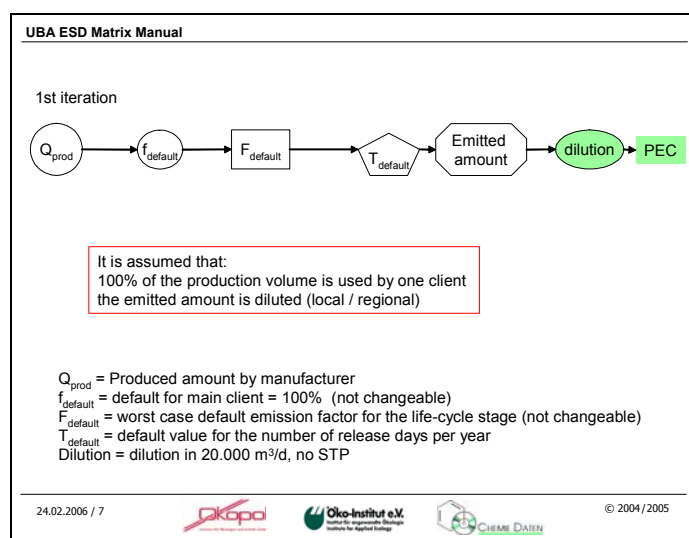


Figure 4.4: 1st iteration: calculation with defaults

In the second iteration some parameters of the calculation can be specified: The fraction of main source (biggest client) and the release days can be selected as defaults from a pick-

¹⁷ All information for the emission estimation is required under REACH (Annex V).

¹⁸ It is a prerequisite for using this manual and the IT-tool that the safety assessor knows at least the industrial process in which the substance is incorporated into a chemical preparation or article.

¹⁹ The manufacturing stage is an exception, as it is assumed that all information for emission estimation is available to the substance manufacturer

²⁰ Assessing the service life step works slightly different and is explained more in detail in the respective chapter.

list²¹. Also additive and process specific defaults for the emission factors can be selected. In the refinement cycle, the emission factors can be overwritten with own values. The safety assessor may use measured or modelled own information. In addition, a municipal sewage treatment plant can be added in deriving the PEC for the aquatic environment.

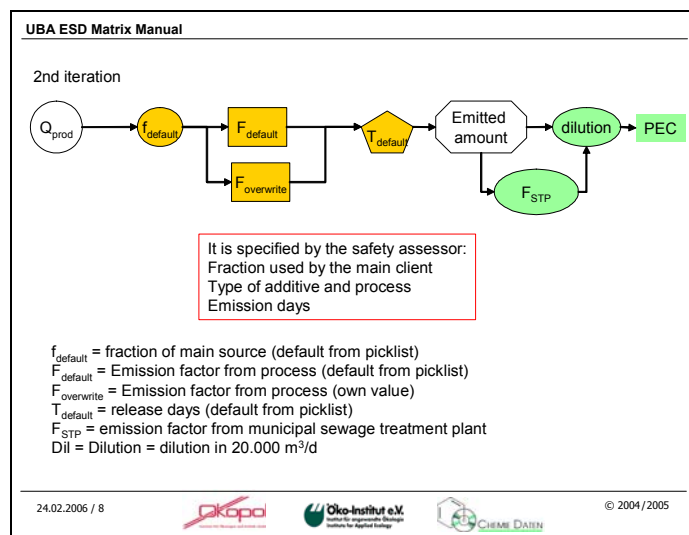


Figure 4.5: 2nd iteration: specific fraction of main source, release days, emission factors, connection to STP and overwriting defaults

In the third iteration, the default values of the fraction of main source and the emission days can be overwritten with own information. In addition, the application of on-site risk management measures can be included in the emission estimation.

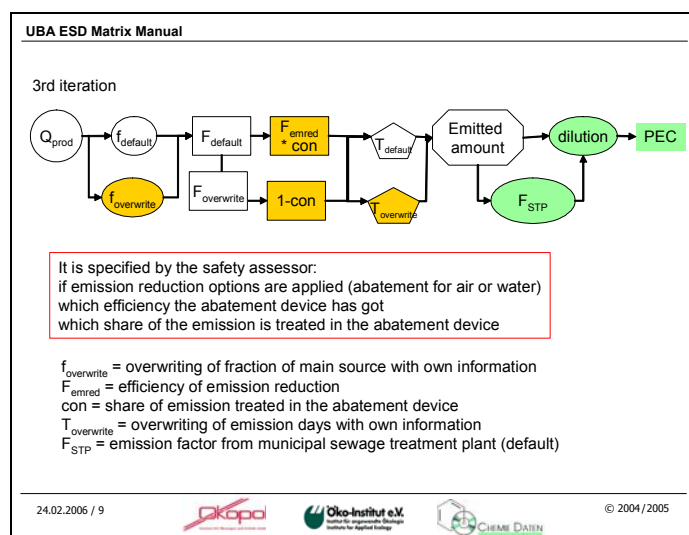


Figure 4.6: 3rd iteration, adding on-site emission reduction measures

²¹ In order to use the pick-lists the substance volume of M/I needs to be known. Thus, DUs may not benefit from the defaults, but can enter their own information in free text.

5 Base information for the assessment

In the beginning of the emission estimation information on the type of industrial use determining the life cycle of a substance, the lifecycle steps, substance properties, substance volume for assessment and the EU market volume are compiled. As first step, the safety assessor has to specify the life cycle of the substance to be assessed. In this case this would be the scenario "additives in plastics".

5.1 Function of the substance

The function of the additive is relevant for the emission factors at all life cycle stages except waste. In this manual and the IT-tool the functions shown in table 5.1 are supported.

Table 5.1: List of additive types supported by the manual and IT-tool²²

Antistatic Agent (inorganic)	Curing agent (liquid)*	Polymeric impact modifier**
Antistatic agent (organic)	Curing agent (solid)*	Preservative (inorganic)**
Antioxidant	Filler	Preservative (organic)**
Blowing agent (liquid or gas)****	Flame retardant (inorganic)	Lubricant (inorganic)****
Blowing agent (solid)***	Flame retardant (organic)	Lubricant (organic)****
Colourant (Dye)	Heat stabiliser (liquid)	UV / weathering stabiliser
Colourant (Pigment)	Heat stabiliser (solid)	Viscosity aid**
Coupling agent*	Plasticizer	

* destroyed during compounding → no conversion, service-life and disposal stage

** check if substance is exempted (polymer? use as biocide according to Directive 98/8/EC?)

*** destroyed during conversion → no service-life and disposal stage

**** destroyed or lost during service-life, no disposal stage

5.1.1 Specification of emission scenario

The life cycle of plastic additives consists of five lifecycle stages²³. The safety assessor may remove lifecycle stages if they are not relevant.

Example: Coupling agents react during compounding → lifecycle stages "conversion", "service life" and "waste" can be omitted (columns).

In reality the processes at different lifecycle stage of an additive can rarely be assigned to single supply chain actors. Nevertheless, in the emission estimation, each stage is calculated separately, facilitating the transparent derivation of emitted amounts and the identification of products and processes where the risks are not adequately controlled. If the safety assessor knows that processes of different life cycle stages occur simultaneously and at the same installation, he should manually sum up the emissions from each process before modelling environmental concentrations and performing the risk characterisation²⁴.

²² If emissions of an additive type not covered by the list shall be estimated, the safety assessor may choose to use default values of a similar additive type or choose the highest factors (worst case) given.

²³ Lifecycle stages which are not applicable are left blank.

²⁴ The risk characterisation is not part of the manual and IT-tool but for demonstration purposes, the PEC/PNEC comparison for the water compartment is supported and explained here.

5.2 Basic information on the substance

Basic substance information is needed throughout the assessment but is compiled only once in the beginning. The following table explains how substance properties influence emissions and for which calculations the information is needed.

Table 5.2: Basic information on the additive

Property	Why is it relevant / needed?
Vapour pressure [Pa]	Determines how easily a substance emits to air. For simplification, the additive is assigned to a volatility group (cf. Table 5.4)
Physical appearance	Determines emissions during raw material handling. Relevant for additives supplied in solid form
LogPow	Characterises the tendency to dissolve in water or in a lipid phase. It is needed to determine emissions from a sewage treatment plant.
Degradability	Determines how much of the additive is degraded in the sewage treatment plant. Relevant for wastewater discharged to the municipal sewage or where on-site wastewater treatment is done (RRM).
Molecular weight [g/mol]	Needed for the calculation of predicted environmental concentrations
Water solubility [mg/l]	Needed for the calculation of predicted environmental concentrations
PNEC [$\mu\text{g/l}$]	Necessary for the PEC/PNEC comparison. The value is to be derived from toxicity test data (not supported by IT-tool nor manual)

The following tables facilitate the identification of the additive's volatility group²⁵. The vapour pressure of a registered additive should be known, as it is required according to Annex V of REACH. If the data is not available, the software EPIWIN can be used to model it.

Table 5.3: Groups of volatility

Low	Substance is solid and vapour pressure $< 10^{-6}$ Pa at 20°C
High	Substance is a gas

Table 5.4: Grouping of volatility according to vapour pressures [Pa]

Volatility group Temperature	High	Medium	Low
20	$V_p > 10^{-5}$	V_p between 10^{-5} and 10^{-6}	$V_p < 10^{-6}$
50	$V_p > 10^{-3}$	V_p between 10^{-3} and 10^{-4}	$V_p < 10^{-4}$
100	$V_p > 0.1$	V_p between 0.1 and 0.01	$V_p < 0.01$
150	$V_p > 10$	V_p between 1 and 10	$V_p < 1$
200	$V_p > 100$	V_p between 10 and 100	$V_p < 10$

Information in the following tables is necessary only for modelling environmental concentrations of a substance.

²⁵ Source: Table 6.1 of OECD emission scenario document, modified

Table 5.5: Groups of degradability

	Criteria
Not degradable	not degradable in test
Ready degradable	pass level 28 days, 10-day window fulfilled
Ready degradable, no 10d	pass level 28 days, 10-day window <u>not</u> fulfilled
Inherently degradable	OECD/EU test result: $k_{bio_{stp}} = 0.1$ hour in the aqueous phase of activated sludge

In addition, the value of the LogPow needs to be known.

The logH is needed for the calculation of the efficiency of wastewater treatment.

$$\text{Henry coefficient} = \frac{VP * MW}{\text{solubility}}$$

Equ. 3: Calculation of Henry coefficient

VP [Pa] = vapour pressure

MW [g/mol] = molecular weight

solubility [mg/l] = water solubility

Table 5.6: Groups of LogH

	Criteria
LogH	< 1
LogH	1-2
LogH	≥ 2

If M/I estimates emissions, the annually imported/produced amount of the substance is needed as input for emission calculations of all lifecycle stages [Q]. If a DU estimates emissions, his annual use amount is needed as "total amount" [Q] for the own and the following lifecycle stages.

The total EU market volume is needed to calculate the environmental background concentrations of the substance. Information sources can be the IUCLID files on the ECB homepage or, in the future, the European Chemicals Agency.

6 Assessment of risk to the aquatic environment

By comparing the predicted environmental concentration (PEC) and the predicted no effect concentration (PNEC) a statement on the risk can be made: if the PEC/PNEC quotient remains under 1, the use of the substance can be regarded safe. If it exceeds 1, either the assumptions of the assessment are too rough and need to be refined or the use is in fact not safe and should not be supported in the future.

Municipal wastewater treatment is part of the derivation of the PEC, rather than the estimation of emissions of the company (cf. Figure 2.1). Therefore, the emission factor from the treatment plant (F_{STP}) is introduced in the derivation of the PEC and not in the emission estimation. In opposite, on-site wastewater treatment is part of the emission estimation and is taken into account in the third iteration at each life cycle stage (F_{emred}).

The way of deriving a PEC described here is simplified and only consists of municipal wastewater treatment and dilution in the environment. For a risk characterisation under REACH appropriate environmental fate models like EUSES²⁶ should be used. The result of the estimation carried out using this tool is an emission to a specific environmental compartment per time to a local or regional environment. This value can be an input to respective fate models in order to estimate environmental fate with a validated model.

6.1 Calculation of regional background concentration

The $PEC_{\text{regional,background}}$ describes which average concentration of a substance is expected in the aquatic regional environment. In order to take account of other emission sources than those related to the own substance volume produced/imported or applied, the regional background concentration is added to the environmental concentrations resulting from local and regional emissions.

For this manual and the IT-tool, a pragmatic way to derive this value has been chosen. It is more simplistic than the method of the current TGD²⁷. The derivation of the regional background concentration is given in the following equation.

$$PEC_{\text{regional background}} = \frac{[Q_{EUprod} * 0.02 * 0.1 * 0.8 * F_{STP}] + [Q_{EUprod} * 0.02 * 0.1 * 0.2]}{dil_{\text{regional}}} * 1000$$

Equ. 4: Modelling of the regional background concentration

Q_{EUprod} [t/a] = EU market volume of the substance

0.022: overall emission factor to water²⁸

0.1: assumption that 10% of EU production volume is used in the region

0.8/0.2: 80% of emission are discharged to a sewage treatment plant, 20% aren't

$dil_{\text{regional}} = 25 * 10^9 \text{ m}^3/\text{a}$ ²⁹

6.2 Derivation of PEC_{local}

The formula is applicable to all local emissions. When using the IT-tool, the sewage treatment plant can be added to the PEC modelling at the second iteration level. Here, a share entering the STP can be specified. The emission factor from the STP is selected automatically by the tool from the substance property information³⁰.

²⁶ <http://ecb.jrc.it/existing-chemicals/>

²⁷ In essence, an overall emission factor to water has been calculated from the reasonable worst case emission factors of the single life cycle stages given in the ESD. This overall emission factor is applied to 10% of the market volume. The emission is sent through the STP following the 20/80 rule and diluted in the TGD regional water volume. The user of the IT-tool only needs to enter the total EU market volume and the substance properties to obtain the $PEC_{\text{regional,background}}$. This approach is deemed sufficient for the IT tool, as under REACH, the background concentrations neither need to be calculated nor to be taken into account by the registrant.

²⁸ The reasonable worst case emission factors integrated in the value are – production: 0.003, formulation: 0.00225, conversion: 0.0025, service life: 0.00837 and waste: 0.006.

²⁹ Value derived from TGD

³⁰ C.f. Chapter 7.6

$$PEC_{local,water} = \frac{[E_{local,water} * con * F_{STP} + E_{local,water} * (1 - con)] * 1000}{dil_{local}}$$

Equ.5: Modelling $PEC_{local,water}$

$PEC_{local,water}$ [mg/l] = predicted environmental concentration in the receiving surface water at local scale

$E_{local,water}$ [kg/d] = daily emission to water [kg/d]

Con = share of wastewater discharged to the municipal STP

F_{STP} = emission factor from municipal sewage treatment plant (c.f. Table 7.11)

dil_{local} : dilution in local aquatic environment = 20,000 m³/d³¹

$PEC_{regional,background}$ [mg/l] = background environmental concentration

Sometimes, emissions are intermittent; that means the release occurs on less than 12 days per month. In these cases, the PNEC can be increased by the factor 10 in the PEC / PNEC comparison³².

6.3 Derivation of $PEC_{regional}$

The formula is applicable to all regional emissions. In the IT-tool, this applies to the service life of plastic additives. In the PEC derivation for the regional environment from outdoor uses, no sewage treatment plant is assumed. The IT-tool does not support the use of a local scenario in the service life stage, thus STP calculations have to be done manually.

$$PEC_{regional,water} = \frac{\sum E_{regional,water} * 1000000}{dil_{regional}}$$

Equ. 6: Modelling of PEC for the regional aquatic environment

$E_{regional,water}$ [t/a] = emissions to water from service life. If different product types with differing lifetimes are assessed, all emissions from them are to be summed up

$dil_{regional}$ [m³/a] = regional dilution, 25 * 10⁹

³¹ The default dilution volume in the tool is set to 20,000 m³ for the local scenario. This is composed of a dilution volume of 2,000 at the sewage treatment plant and a 1:10 dilution in the receiving surface water. The dilution volume is not changed when the emitted water is not treated in an STP. It is not possible to change the dilution in the STP and the dilution in the receiving surface water separately, but only the total water volume can be changed. Changing the dilution volume is possible at iteration level 2 and 3 in the IT-tool.

³² The ecotoxicological reason behind is that the environment has time to recover between releases.

7 Assessment of particular life cycle stages

In the following chapters, the emission estimation for each life cycle stage is explained in detail. This does not include the calculation of predicted environmental concentrations; for this the safety assessor is referenced to Equation 4 and 6.

7.1 Manufacture of the additive

7.1.1 First / second iteration

The first and second iteration are the same for the lifecycle stage manufacture of the additive, as it is assumed that no default calculation is needed.

$$E_{local,prod} = \frac{Q * F_{local,prod} * 1000}{T}$$

Equ. 7: Emissions during substance production

E [kg/d] = Emission to the environment

Q [t/a] = own production volume

T [d/a] = release days

F_{local,prod} = default emission factor for production

No defaults are provided for the release days as own information should be available. The emission factor (F) can be selected from Table 7.1. Please note that the emission factors are comparably high.

Table 7.1: Emission factors³³ for the production of additives [source: TGD Table A1.1]

Compartment	Volatility	Emission factor F _{prod}
Air	Low	0.00001
	Medium	0.0001
	High	0.001

Compartment	EU market volume	Emission factor F _{prod}
Water	< 1000 t/a	0.02
	> 1000 t/a	0.003

Compartment		Emission factor F _{prod}
Soil		0.0001

As refinement of the calculation, it is possible to overwrite the emission factors and release days with own values. These could be measured values or derived from material flow analysis etc. For emissions to soil: if the installation and filling stations are equipped with troughs or foils to avoid leaking to soil, the emission factor can be set to the value '0'.

³³ There is no information provided in the TGD on whether these factors include integrated risk reduction measures or onsite abatement used in the production.

7.1.2 Third iteration

In the third iteration on-site emission reduction measures can be taken into account. The emission factor F_{emred} (substance-specific efficacy of emission reduction) is combined with the share of the emission entering the abatement device.

$$E_{local,prod} = \frac{[Q * (1 - con) + Q * con * (1 - F_{emred})] * F_{local,prod} * 1000}{T}$$

**Equ. 8: Determination of emissions
during substance production with risk management measures**

E [kg/d] = Emission to the environment

Q [t/a] = own production volume

con = fraction of emission captured by the respective emission treatment device

F_{emred} = efficacy of risk management (fraction of emission reduction (100% = 1))

$F_{local,prod}$ = emission factor for production

T [d/a] = release days

7.2 Formulation (production of master batches and compounding)

If the additive is contained in preparations in concentrations below the lowest limit value³⁴ of the Preparations Directive (99/45/EC) only the manufacturing of the additive and the formulation process have to be assessed. Emissions from formulation are calculated according to the equation below.

$$E = \frac{Q * f_{mainsource} * F_{local,form} * 1000}{T}$$

$$F_{local,form} = F_{rawmat} + F_{comp}$$

Equ.9: Emissions from formulation

E [kg/d] = local emissions from formulation per day

Q [t/a] = production / import volume of the substance³⁵

$f_{mainsource}$ = parameter adjusting the substance amount used at second iteration level; specification of share of production/import volume of M/I which is used at the local site by the formulator

$F_{local,form}$ = emission factor from formulation

T [d/a] = number of release days at main source

The following description is made from the perspective of the substance manufacturer / importer. If the formulator carries out the assessment, he enters the substance volume he himself handles in the section 'substance information'. The fraction of main source consequently is 1 for assessing his own life cycle stage.

³⁴ cf. Article 13 of REACH

³⁵ If a formulating company estimates emissions, the own use volume is to be entered as share of the production volume of M/I by changing the value for fraction of main source.

7.2.1 First iteration formulation

In the first iteration, the entire substance volume is assumed to be used ($f_{\text{mainsource}} = 1$). The following values are used for the remaining parameters³⁶.

$F_{\text{Water}} = 0.00675$

$F_{\text{Air}} = 0.01025$

$F_{\text{Soil}} = 0.01$

$T = 20 \text{ [d/a]}$

7.2.2 Second iteration formulation

The IT-tool does not support process integrations for polymerisation/compounding and compounding/ conversion. In these cases, emissions can be estimated by assessing the steps separately and adding up the emissions afterwards.

In the second iteration, default values for the release days, the fraction of main source³⁶ and the process and additive-specific emission factors (F) can be selected. Emissions from formulation arise from two steps: the materials handling (F_{rawmat}) and the compounding (F_{comp}) itself. Therefore, two factors are summed up to derive the overall emission factor from formulation. Emissions depend on the dustiness and volatility of the substance, as well as the degree of process containment. Default values for the estimation are:

f = fraction of M/I volume used at local site (cf. Table 7.2 / 7.3).

T = amount of release days (defaults cf. Table 7.2 - 7.4)

F_{form} = emission factor to the environment: consists of a factor for raw materials handling and for the formulation process

F_{rawmat} = emission factor for raw materials handling (defaults cf. Table 7.5)

F_{comp} = emission factor for compounding process (defaults cf. Table 7.6)

The default values for the fraction of main source and for the release days are derived from the tables, by selecting the row with the applicable tonnage ranges of the final product (compounded polymer). **The values refer to the total amount of compounded polymer that can be produced with the total annual production volume of the additive manufacturer.** To calculate this amount, the average concentration of the additive in the polymer compound needs to be known.

$$\text{Amount} = \frac{\text{Total production volume of M / I}}{\text{content in polymer}}$$

Equ. 10: Determination of defaults for release days and fraction of main source

Amount [t/a] = amount of polymer preparation containing the total production volume of M/I

Content in polymer = additive concentration in polymer product

³⁶ The emission factors include emissions from raw materials handling and compounding and are derived from the OECD Emission scenario document. The release days are taken from Table B2.8 of the TGD. It is recognized that these factors are overly conservative.

Table 7.2: Fraction of main source and release days for additives ³⁷

All HPV additives except curing agents & polymeric impact modifiers		
Calculated amount of polymer compound that can be formulated with the total annual production volume of the additive of M/I. Calculation is based on the average percentage of the additive in the polymer. [t/a]	Fraction of main source (formulator) (f)	Release days (T)
< -3500	1	300
3500-10000	0.8	300
10000-25000	0.7	300
25000-50000	0.6	300
≥ 50000	0.4	300

Table 7.3: Fraction of main source and release days for additives.

All LPV additives except curing agents & polymeric impact modifiers		
Calculated amount of polymer compound that can be formulated with the total annual production volume of the additive of M/I. Calculation is based on the average percentage of the additive in the polymer. [t/a]	Fraction of main source (formulator) (f)	Release days (T)
< 5	1	20
5-50	1	60
50-100	1	100
100-500	0.8	200
500-1000	0.6	220

Table 7.4: Fraction of main source and release days for additives

HPV-chemicals used as curing agents & polymeric impact modifiers		
Calculated amount of polymer compound that can be formulated with the total annual production volume of the additive of M/I. Calculation is based on the average percentage of the additive in the polymer. [t/a]	Fraction of main source (at formulator's level) (f)	Release days (T)
–		
< 25000	1	300
25000-50000	0.75	300
≥ 50000	0.4	300

Example: A manufacturer produces a plasticizer with a total annual EU market volume of 8000 t. He knows that the average concentration in the polymer is 20%. Thus, 40000 t/a of polymer compounds can be produced and the fraction of main source select is 0.4 and the release days are 300.

When selecting the emission factors, please note that many additive types appear more than once in most of the following tables, as they are used in different physical states or in different types of processes. When assessing a liquid additive which is only listed with reference to particle sizes (40µm or other forms of physical appearance), please select the value for

³⁷ Tables 7.2, 7.3 and 7.4 derived from the TGD, Tables B2.3, B2.8 and B2.9

> 40µm. When selecting emission factors from Table 7.5, it is important to consider both the type of additive and its physical appearance; in Table 7.6 the process type and the volatility are relevant for the emission factor.

Table 7.5: Emission factors raw materials handling (F_{rawmat})³⁸

Additive type	Physical appearance	F_{Air}	F_{Water}	F_{Waste}
Antioxidant, anti-static agent, blowing agent, colourant, curing agent, fillers, flame retardant, heat stabiliser, polymeric impact modifier, preservative, lubricant, UV and weathering stabiliser, viscosity aids	< 40 µm	0	0.006	0.01
Antioxidant, anti-static agent, blowing agent, colourants, curing agent, filler, flame retardant, heat stabiliser, polymeric impact modifier, preservative, lubricant, UV and weathering stabiliser, viscosity aids	> 40 µm	0	0.002	0.0001
Filler	discontinuous fibre strands	0	0.006	0.001
Filler	continuous fibre strands or mats	0	0	0.0001
Polymeric impact modifier	bales and strips	0	0	0
Curing agent, heat stabiliser	liquids	0	0.001	0
Blowing agent	liquids or gases	0.01	0	0
Plasticizer, coupling agent	all types	0	0.001	0

Table 7.6: Emission factors for formulation (F_{comp})

Additive type	Blending process	Volatility	F_{Air}	F_{Water}
Anti-static agent, inorganic, particle < 40µm	Dry, Banbury and plastisol	involatile	0	0.0005
Anti-static agent, inorganic, particle > 40µm	Dry, Banbury and plastisol	involatile	0	0.0001
Anti-static agent, organic, particle < 40µm	Dry, Banbury	low medium high	0.00001 0.00005 0.00025	0.00051 0.00055 0.00075
Anti-static agent, organic, particle > 40µm	Dry, Banbury	low medium high	0.00001 0.00005 0.00025	0.00011 0.00015 0.00035
Blowing agent (liquid)	No separate emission	all groups	--	--
Blowing agent (solid), particle < 40 µm	Independent of process	all groups	0	0.0005
Blowing agent (solid), particle > 40 µm	Independent of process	all groups	0	0.0001
Colouring agent, dye, particle < 40 µm	Independent of process	all groups	0.00001	0.00051
Colouring agent, dye, particle > 40 µm	Independent of process	all groups	0.00001	0.00011
Colouring agent, pigment < 40 µm	Independent of process	all groups	0	0.0005
Colouring agent, pigment > 40 µm	Independent of process	all groups	0	0.0001

³⁸ Default values of Table 7.4, 7.5 and 7.6 are derived from OECD ESD

Additive type	Blending process	Volatility	F _{Air}	F _{Water}
Coupling agent	Independent of process	Low	0.00001	0.00001
		Medium	0.00005	0.00005
		High	0.00025	0.00025
Curing agent (liquid)	Independent of process	all groups	0.00005	0.00005
Curing agent (solid), particle size < 40µm	Independent of process	all groups	0	0.0005
Curing agent (solid), particle size > 40µm	Independent of process	all groups	0	0.0001
Fillers, particle < 40µm or discontinuous fibre strands	Independent of process	all groups	0	0.0005
Fillers, particle > 40µm or continuous fibre and mats	Independent of process	all groups	0	0.0001
Flame retardant (inorganic), particle < 40µm	Independent of process	all groups	0	0.0005
Flame retardant (inorganic), particle > 40µm	Independent of process	all groups	0	0.0001
Flame retardant, (organic), particle < 40µm	Independent of process	Low	0.00001	0.00051
		Medium	0.00005	0.00055
		High	0.00025	0.00075
Flame retardant, (organic), particle > 40µm	Independent of process	Low	0.00001	0.00011
		Medium	0.00005	0.00015
		High	0.00025	0.00035
Heat stabiliser (solid), particle < 40µm	Dry, Banbury	low	0.00001	0.00051
		medium	0.00005	0.00055
		high	0.00025	0.00075
Heat stabiliser (solid), particle < 40µm	Independent of process	involatile	0	0.0005
Heat stabiliser (solid), particle < 40µm	Plastisol blending	all groups	0	0.0005
Heat stabiliser (solid), particle > 40µm	Dry, Banbury	low	0.00001	0.00011
		medium	0.00005	0.00015
		high	0.00025	0.00035
Heat stabiliser (solid), particle > 40µm	Independent of process	involatile	0	0.0001
Heat stabiliser (solid), particle > 40µm	Plastisol blending	all groups	0	0.0001
Plasticiser	Dry / Banbury blending	Low	0.00001	0.00001
		Medium	0.00005	0.00005
		High	0.00025	0.00025
Plasticizer	Plastisol blending	all groups	0	0
Polymeric impact modifiers, bales and strips	Independent of process	all groups	0	0
Polymeric impact modifiers, particle < 40µm	Independent of process	all groups	0	0.0005
Polymeric impact modifiers, particle > 40µm	Independent of process	all groups	0	0.0001
Preservative, particle < 40µm	Independent of process	Low	0.00001	0.00051
		Medium	0.00005	0.00055
		High	0.00025	0.00075
Preservative, particle > 40µm	Independent of process	Low	0.00001	0.00011
		Medium	0.00005	0.00015
		High	0.00025	0.00035

Additive type	Blending process	Volatility	F _{Air}	F _{Water}
Lubricants, particle < 40µm	Independent of process	Low	0.00001	0.00051
		Medium	0.00005	0.00055
		High	0.00025	0.00075
Lubricants, particle > 40µm	Independent of process	Low	0.00001	0.00001
		Medium	0.00005	0.00015
		High	0.00025	0.00035
Viscosity aid, particle < 40 µm	Independent of process	all groups	0	0.0005
Viscosity aid, particle > 40 µm	Independent of process	all groups	0	0.00001

As refinement option, the additive and process specific emission factors can be overwritten with own information.

7.2.3 Third iteration formulation

In the third iteration the default values selected for determining the fraction of main source³⁹ and the release days as well as the emission factors can be overwritten with own information. In addition, on-site emission reduction measures can be taken into account. The emission factor F_{emred} depends on i) the of the total waste gas or waste water entering the emission reduction device and ii) its efficiency.

$$E_{local,emred} = E * (1 - con) + E * con * (1 - F_{emred})$$

$$E = \frac{Q * f_{mainsource} * F_{localform}}{T}$$

Equ. 11: Emission factor after abatement equipment

F_{emred} = factor for the efficiency of on-site emission reduction measures.

Con = share of emission captured for treatment in the emission treatment device

7.3 Industrial use (Conversion processes)

The emission estimation of this life cycle stage is not relevant for coupling agents and curing agents, as these react during compounding⁴⁰.

The following description is made from the perspective of the substance manufacturer / importer. If the tool is used for the assessment by an industrial user, he enters the substance volume he assesses in the section on substance information. Consequently, for assessing his own life cycle stage, the fraction of main source is to be set to 100 %.

$$E = \frac{Q * f_{mainsource} * F_{local,conv} * 1000}{T}$$

Equ.12: Emissions during conversion

³⁹ Note that here the share of the substance volume of M/I is to be entered and not the absolute amount of the substance used.

⁴⁰ Consequently the life cycle stages conversion, service life and waste are not relevant either.

E [kg/d] = local emissions from conversion per day
Q [t/a] = production / import amount of M/I
f_{mainsource} = parameter adjusting the substance amount used at second iteration level; specification of share of production/import volume of M/I which is used at the local site by the formulator
F_{local,conv} = emission factor from conversion → 1st iteration conservative default, 2nd iteration emission factor is additive specific
T [d/a] = number of release days at main source

7.3.1 First iteration conversion

In the first iteration, the $f_{\text{mainsource}}$ is set to the value 1 in Equation 12, as it is assumed that the entire substance amount is used in one process. The following values are used for the remaining parameters⁴¹.

F_{local,conv,air} = 0.0025
F_{local,conv,water} = 0.025
F_{local,conv,waste} = 0.10
T = 10 [d/a]

7.3.2 Second iteration conversion

In the second iteration, default values for the release days, the fraction of main source⁴² and the emission factors can be selected. The default values are given below:

f = Fraction of production volume used by main client (defaults cf. table 7.7)
T [d/a] = amount of release days at the main client (defaults cf. table 7.7)
F = emission factor to the environment: during conversion

Table 7.7: Factors for fraction of main source and release days for conversion processes⁴³

Amount of additive produced [t/a]	Fraction of main source (at converter's level) f	Release days T [d/a]
0 – 9.99	0.5	Q
10 – 49.9	0.35	0.35*Q
50 – 499	0.25	0.1*Q
500 – 4999	0.15	0.06*Q
5000 – 24999	0.12	300
> 25000	0.05	300

For plasticizers and heat stabilisers default values are given also for cases where the further processing type is unknown. For all other additive types where the processing type or prod-

⁴¹ The emission factors are derived from the OECD ESD by taking the value of the process and additive type with the highest emission. The values for the release days are taken from the TGD, Table B3.9. It is recognized that these values are overly conservative.

⁴² Note that Table 7.7 relates to the produced/imported substance amounts. Thus, if a DU makes the assessment (who is not the converter himself), can only make use of the defaults, when he is aware of the substance's production / import volume

⁴³ Defaults for fraction of main source and release days taken from the TGD, Table B3.9.

ucts are unknown select the highest emission value for the respective additive type as default.

Table 7.8: Emission factors conversion⁴⁴

Additive type	For product / process	F _{Air}	F _{water}
Anti-static agent (inorganic), colouring agent (pigment), Filler, Flame retardant (inorganic), , Preservative (inorganic), Lubricant (inorganic)	grinding / machining	0	0.025
Anti-static agent (inorganic), colouring agent (pigment), Filler, Flame retardant (inorganic), Heat stabiliser (solid), Preservative (inorganic), Lubricant (organic)	all forms other than woven mats	0	0.0001
Blowing agent (solid), Curing agent, Polymeric impact modifier, Viscosity aid (gaseous reaction product not taken into account)	all materials	0	0
Blowing agent, (liquid & gas)	thermoplastic materials	1 ⁴⁵	0
Filler	woven mats	0	0
Lubricant (inorganic)	other processes than grinding / machining	0	0.0001

Additive type	Process	Volatility	F _{Air}	F _{water}
Antioxidant, Anti-static agent, (organic), Flame retardant (organic), Preservatives (organic), Lubricant, UV and weathering agent	Open process, solid article	Low	0.0005	0.00005
		Medium	0.0025	0.00025
		High	0.0125	0.00125
Antioxidant, Anti-static agent, (organic), Flame retardant (organic), Preservatives (organic), Lubricant, UV and weathering agent	Open process, foamed article	Low	0.001	0.0001
		Medium	0.005	0.0005
		High	0.025	0.0025
Antioxidant, Anti-static agent, (organic), Flame retardant (organic), Preservatives (organic), Lubricant, UV and weathering agent	Partially open process	Low	0.0003	0.00003
		Medium	0.0015	0.00015
		High	0.0075	0.00075
Antioxidant, Anti-static agent, (organic), Flame retardant (organic), Preservatives (organic), Lubricant, UV and weathering agent	Closed process	Low	0.0001	0.00001
		Medium	0.0005	0.00005
		High	0.0025	0.00025
Colouring agent (dye)	Open process, solid article	All	0.0005	0.00005
Colouring agent (dye)	Open process, foamed article	All	0.001	0.0001
Colouring agent (dye)	Partially open process	All	0.0003	0.00003
Colouring agent (dye)	Closed process	All	0.0001	0.00001
Heat stabiliser (liquid), Plasticiser	Calendering, film blowing	Low	0.0005	0.00005
		Medium	0.0025	0.00025
		High	0.0125	0.00125
Heat stabiliser (liquid), Plasticiser	Extrusion, injection moulding	Low	0.0001	0.00001
		Medium	0.0005	0.00005
		High	0.0025	0.00025

⁴⁴ The default values are taken from the OECD ESD.

⁴⁵ According to the ESD, the factor for raw materials handling, which is 0.01 has to be subtracted from the '1'. For reasons of simplification this has been disregarded.

Additive type	Process	Volatility	F _{Air}	F _{water}
Heat stabiliser (liquid), Plasticiser	Spread coating	Low	0	0.00005
		Medium	0	0.00025
		High	0	0.00125
Heat stabiliser (liquid), Plasticiser	Process closed, specific type unknown	Low	0.00001	0.00001
		Medium	0.00005	0.00005
		High	0.00025	0.00025
Heat stabiliser (liquid), Plasticiser	Process partially open, specific type unknown	Low	0.00003	0.00003
		Medium	0.00015	0.00015
		High	0.00075	0.00075
Heat stabiliser (liquid), Plasticiser	Process open, specific type unknown	Low	0.00005	0.00005
		Medium	0.00025	0.00025
		High	0.00125	0.000125

As refinement option, the emission factors can be overwritten with own information. In addition, if the processing temperature during conversion is below 200 °C, the emission factor can be reduced by the factor 10.

7.3.3 Third iteration conversion

In the third iteration the default values for the fraction of main source, the release days and the additive-specific emission factors can be overwritten with own information. In addition, on-site emission reduction measures can be taken into account (cf. Chapter 7.2.3).

$$E = \frac{Q * f_{\text{mainsource}} * F_{\text{local,conv}}}{T}$$

$$E_{\text{local,emred}} = E * (1 - \text{con}) + E * \text{con} * (1 - F_{\text{emred}})$$

Equ. 13: Emission factor after abatement equipment

F_{emred} = efficacy of on-site emission reduction measures. Efficiency 100% = 1

7.4 Service life

The currently available models and default values for estimating emissions from service life of articles are conservative and frequently not available at all. Research is still necessary to further develop the emission estimation at this life cycle stage.

In the current implementation of the IT-tool when the M/I assesses the service life of the additive, a common EU market is assumed, since it is unlikely that M/I sells plastic additives exclusively to a regional market. Thus, 10% of the M/I production volume enters into the region. If a formulator or converter assesses service life, 100 % of the substance volume he handles is to be taken as a basis for the estimation, as the likelihood of regional markets is much higher than for M/I⁴⁶.

⁴⁶ The IT-tool asks the user at this stage to identify his role and automatically sets the respective default value for adjusting the calculation.

For the additive types polymeric impact modifier, curing agent, coupling agent, blowing agent (chemical and physical) or viscosity aid, no assessment of the service life and the waste disposal are necessary (they are emitted or destroyed in the prior processes).

7.4.1 PEC modelling in the service life stage

The PEC modelling in the IT-tool is currently possible only for outdoor uses in the regional environment. In the calculation of the PEC value for emissions from outdoor uses, no sewage treatment can be applied when using the IT-tool.

Additives may be used only in indoor products or in indoor and outdoor products at the same time. Indoor emissions to water still occur at regional scale, but may (partially) be treated in an STP. The safety assessor can carry out a manual estimation of emissions from indoor uses: the additive amount used in indoor products is multiplied with the respective indoor emission factors provided in the pick-list and an emitted amount is obtained. For additives which are readily biodegradable or additives with a log Pow > 5 this emitted amount may be reduced by 70%. For additives which are inherently biodegradable and have a logPow < 4 the amount may be reduced by 30% and if the additive is readily biodegradable or and has a log Pow between 4 and 5 the emission may be reduced by 50%.

A local scenario is not yet implemented in the IT-tool for the service life stage. However, if emissions occur locally the PEC modelling can be performed manually using the generic formula for local emissions. Here the settings are different from those of the local scenarios in industrial manufacture and use of the substance. As default values for the parameters use: 365 release days (T), 100% of the substance amount is used in the region (Q) and fraction of main source (f) = 0.002⁴⁷. Treatment in a municipal sewage treatment plant is assumed⁴⁸.

$$E = Q * 0.1 / (1) * F_{service} * lifetime$$

Equ. 14: Emissions during service life

7.4.2 First iteration service life

In the first iteration, the value for the lifetime is set to 1. Further defaults are⁴⁹:

$$F_{service,water} = 0.032$$

$$F_{service,air} = 0.01$$

⁴⁷ The fraction of the registrant's production volume contained in plastic articles disposed off locally derived from the TGD. If F/DU carries out the assessment with his own substance volume used, the 0.2% is to be exchanged with 100% since a converter may have a regional market.

⁴⁸ The standard assumption that 80% of the substances are discharged to a municipal sewage can be reduced, depending on the type of application of the additive in the end product.

⁴⁹ The worst case emission factors of the OECD ESD are given here as default values for the first iteration. The factors for slip-promoters and antistatic agents were not taken into account.

7.5 Second iteration service life

In the second iteration, additive specific emission factors for service life of articles can be chosen. The emission factors need to be linked to the life time of the products (multiplication). For organic additives used in outdoor applications, the default lifetime of 20 years (c.f. Table 7.9), can be reduced using Table 7.10 for certain types of outdoor products.

Table 7.9: Defaults for emission factors and lifetimes during outdoor service life

Additive type	F(water)	Multiply with service life (water)	F(air)	Multiply with service life (air)
Inorganics: Fillers, pigments, anti-static agents and flame retardants	0.0001	no	0	Not applicable
Indoor Organics: Plasticisers, antioxidants, dyes, stabilisers and flame retardants	0.0005	no	0.0005	no
Outdoor Organics: Plasticisers, antioxidants, dyes, stabilisers and flame retardants	0.0016	Yes, 20 years	0.0005	no
Others: Slip promoters (lubricants) and organic anti-static agents	1	no	0.083	Yes, 20 years

Table 7.10: Average service lifetimes for outdoor products

Example of product types	Average lifetime [a]	Value for calculation [a]
Articles used in agriculture	1	1
Shoes	2 to 5 years	5
Outdoor furniture	5 to 10 years	10
Plastic used in cars, construction materials and outdoor cables	10 to 20 years	20

7.5.1 Third iteration

At the third iteration level for service life, the substance amount can be separated according to different product types by defining the product specific share of the total substance volume. This means, the additive amounts used in products with indoor and outdoor applications or in products with long or short service lifetimes can be assessed separately. However, the emission amounts to the regional environment have to be summed up after the separate assessments.

Accordingly, the safety assessor can overwrite the emission factors and service lifetimes with product-specific emission factors and service life times. The assessor can enter measured or modelled data on additive emissions from products⁵⁰. Therefore, these values are called product-specific emission factors and product specific service lifetimes. The safety assessor thus should check if he has got information specific for the product type that he aims to assess.

⁵⁰ Note that the emission factors relate to one year and the IT-tool automatically multiplies with the lifetime of the product! If e.g. the information on additive emissions from the product relate to the service life time of the product (e.g. 1% per 15 years) the assessor may either enter 1% for the emission factor and enter a life time of 1 year or enter an emission factor of 0.067% and enter a life time of 15 years.

7.6 Disposal

At present, no appropriate emission estimation methods have been developed in the frame of the TGD or ESDs, which could be used for the disposal stage. This chapter therefore reflects the basic structure of emission estimation and provides first assumptions for emission factors derived from risk assessments carried out under EU existing substances program.

The waste stage is relevant for the following additive types: Fillers, Antistatic agent (organic, inorganic), flame retardant (organic, inorganic), preservative (organic, inorganic), heat stabiliser (solid, liquid), plasticizer, lubricant (= slip promoter, organic), viscosity aid, colourant (dye, pigment), UV-stabiliser, polymeric impact modifier.

Wastes occurring during industrial processing are not submitted to the waste module by the IT-tool. Only the article waste is used as input to the waste stage. If emissions from waste disposal of industrial processing waste shall be estimated, the input amount has to be overwritten with the emissions 'to waste' estimated in the respective lifecycle stage.

The current IT-tool does not support the modelling of PECs at regional scale, but only at local scale. If the safety assessor wants to manually derive the PEC_{regional} (emission factors are given in the following table), the following formula and setting should be used:

Regional scenario:

$$\frac{E_{\text{regional}}}{T} = \frac{Q * 0.1 * F_{\text{disp}}}{T}$$

Equ.15: Emissions from disposal operations, regional scenario

The value 0.1 reflects that a common EU market is assumed from M/Is perspective since usually there is no regional market for plastic additives where M/I would sell his total production volume. If the calculation is performed from F's or IU's perspective 100% of the volume are assumed since the compounder or converter may have a regional market and hence no "dilution" across the whole market would occur. 365 release days should be assumed.

Local scenario:

$$E_{\text{local}} = \frac{Q * f_{\text{mainsource}} * F_{\text{disp}}}{T}$$

Equ. 16: Emissions from disposal operations, local scenario

E_{local} [kg/d] = emission to local environment from waste disposal

Q [t/a] = amount of the substance entering the waste disposal operation

f = fraction of the registrant's production volume contained in articles entering a waste disposal facility = 0.002⁵¹ or 1 (DU perspective)

F_{disp} = emission factor from disposal operation

T [d/a] = release days per year from disposal operations

⁵¹ It is assumed that the maximum fraction of the registrant's production volume contained in articles in a municipal waste facility can be determined by the fraction of main source for domestic use of chemicals (B tables, = 0.002). However, if the calculation is carried out from F's or IU's perspective 100% is assumed by default since the compounder or the converter may possibly serve a regional market. In the third iteration this value can be further adjusted.

7.6.1 1st iteration disposal

The default values used in the 1st iteration are given below.

Q = produced/imported amount by M/I

F_{mainsource} = 0.002

F_{water} = → 0.048⁵²

F_{air} = → 0.01

F_{soil} = → 0

T = → 365

7.6.2 2nd iteration disposal

In the second iteration step, for specific additive groups and disposal techniques emission factors can be selected from the following table. Note that some of the emission factors relate to regional emissions, where the PEC derivation cannot be performed by the IT-tool.

Table 7.11: Additive-specific emission factors for disposal techniques

Additive groups Disposal technique	Additives containing toxic metals (Cd, Pb, Zn, Co, Sb, Sn)	Organic additive with halogen content > 3%	Organic additive with halogen content < 3%
Waste remaining in the environment Regional	F _{air} = F _{water} = 0.025 F _{soil} = 0	F _{air} = 0 F _{water} = 0.025 F _{soil} = 0	F _{air} = 0 F _{water} = 0.025 F _{soil} = 0
Shredder process Local	F _{air} = 0.005 F _{water} = 0 F _{soil} = 0	F _{air} = 0.005 F _{water} = 0 F _{soil} = 0	F _{air} = 0.005 F _{water} = 0 F _{soil} = 0
Thermal Treatment for material separation, other than incineration; temperature > 150	No flag	Flag: Exposure scenario must contain a statement on prevention of Dioxine formation	No flag
Incineration Local Main source 0.2%, 365 d	F _{air} = 0.001 F _{water} = 0 F _{soil} = 0	F _{air} = 0 F _{water} = 0 F _{soil} = 0	F _{air} = 0 F _{water} = 0 F _{soil} = 0
Incineration, slag is used in road construction Regional	F _{air} = 0.001 F _{water} = 0.002 F _{soil} = 0	F _{air} = 0 F _{water} = 0 F _{soil} = 0	F _{air} = 0 F _{water} = 0 F _{soil} = 0
Direct landfill of plastic waste (construction waste) Local Main source 0.2%, 365 d	F _{air} = 0 F _{water} = 0.048 ⁵³ F _{soil} = 0	F _{air} = 0 F _{water} = 0.001 F _{soil} = 0	F _{air} = 0 F _{water} = 0.001 F _{soil} = 0
Incineration as secondary fuel / co-incineration	Flag: Exposure scenario must contain a statement on the prevention of contamination of the product by metals	Flag: Exposure scenario must contain a statement on prevention of Dioxin formation	No flag
Other techniques	F _{air} =	F _{air} =	F _{air} =

⁵² Organic additives, 30 years, open in the environment

⁵³ assumption: landfill operation up to 30a after end of service life.

Additive groups Disposal technique	Additives containing toxic metals (Cd, Pb, Zn, Co, Sb, Sn)	Organic additive with halogen content > 3%	Organic additive with halogen content < 3%
	F _{water} = F _{soil} =	F _{water} = F _{soil} =	F _{water} = F _{soil} =
Recycling by standard plastic conversion process	F _{air} = 0.0025 F _{water} = 0.025 F _{soil} = 0	F _{air} = 0.0025 F _{water} = 0.025 F _{soil} = 0	F _{air} = 0.0025 F _{water} = 0.025 F _{soil} = 0

7.6.3 3rd iteration disposal

In the third iteration, the assessor can overwrite the default values for the emission factors with own information.

7.7 Standard model for wastewater treatment

This chapter supports the selection of emission factors from sewage treatment plants. The safety assessor needs information on the degradability, the water solubility, molecular weight and the logPow to find the emission factor, applicable for his substance. This factor can be used for all lifecycle steps, when a municipal sewage treatment plant exists. Also if on-site wastewater pre-treatment in a biological treatment plant is carried out the respective emission factors can be used. The factors do not apply to specific treatment devices.

Table 7.12 also gives factors for emissions to sludge, which have not appeared yet in any other estimation module: when doing a detailed assessment of emissions, sludge produced in sewage treatment may be an important source of emissions to the environment, e.g. if it is used as fertiliser. The table thus indicates whether sewage treatment sludge should be included in an assessment (high emission factors) or not. Further calculations are not supported by the IT-tool or this manual.

Table 7.12: Factors for the removal of a substance in a wastewater treatment plant

	Non biodegradable			Inherent biodegradable			Ready biodegradable (10 day window not fulfilled)			Ready biodegradable (10-day window fulfilled)		
	F _{water}	F _{Air}	F _{Sludg}	F _{water}	F _{Air}	F _{Sludg}	F _{water}	F _{Air}	F _{Sludg}	F _{water}	F _{Air}	F _{Sludg}
LogP <3	100%		1%	59%		1%	33%		1%	13%		0%
LogH ≤1		15%			10%			6%			3%	
LogH 1-2		64%			50%			36%			19%	
LogH >2		95 %			91%			85%			68%	
LogP 3-4	96%		21%	57%		19%	32%		17%	12%		16%
LogH ≤1		14%			9%			6%			3%	
LogH 1-2		62%			49%			35%			18%	
LogH > 2		92%			89%			82%			66%	
LogP 4-5	39%		61%	28%		56%	18%		51%	8%		47%
LogH ≤1		5%			4%			3%			1%	
LogH 1-2		28%			23%			17%			9%	
LogH > 2		51%			49%			46%			37%	

	Non biodegradable			Inherent biodegradable			Ready biodegradable (10 day window not fulfilled)			Ready biodegradable (10-day window fulfilled)		
	F _{water}	F _{Air}	F _{Sludg}	F _{water}	F _{Air}	F _{Sludg}	F _{water}	F _{Air}	F _{Sludg}	F _{water}	F _{Air}	F _{Sludg}
LogP > 5	15%		85%	13%		83%	11%		79%	7%		72%
LogH ≤ 1		1%			1%			7%			1%	
LogH 1- 2		9%			8%			7%			4%	
LogH >2		27%			26%			25%			20%	