

How to use EUSES 2.2.0

September 2019



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European Chemicals Agency

Mailing address: P.O. Box 400, FI-00121 Helsinki, Finland Visiting address: Annankatu 18, Helsinki, Finland

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1. Background

This document is not meant as a software manual but as a guide describing the changes and new features in the EUSES software version 2.2.0 compared to the previous version EUSES 2.1.2 (2012) and **explaining the reasoning and way of how certain parameters and scenarios have been implemented in the existing limited EUSES software settings**.

For the scientific background on the implemented emission scenarios and SimpleTreat module, as well as on other exposure modules, please consult the existing guidance referred to in Table 1.

Table 1: Overview on relevant guidance explaining the background for the implementations in EUSES

Module	Relevant guidance	Link
Release	Emission Scenario Documents (ESD)	https://echa.europa.eu/guidance- documents/guidance-on-biocides- legislation/emission-scenario-documents
	Technical Agreement for Biocides (TAB)	https://webgate.ec.europa.eu/s- circabc/faces/jsp/extension/wai/navigation/ container.jsp
Fate and distribution	Guidance on the Biocidal Products Regulation Volume IV Environment - Assessment and Evaluation (Parts B + C)	https://webgate.ec.europa.eu/s- circabc/faces/jsp/extension/wai/navigation/ container.jsp
	SimpleTreat 4.0 manual	https://www.rivm.nl/en/soil-and- water/simpletreat
	EUSES chapter III model calculations (for non-updated parts in EUSES 2.2.0)	https://echa.europa.eu/documents/10162/ 16908203/pt4_food_contact_materials_en. pdf/6d9730f0-7ba1-4a34-aad4- 1b8d5ec9ec7f

2. Introduction and scope of EUSES 2.2.0

The European Union System for the Evaluation of Substances (EUSES) is a software that helps chemical companies, authorities and research institutes to carry out qualitative assessments of the risks posed by chemical substances to the environment. It implements the technical guidance for the EU legislation for industrial chemicals and biocides. It dates back to 1994 and the last version was released in 2012.

In the EUSES version 2.2.0, the software was updated as an intermediate step to provide a software solution until the major EUSES update (planned to take place between 2020 and 2022) is finalised. The major update will result in a merge of the existing tools CHESAR and EUSES into a new state-of-the-art software tool.

In the intermediate update (resulting in this EUSES version 2.2.0), the software and the user interface as such, as well as the structure of the implemented modules was not changed; only some missing features were added.

The previous version, EUSES 2.1.2, implemented Emission Scenario Documents (ESDs) covering product types (PT) for biocides that were prepared before 2012. More ESDs have been developed since then and already existing ESDs have been updated. In EUSES 2.2.0, missing emission scenarios developed after 2012 have been implemented, and the previously implemented emission scenarios have been re-structured for harmonisation reasons.

In addition, the processing of direct releases was included in the fate and distribution as well as the risk characterisation module. A full risk assessment can now also be performed with EUSES for uses specifically with biocides, resulting in direct releases to soil and surface water (in EUSES 2.1.2 PEC values were calculated in the release module but were not necessarily further processed in the software).

Furthermore, the new version of SimpleTreat (v4.0) was included in EUSES 2.2.0 in addition to SimpleTreat 3.1. Ideally, Simple Treat 4.0 should be used for the exposure assessment of biocides.

The following figure summarises the main changes in EUSES 2.2.0 compared to the previous EUSES version:



This "How to use EUSES 2.2.0" manual is structured as follows:

- Section 3 provides explanations on general functions of EUSES 2.2.0.
- In section 4, specific ways of implementations in the release module cross-PT as well as PT specific – are described.
- Section 5 contains details on the changes in the fate and distribution module, i.e. the inclusion of direct release pathway in EUSES 2.2.0, as well as the implementation of SimpleTreat 4.0.

3. General functions

3.1 Running a study in EUSES 2.2.0

When running a new study in EUSES, start the assessment via "File" in the menu bar and then select "New Study".

Use the interactive mode when navigating in EUSES: under "Assess" in the menu bar, select "Interactive mode assessment" and then use the "Next" and "Prev" buttons to move back and forth in the assessment.

If you run an assessment for a substance under REACH, no adaptations in the "Assessment type" windows are needed (as by default sections I, Ia, Ib, II, III, IIIa and IIIb checkboxes are selected). If you run an assessment for a biocidal substance, the following setting is recommended:

 Assessment of biocides on local scale only I. Environmental Ia. I Local scale Ib. Regional scale II. Predators exposed via the environment III. Man exposed via the environment 	Run mode C Direct C Interactive C Outline Hydrocarbon-Blocks Defaults	
IIIa. Local scale IIIb. Regional scale IV. Man exposed via consumer products V. Man exposed at the workplace (EASE) Prev Next	↓ Add defaults	

3.2 Importing files from EUSES 2.1.2

When importing a file created in EUSES 2.1.2, not all the information in the file will be imported into EUSES 2.2.0. Due to the changes introduced in the release module and implementation of SimpleTreat 4.0, some related information will not be imported. Following is the description of the compatibility between EUSES versions module by module.

💭 EU	SES 2.2.0)		
File E	dit As	sess	Defaults	S
Ľ	e		B	
new	open	save	edit	s
-0 -0 -0 -0 -0 -0) Study i Asses Default Substa Releas Distrib Exposu	sment ince e estil ution ure	t type	

- From Study identification information will be imported from 2.1.2 to 2.2.0
- From Assessment type information will be imported from 2.1.2 to 2.2.0
- From Defaults information will be imported from 2.1.2 to 2.2.0
- From Substance:
 - EUSES 2.2.0 will recalculate the Vapour Pressure and Water solubility at 25°C. The test temperature values will be lost
 - The information from "Degradation and transformation input" →tab "STP" is not imported from 2.1.2 to 2.2.0
- From Release estimation information will **not** be imported from 2.1.2 to 2.2.0 (with few exceptions, i.e. parameters with the same name)
- From Distribution and Exposure information will **not** be imported from 2.1.2 to 2.2.0
- From Effects information will **not** be imported from 2.1.2 to 2.2.0
- From Risk characterisation information will **not** be imported from 2.1.2 to 2.2.0 (as a consequence of the above)

Due to the changes in the fate and distribution modules, we recommend that you avoid importing files from the older EUSES version; instead, a new assessment should be performed in EUSES 2.2.0.

3.3 Help button

This functionality was available in former EUSES versions (but no longer in EUSES 2,1,2) and it was out of scope for EUSES 2.2.0. Therefore, we refer the user to the different guidance documents available on ECHA website noted in previous Table 1.

3.4 Layout

The tabs in the release module have been renamed and reorganised in a harmonised way: there is always at least an input tab and an output tab. The output tab contains the final output of the release module, i.e. local emission values used in subsequent calculations. When needed, the input parameters are distributed over several tabs.

In some Product Types (PT), there is one tab for the tonnage approach and another tab for the consumption approach. In such cases, the user must select upfront between the two approaches, and only the relevant tab will be enabled for entering input parameters.

Note that within a given input tab some input parameters will be enabled/disabled depending on earlier selections made by the user.

Example: In the screenshot example below, the parameters "Application rate of the product (fluid)" and "Density of liquid product" will be enabled once the selection for "Applied formulation state" is "Fluid". At the same time, "Application rate of the product (solid)" will be disabled.

Release fractions and emission days [1 "", IC=15/UC=39]			— 🗆	×				
Industrial use								
Product type (8) Wood preservatives, (8.1.1) Industrial preventive proc	esses, Automa	ted spraying						
General input Application Storage Output								
Area of wood treated per day	??	[m2.d-1]	u					
Applied formulation state	Solid		▼ S					
Application rate of the product (solid)	Solid Fluid							
Application rate of the product (fluid)	??	[l.m-2]	u					
Fraction of substance in the product	??	[-]	u					
Density of liquid product	1E+03	[kg.m-3]	d					
Quantity of the substance applied per m2 of wood	??	[kg.m-2]	o					
Water solubility at 20 C 5 [mg.I-1]								
Fraction released to wastewater	3E-03	[-]	d					
Vapour pressure at 20 C	5	[Pa]	0					
Fraction released to air	0.25	[-]	d					
Fraction of spray drift deposition	1E-03	[-]	d					
Parameters required for the distribution module or for calculation of PECs								
Number of emission days 300 [d.yr-1]								
	Indo	X A <u>b</u> ort	? H	elp				

If text is greyed out within a tab, it is either not relevant for the scenario or there are input values missing (which will trigger the parameter to be enabled).

3.5 Overwriting values in EUSES

Default values (identified with "d" on the right hand side of a parameter row – see screenshot above) can be overwritten. Any modified default value must, however, be duly justified in the assessment report or CSR.

Output values (identified with "o" on the right of a parameter row) can also be overwritten. Changing output values does not affect any previously calculated values. The overwritten output values will only be used in subsequent calculations.

Both overwritten default and output values will be marked as set values (identified with "s" on the right hand side of a parameter row).

Note that values overwritten in output fields (values set by the user) are not recalculated in case any input parameter is changed after that! In this situation, in order to force the tool to recalculate the output value in accordance with the new input value, the set value in the output field needs to be deleted, then press "Enter".

Since overwriting values may lead to mistakes, we recommend you mark set values by a colour code via "System" in the menu bar, then click on "Options" and change the colour of set values ("Status Set") under "Parameter status colours".

4. Notes on the release module for biocides assessment

EUSES 2.2.0 contains new or updated release scenarios for Product Types (PT) 1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 18, 19 and 22. For PT 3 and 18 not all the scenarios were implemented. See the full list of scenarios implemented or updated in Appendix 1.

The new scenarios can be accessed from the window "Biocide scenario input data".



For detailed background information on new ESDs and changes in existing ESDs, please refer to the ECHA webpage on Emission Scenario Documents¹ and the TAB².

4.1 Cross-PT related items

4.1.1 Number of emission days (Temission)

Temission, the number of emission days, is an input parameter for the fate and distribution module and in some cases also for the release module. In case it is only relevant for the fate and distribution module, Temission is not necessarily provided in the ESDs. In such cases, it was added in the release module of EUSES 2.2.0 together with an explanatory note as shown in the following screenshot.

¹https://echa.europa.eu/guidance-documents/guidance-on-biocides-legislation/emission-scenario-documents ² https://webgate.ec.europa.eu/s-circabc/faces/jsp/extension/wai/navigation/container.jsp

Release fractions and emission days [1 "", IC=15/UC=39]							
Industrial use Private use							
Product type (1) Human Hygiene							
General input Consumption input Tonnage input Output							
Type of end-product	elect		- u				
Number of inhabitants feeding one STP	1E+04	6	d				
Fraction released to wastewater	1	6	d				
Substance in biocidal product	??	[g.l-1]	u				
C	onsumption per inhabitant pe	r day	▼ d				
Consumption per inhabitant per day	??	[ml.d-1]	u				
Consumption per application	??	[ml]	u				
Number of applications	??	[d-1]	u				
Fraction of inhabitants using end-product	??	[-]	u				
Market penetration factor	0.5	[-]	d				
Density of the product	1E+03	[kg.m-3]	d				
Parameters required for the distribution module or for c	alculation of PECs						
Number of emission days	365	[d.yr-1]	d				

For a more detailed overview please refer to Appendix 2 where:

- Table 2 of Appendix 2 lists the scenarios where the number of emission days was added in the release module.
- Table 3 of Appendix 2 includes the emission scenarios where the number of emission days was already available in the emission scenario.

4.1.2 Assessment periods in PT 6, PT 8 and PT 10 (service life)

Service-life-related emission scenarios resulting in direct emissions to soil or surface water —following leaching from a treated commodity— now include an intermediate assessment period of 365 days (new TIME 2 as agreed by the BPC Environment WG). Concerning the applicability of TIME 2 for decision-making, please refer to the information provided in the latest version of the TAB.

In total, three assessment periods, TIME1, TIME2, and TIME3, are considered, which include also the initial concentration at t=0, i.e. releases from spillage during application. As a result, $Q^*_{leach, time 1}$, $Q^*_{leach, time 2}$, and $Q^*_{leach, time 3}$ are defined as the cumulative amounts leached over 0-30 days for TIME1, 0-365 days for TIME2, and total service life for TIME3.

This is, amongst others, relevant for e.g. scenario

- (6.2) Paints and coatings service life countryside scenario;
- (8.3.1) Treated wood in service UC3; and
- (10.3) Service life house in the countryside.

4.1.3 Service life in scenarios 7.2 and 9.3 (Polymerised materials) and tonnage based approaches

Scenarios 7.2 and 9.3 are based on the A & B tables for general chemicals (TGD, 2003; also reported in Appendix 6 of Vol. IV Part B+C), for which also a regional assessment is performed under REACH. Specifically, the direct emissions to surface water resulting from the service-life lifecycle step in scenarios 7.2 and 9.3 (Polymerised materials), are processed at the regional scale. These emissions are therefore disregarded in subsequent calculations for biocides since (for biocides only) a local assessment is performed. The same rule was applied for scenarios using a tonnage based approach (e.g. formulation step in PT 6) resulting in direct release to soil or surface water.

Release fractions and emission days [1 "", IC=15/UC=39]				\times
Service life				
Product type [7] Film preservatives, [7.2] Polymerised materials				1
Intermediate results Fraction of tonnage released to air Fraction of tonnage released to wastewater Fraction of tonnage released to surface water	5E-04 0 0.016	[-] [-]	0	
<u>Final output</u> Local emission to air Local emission to wastewater Local emission to surface water	7.51E-10 0 <mark>2.4E-08</mark>	[kg.d-1] [kg.d-1] [kg.d-1]	0 0 0	

If a regional assessment is needed, the assessment should be done using the general chemical setting of running EUSES (i.e. do not choose "Assessment of biocides on local scale only" in the "Assessment type" window. If not chosen, the checkbox "regional scale" is automatically selected - see explanation provided in section 3.1).

4.1.4 Display of emissions to air and subsequent deposition to soil

In scenarios covering uses resulting in emissions to air, the amount released is indicated in the Study > Release estimation > Local ("Local emissions") screen. In subsequent windows, the release to air is covered under the Study > Release estimation > Local > [life cycle stage] > "Release via STP" tab, and is considered as indirect release in the current software setting.

💭 Local e	missions									
									Ŧ	
Usage	Step	Emis. Air	Emis. Water	Biocides	Show	Intermittent	Release via STP	Direct release		
1 "" (15/39)	5 Serv	9.23E-08 [kg.d-1]	9.23E-08 [kg.d-1]	Yes	Yes	No	Yes	No		
Edi		Release via STP Local emission Emission to ai Local emission Emission to wa	ns [1 "", IC=15/UC to air r calculated by sp to wastewater ater calculated by ocides scenario a step in further calculater	ecial scena special sce vailable	nio		9.23E-08	[kg.d-1] Yes [kg.d-1] Yes		×
		☐ Intermitten	t release		X !	Cancel			? н	elp

In case of releases to wastewater, the STP will be a source of indirect emissions to air. When a scenario has emissions to air from both the use of the substance and from the STP, the highest of the values will be used in subsequent calculations. The amount of substance released to air, either from the use or from the STP, will then be further distributed to soil due to deposition and reported in the "Release via STP" tab.

If deposition to soil from air occurs as a direct release to soil e.g. due to drift, the Study > Distribution > Life cycle steps > [life cycle stage] > Local concentrations and depositions [life cycle stage] > "Release via STP" tab reports the local concentration following deposition (as previously described) and the "Direct releases" tab reports the direct emissions to soil following e.g. drift.

Local concentrations and depositions [1 "", IC=15/UC=39] [Industrial u			\times	
Release via STP Direct release				
Air Water, sediment Soil, groundwater				
Concentration in air during emission episode	2.78E-04	[mg.m-3]	0	
Annual average concentration in air, 100 m from point source	7.62E-07	[mg.m-3]	0	
Total deposition flux during emission episode	[mg.m-2.d-1]	o		
Annual average total deposition flux 1.88E-06 [mg.m-2.d-1				
	1	1		
<u>Prev</u> <u>Next</u> <u>Prinish</u> <u>SUnd</u>	lo 🛛 🗡	Abort	<u>? Н</u> еlp	

Local concentrations and depositions [1 "", IC=15/UC=39] [Industrial use]	_		×
Release via STP Direct release			
Freshwater <mark>Soil</mark>			
Local concentration in soil due to drift 1.96E+06	[mg.kg ww t-1]	0	
▲ Prev ▶ Mext ▶ Einish ★ Undo	A <u>b</u> ort	? <u>Н</u> ец	2

Since two different soil compartments are considered, the two releases cannot be combined.

Another related aspect is that in scenarios that result in emissions to air only, e.g. 8.4 Indoor fumigation, the emissions to air will be reported in STP related windows, although there are no emissions to wastewater (see example in the following screenshot). This implementation results from limitations of the existing software settings.

Release fractions and emission days [1 **, IC=15/UC=	=39]	0 X	💭 Local en	nissions							
[Industrial use]											
Product type [8] Wood preservatives, [8.4] Indoor	fumigation		Usage	· ·	Emis. Air	Emis. Water	Biocides	Show	Intermittent	Release via STP	Direct release
Local emission to air	<mark>9.79</mark> [kg.d·1]	- o	1 (15/39)	3 Indus 5	9.79 [kg.d-1]	0 [kg.d-1]	Yes	Yes	No	No	No
			Edit	:							
	😏 Undo 🗙 Abort	? Help	♦ Pre	rv 🛛	• <u>N</u> ext	H	<u>F</u> inish		X Abo	t	? <u>Н</u> еlp
	Local concentrations and depo Release via STP Air Water, sediment Soil, grou Concentration in air during em Annual average concentration Total deposition flux during en Annual average total depositio Prev Next	undwater ission episode n in air, 100 m nission episod on flux	e I from point s		2.72E-03 7.46E-06 2.94E-03 8.05E-06	[mg.m-3]	1-1] 1-1]				

4.1.5 Secondary poisoning

The updated release module in EUSES 2.2.0 and the secondary poisoning module are not linked. Assessment of secondary poisoning needs to be performed outside of EUSES.

4.2 PT specific notes

4.2.1 PT 1 Human hygiene

4.2.1.1 Releases to air

For all scenarios in PT 1, for both private uses and industrial uses, releases to air have been implemented in EUSES 2.2.0 by adding also 'a fraction released to air' in the scenario and equations, if relevant. The ESD for PT 1 only foresees releases to wastewater. However, active substances used in PT 1 may be highly volatile and therefore releases to air are relevant.

4.2.2 PT 2 Disinfectants and algaecides not intended for direct application to humans or animals

4.2.2.1 Scenario 2.9.2 Wall treatment against algae (service life) (location: countryside)

The output tab of the release module covers all contributions to the release from the treatment of a house façade against algae: releases from application (spray drift, run-off, rinsing) and releases from leaching during service life.

In a Tier 1 assessment, all emissions are summed up, as they all end up in a soil volume of 13 m³ adjacent to the treated surface.

The scenario was implemented according to the very similar scenarios for in-situ outdoor spraying in the ESD for PT 10 and the OECD ESD for PT 8³. The latter considers the following input parameters for the soil volume: "soil volume adjacent to treated surface" and "soil volume receiving drift from façade spraying and rinsing in Tier 1", which both have been implemented in EUSES.

In order to keep full flexibility in changing any default values for either the receiving compartment due to run-off or due to spray drift, the calculations have been implemented separately. The concentrations in soil are calculated using the respective default values for the adjacent and distant soil volume value as follows:

- Concentrations in soil due to run-off (Tier 1) and leaching are calculated using the parameter "Soil volume adjacent to treated surface".
- Concentrations in soil due to spray drift (Tier 1) are calculated using the parameter "Soil volume receiving drift from façade spraying and rinsing in Tier 1".

In the Local concentrations and depositions window, the total concentrations are calculated. The total concentrations are then used to determine the predicted environmental concentration (PEC) and risk characterisation ratio (RCR).

In a Tier 2 assessment it is assumed that the soil around the building is covered by a plastic sheet (assumed width of 100 cm), as provided in the PT 8 scenario 'In-situ spraying (outdoor)'.

The Tier 2 concentration at the end of the day of application and rinsing due to spray drift, is calculated using the parameter "Soil volume receiving drift from façade spraying in Tier 2".

³ OECD ESD for PT 8 (in-situ outdoor spraying), based on which this scenario was developed.

4.2.2.2 Releases to air

For the scenarios under PT 2.1 Sanitary sector, private and institutional areas and PT 2.3 Industrial areas, releases to air have been implemented in EUSES 2.2.0 by adding also 'a fraction released to air' in the scenario and equations. The ESD for PT 2 only foresees releases to wastewater for those scenarios. However, active substances used in PT 2 may be highly volatile and therefore releases to air are relevant.

4.2.3 PT 3 Veterinary hygiene

4.2.3.1 Scenario (3.5) Disinfection in hatcheries

The implementation of this scenario in EUSES 2.2.0 deviates from the ESD. The ESD has a mistake that will be corrected by a TAB entry.

The equations implemented in EUSES for estimating the releases from the scenario can be found in Appendix 3.

4.2.4 PT 4 Food and feed area

4.2.4.1 Scenario (4.1) Food, drink and milk industries – Cleaning in process (CIP, brewery)

In scenario (4.1) Food, drink and milk industries – Cleaning in process (CIP, brewery), subsequent treatment by an on-site or off-site STP can be selected. If the on-site STP is selected, the concentration in surface water is calculated in the Study > Distribution > Life cycle steps > [life cycle stage] > "Local concentration and depositions" window and is in the current software setting treated as direct release.

4.2.5 PT 7 Film preservatives

The emission scenarios for PT 7 implemented in EUSES 2.2.0 were based on the following scenarios:

- The emission scenario for PT 7.2 Polymerised materials is implemented according to EUSES 2.1.2, no changes have been introduced.
- The emission scenario for PT 7.3 is based on the scenario PT 9.4 Rubber products, as described in the ESD for PT9: Emission scenarios for biocides used as preservatives in rubber and polymerised materials (EUBEES, 2004).
- The emission scenario for PT 7.4 is based on the scenario PT 9.5 Roof membranes as described in the document "Use-based approaches for the estimation of environmental exposure due to roof membranes" (UBA, 2014).
- The emission scenario for PT 7.5 is based on the scenario PT 9.6 Paper and cardboard as described the ESD for PT 6, 7 & 9: Emission scenarios for biocides used in paper coating and finishing (EUBEES, 2001).

4.2.6 PT 8 Wood preservatives

4.2.6.1 Scenario 8.3.1 Treated wood in service - UC 3

The scenario (8.3.1) Treated wood in service – UC 3 covers the life cycle stage "Service life" which gives the opportunity to include also releases from in-situ treatment (i.e. brushing) in the assessment.

This has been implemented as a specific inner tab, where for parameter "Cover in situ treatment" the user selects "Yes". In spite of this choice, the industrial treatments to pre-treat wood in a factory are also available under the inner tab "Service life" and drop-down list for the parameter "Select application methods/process". Do not select any of the industrial application methods when assessing in-situ treatment within service life. That is, when assessing in-situ treatment make sure to select "In-situ brushing" in the inner tab "Service life".

Release fractions and emission days [1 "", IC=15/UC=3	9]	_		Release fractions and emission days [1 "", IC	=15/UC=39]		_	o x
Service life				Service life				
Product type (8) Wood preservatives, (8.3.1) Treated	1 wood in service - UC 3			Product type (8) Wood preservatives, (8.3.	1) Treated wood in servi	ce - UC 3		
Input Output				Input Output				
Select scenario	House scenario		▼ s	Select scenario	House scenario	D	-	s
Volume of wet soil	13	[m3]	d	Volume of wet soil		13	[m3]	d
Bulk density of soil	1.7E+03	[kgwwt.m-3]	d	Bulk density of soil		1.7E+03	[kgwwt.m-3]	d
Water volume under bridge	1E+03	[m3]	d	Water volume under bridge		1E+03	[m3]	d
In situ treatment Service life Cumulative quantities				In situ treatment Service life Cumulative quantiti	es			
Cover in situ treatment	Yes		▼ s	Leachable wood area		125	[m2]	d
Area of wood treated per day	125	[m2.d-1]	d	Select application method/process	In-situ brushing	9	•	· S
Application rate of the product	??	[l.m-2]	u	Initial assessment period	Select Vacuum pressu	ire treatment		d
Fraction of substance in the product	??	E	u	Intermediate assessment period	Double vacuum Automated spra	n pressure treatm aving	ent	d
Density of the product	1E+03	[kg.m-3]	d	Service life	Dipping/flow c	oating		d
Select professional user or amateur user	Select		- u	Cumulative quantity of substance leached				• · ·
Fraction of product lost to soil/water during application	ion ??	[-]	u	- over the initial assessment period		??	[mg.m-2]	u
				- over the intermediate assessment period	d	??	[mg.m-2]	u
				- over the service life		??	[mg.m-2]	u
				Fraction released to soil		0.3	[-]	d
				Fraction released to wastewater		0.7	[-]	d
Parameters required for the distribution module or for	calculation of PECs			Parameters required for the distribution mo	dule or for calculation of	PECo		
Number of emission days	365	[d.yr-1]	d	Number of emission days		365	[d.yr-1]	d
}						1		1-
▲ Prev ▶ Next ▶ Finish	5 Undo	X Abort	? <u>H</u> elp		🕈 Einish 🔄 🖞	Indo 🔰	🕻 A <u>b</u> ort	? <u>H</u> elp

4.2.6.2 Scenario 8.9 Railway sleepers

As an output of this scenario, EUSES calculates only the application rates on 1 hectare to be used as input parameters for FOCUS models⁴ and no further assessment is done in EUSES. These are calculated over an intermediate and longer assessment periods. The initial assessment period of 30 days is not covered in the emission scenario (i.e. no input for PEARL⁵/PELMO⁶ is calculated), since it covers a time span of less than one year and can therefore not be simulated with PEARL/PELMO.

4.2.7 PT 9 Preservatives for liquid-cooling and processing systems

The emission scenarios for PT 9 implemented in EUSES 2.2.0 were based on the following scenarios:

- The emission scenario for PT 9.1 Textile and fabrics, is implemented according to the ESD for PT 9 & 18: Emission scenario document for biocides used as preservatives in the textile processing industry.
- The emission scenario for PT 9.2 Leather, is implemented according to the ESD for PT 9: Emission scenarios used as preservatives in the leather industry.
- The emission scenario PT 9.3 Polymerised materials, is implemented according to the scenario for PT 7.2 as it was implemented in EUSES 2.1.2.

⁴ <u>https://esdac.jrc.ec.europa.eu/projects/focus-dg-sante</u>

⁵ <u>https://esdac.jrc.ec.europa.eu/projects/pearl</u>

⁶ <u>https://esdac.jrc.ec.europa.eu/projects/pelmo</u>

- The emission scenario for PT 9.4 Rubber products, is implement according to the ESD for PT 9: Emission scenarios for biocides used as preservatives in rubber and polymerised materials (EUBEES, 2004).
- The emission scenarios for 9.5 Roof membranes, are implemented according to "Usebased approaches for the estimation of environmental exposure due to roof membranes" (UBA, 2014).
- The emission scenario for 9.6 Paper and cardboard, is implemented according to the ESD for PT 6, 7 & 9: Emission scenarios for biocides used in paper coating and finishing (EUBEES, 2001).

4.2.8 PT 10 Construction material preservatives

4.2.8.1 Soil volumes

The default values and soil volume derivation in PT 10 countryside scenarios covering direct releases to soil have been set in line with the emission scenarios for PT 8 for in-situ outdoor spraying.

4.2.8.2 Scenario 10.4 Service life - city scenario

According to the ESD for PT 10, some masonry preservatives can be applied in form of a paint (ESD Table 5). Therefore, the pick-list in EUSES has been extended to include products such as "paints applied on façade (outdoor)".

4.2.9 PT 11 Preservatives for liquid-cooling and processing systems

The emission scenarios for PT 11 are implemented content-wise in line with the previous EUSES version 2.1.2, since no recent changes in the emission scenarios were performed.

Discussions on any potential adaptations of the emission scenarios are ongoing, but were not agreed on at the time when EUSES 2.2.0 was released.

Note that the emission estimation for soil in PT 11 was under discussion at the time when EUSES 2.2.0 was prepared. It was therefore not fully implemented (i.e. it was not implemented for PT 11.1 and for PT 11.2 if release via STP is considered, due to conflicting settings in the STP module). This will be updated in a future release.

4.2.10 PT 12 Slimicides

4.2.10.1 Scenario 12.1 Paper production

The following note is related to the inner tab "Input for degradation" – Hydraulic retention times:

The concentration in the effluent of the on-site treatment is calculated using the following equation:

 $Clocal_{effl-treat} = C_{infl-ps} * (1 - F_{ads,settling} - F_{ads,cm}) * e^{-kdeg2*(Tps+Tcm)}$

The concentration in the influent to the STP is calculated using the following equation:

 $Clocal_{infl-WWTP} = C_{paper} * (1 - F_{ads,settling}) * e^{-kdeg1*(Tpr+Tps)}$

These are the equations provided on pages 44 and viii of the ESD for PT 12, slightly modified to correct the parameter "hydraulic retention time". The original equations used parameter

hydraulic retention time for primary settling and chemical/mechanical treatment Ttreat in Table 5.3 on p. 43 of the ESD for PT 12 (and Table C on p. viii) which is not correct. As given in the original scenario described on p. 74 Table 4.2 in the ESD, the parameter Ttreat should be divided into two parameters:

- hydraulic retention time for primary settling Tps = 0.167 d; and
- hydraulic retention time for chemical/mechanical treatment Tcm = 0.167 d.

This lead to changes in the equations in the ESD implemented in EUSES as described above.

4.2.11 PT 14 Rodenticides

4.2.11.1 Scenario 14.1 Sewer systems

The scenario (14.1) Sewer systems combines the scenarios "Emission to STP " and "Emission to surface water bodies" of the ESD ("Revised Emission Scenario Document for Product Type 14 – Rodenticides, August 2018).

To assess each of the two scenarios through this single implementation:

- The fraction of active ingredient released directly and the fraction of active ingredient released indirectly are purposely made independent. Therefore, in case one default value is changed, the other default value will not automatically change.
- In order to assess the scenario "Emission to surface water bodies" via a rainwater sewer, it is necessary to:
 - Artificially set the "Effluent discharge rate of local STP" to 0.6x10⁶ l.d⁻¹: in Study
 > Sewage treatment > "Sewage treatment defaults" → tab "General", set the number of inhabitants feeding one STP to 3000 eq, so that the Effluent discharge rate of the local STP is 6x10⁵ l.d⁻¹;
 - In the Study > Distribution > Sewage treatment > [Industrial use] > Input and configuration > "Local STP input and configuration" → tab "Input", set the "Use or bypass STP (local freshwater assessment)" to "Bypass STP".

odel version General Raw sewage Primary settler Activate	a sidaye tarik Solidshiquid:	s separator	
Number of inhabitants feeding one STP	3E+03	[eq]	s
Sewage flow	0.2	[m3.d-1.pers	on-1] d
Effluent discharge rate of local STP	6E+05	[l.d-1]	o
pH	7	[-]	d
Temperature correction for STP degradation	Yes		▼ d
Temperature of air above aeration tank	15	[oC]	d
Temperature of water in aeration tank	15	[oC]	d
Height of air column above STP	10	[m]	d
Regional and continental defaults			
Number of inhabitants of region	2E+07	[eq]	d
Number of inhabitants of continental system	3.5E+08	[eq]	0
Windspeed in the system	3	[m.s-1]	d
<u>✓ 0K</u>	cancel		? <u>Н</u> еlp
Local STP input and configuration [1*", IC=15/UC=39] [Industrial us			? <u>H</u>elp
Local STP input and configuration [1*", IC=15/UC=39] [Industrial us			
Local STP input and configuration [1"", IC=15/UC=39] [Industrial us	:e]	Hass STP	>
OK Local STP input and configuration [1 "", IC=15/UC=39] [Industrial us at STP Configuration] se or bypass STP (local freshwater assessment) se or bypass STP (local marine assessment)	:e]	Hass STP	>
Local STP input and configuration [1"", IC=15/UC=39] [Industrial us at STP Configuration] se or bypass STP (local freshwater assessment)	:e]	oass STP	>
Local STP input and configuration [1 "", IC=15/UC=39] [Industrial us at STP Configuration] se or bypass STP (local freshwater assessment) se or bypass STP (local marine assessment) bocal emission to wastewater	se]] 	Dass STP 71 [kg.d-1] 36 [mg.l-1]	>
Local STP input and configuration [1 "", IC=15/UC=39] [Industrial us at STP Configuration] se or bypass STP (local freshwater assessment) se or bypass STP (local marine assessment) occal emission to wastewater oncentration in untreated wastewater	se] Byy 0.4	Dass STP 71 [kg.d-1] 36 [mg.l-1]	>
Local STP input and configuration [1 "", IC=15/UC=39] [Industrial us at STP Configuration] se or bypass STP (local freshwater assessment) se or bypass STP (local marine assessment) bocal emission to wastewater oncentration in untreated wastewater bocal emission entering the STP	se] By 0.4 0.2 0.4	71 [kg.d-1] 36 [mg.l-1]	>
Local STP input and configuration [1 "", IC=15/UC=39] [Industrial us at STP Configuration] se or bypass STP (local freshwater assessment) se or bypass STP (local marine assessment) ocal emission to wastewater oncentration in untreated wastewater oncentration in untreated wastewater ocal emission entering the STP hemical class ow (apparent octanol-water partition coefficient at actual pH)	se] By 0.4 0.2 0.4	71 [kg.d-1] 36 [mg.l-1] 71 [kg.d-1]	
Local STP input and configuration [1 "", IC=15/UC=39] [Industrial us at STP Configuration] se or bypass STP (local freshwater assessment) se or bypass STP (local marine assessment) ocal emission to wastewater oncentration in untreated wastewater ocal emission entering the STP hemical class ow (apparent octanol-water partition coefficient at actual pH) Ka (acid dissociation constant)	se] [J] [By] [0.4 [0.2 [0.4] [Ne	71 [kg.d-1] 36 [mg.l-1] 71 [kg.d-1] 444	> >
Local STP input and configuration [1 "", IC=15/UC=39] [Industrial us at STP Configuration] se or bypass STP (local freshwater assessment) se or bypass STP (local marine assessment) bocal emission to wastewater oncentration in untreated wastewater occal emission entering the STP hemical class ow (apparent octanol-water partition coefficient at actual pH) Ka (acid dissociation constant) artition coefficients	se] By 0.4 0.2 0.4 Ne ?? 7	Joans STP [kg.d-1] 71 [mg.l-1] 71 [kg.d-1] 71 [kg.d-1] utral [-] [-] [-]	
Local STP input and configuration [1 "", IC=15/UC=39] [Industrial us at STP Configuration] se or bypass STP (local freshwater assessment) se or bypass STP (local marine assessment)	se] [J] [By] [0.4 [0.2 [0.4] [Ne	200855 STP 71 [kg.d-1] 36 [mg.l-1] 71 [kg.d-1] utral [-] [-] [l.kg-1]	>
Local STP input and configuration [1 "", IC=15/UC=39] [Industrial us at STP Configuration] se or bypass STP (local freshwater assessment) se or bypass STP (local marine assessment) ocal emission to wastewater oncentration in untreated wastewater ocal emission entering the STP hemical class ow (apparent octanol-water partition coefficient at actual pH) Ka (acid dissociation constant) artition coefficients rganic carbon-water partition coefficient	se]	File [kg.d-1] 36 [mg.l-1] 71 [kg.d-1] utral [-] [-] [.kg.d-1] 33 [l.kg.dutt	> •

4.2.12 PT 18 Insecticides, acaricides and products to control other arthropods

4.2.12.1 Scenario 18.2.1 Indoor, spray application

Concerning the parameter "Quantity of commercial product applied per $m^{2"}$ in the "Application tab": if there is a dilution step before the application, this can currently not be reflected in EUSES. Therefore, the quantity of commercial product used (per m^2/m^3) needs to be calculated beforehand (outside EUSES).

4.2.12.2 Scenario 18.3.4 Outdoor, spot application

The scenario (18.3.4) Outdoor, spot application is described regarding the life cycle stage as "Industrial use", covering however both professional and non-professional uses.

4.2.12.3 Assessment of releases to waste

The emissions to waste are not relevant for the biocides assessment. Therefore, the calculation of local emission to solid waste, even if described in the ESD, was not implemented. Namely, it was not implemented for PT 18.2.1 – Indoor, spray application, PT 18.2.2 – Indoor, gel application, PT 18.2.3 – Indoor, powders/dusting, 18.2.4 – Indoor, injection and 18.2.6 – Indoor, diffusers.

4.2.12.4 Private uses for outdoor flying insects and nest applications

For outdoor flying insects' uses and outdoor nest application for hornets and wasps, only industrial use, which is used as surrogate for professional use, is covered (18.3.1 Outdoor, flying insects and 18.3.3 Outdoor, nest spraying).

Private uses for outdoor flying insects and nest applications were not implemented in EUSES in line with the ESD for PT 18. According to the ESD for PT 18 (p.108), regarding the outdoor treatments to control flying insects (mosquitoes, flies and hornets or wasps),

the "general public may use insecticide sprays, typically aerosol sprays, to control flying insects such as flies or mosquitoes, but in outdoor conditions, the efficacy of such treatment is of local and time-limited action. Due to the limited scale of the application and the dilution of the application in the air compartment, no specific scenario will be developed for this application. Diffuse releases by the general public have to be considered together with indoor applications. Because equipment for the application of outdoor insecticide using sprayers or foggers for adult mosquitoes control are expensive and complex, these more extensive treatments are often performed by professional."

4.2.13 PT 19 Repellents and attractants

4.2.13.1 Scenario 19.1 Insect repellents applied to human skin and garments

Concerning body surface treated areas, the implementation in EUSES follows the most recent agreements at ENV WG-V-2018 and HEAdoc recommendation of January 2018 for the treated skin area. Therefore the surface area corresponding to "Head+Arms+Hands+Legs+Feet" is 55% of the total surface area for a standard adult person (16600 cm2), i.e. 9130 cm2.

In this respect, the implementation in EUSES deviates from the ESD for PT 19 where "Head+Arms+Hands+Legs+Feet" corresponds to 64.2% of the total surface.

This is relevant for scenario (19.1) Insect repellents applied to human skin and garments, and in particular, for the calculation of the release of repellents used on human skin based on average consumption (indoor use, inner tab – Indoor - consumption), and release of repellents used on human skin due to swimming activities in surface water bodies (inner tab - Outdoor - swimming).

4.2.14 Default scenarios

In preparation of the major EUSES update, ECHA is currently developing core scenarios by grouping certain emission scenarios. As a testing possibility, two default (core) scenarios have been implemented in EUSES 2.2.0 which can be applied in cases where no emission scenario exists for a specific use.

Default Scenario 1 covers any kind of indoor applications to a surface or volume. Releases to either wastewater and air can be calculated.

Default Scenario 2 covers any kind of outdoor applications to a surface, yet currently without the possibility to assess the subsequent service life. Releases to either soil or surface water can be calculated.

5. Notes on the fate and distribution module

The following main changes have been made in the fate and distribution module: inclusion of direct release as exposure pathway in addition to release via the STP, and implementation of the new SimpleTreat version, i.e. SimpleTreat 4.0. These are described in sections 5.2 and 5.3 below.

5.1 Release rates and degradation constants

5.1.1 Rate constants for biodegradation

When a substance is not readily biodegradable, the default value for the following rate constants is set to $6.93 \times 10^{-7} d^{-1}$ (DT50 \triangleq 1 000 000 d):

- Rate constant for biodegradation in surface water;
- Rate constant for biodegradation in aerated sediment;
- Rate constant for biodegradation in bulk soil.

These rate constants can be found in the screen Study > Substance > "Degradation and transformation input". In case a simulation study is available, the default values can be overwritten for the relevant compartment with measured values.

5.1.2 Total rate constants for degradation

Nothing has changed regarding the way the total rate constant for degradation in bulk soil, bulk salt water and bulk sediment are calculated:

• Total rate constant for degradation in bulk soil

The Total rate constant for degradation in bulk soil is equal to the sum of the Rate constant for biodegradation in bulk soil and the Rate constant for abiotic degradation in bulk soil. Note that the latter can be found in the defaults screen Study > Defaults > "Degradation and transformation rates default" and is equal to zero by default.

• Total rate constant for degradation in bulk salt water

The Total rate constant for degradation in bulk saltwater is the sum of the Rate constant for hydrolysis in surface water and the Rate constant for photolysis in surface water plus the Rate constant for biodegradation in saltwater.

• Total rate constant for degradation in bulk sediment

The Total rate constant for degradation in bulk sediment is the sum of the following three elements:

(a) Rate constant for biodegradation in aerated sediment multiplied by Fraction of sediment compartment that is aerated;

(b) Rate constant for anaerobic biodegradation in sediment multiplied by (1 - Fraction of sediment compartment that is aerated);

(c) Rate constant for abiotic degradation in bulk sediment.

Note that the Rate constant for anaerobic biodegradation in sediment, Fraction of sediment compartment that is aerated, and the Rate constant for abiotic degradation in bulk sediment, can be found in the defaults screen Study > Defaults > "Degradation and transformation rates

default".

5.2 Direct release

The previous EUSES versions provided only limited possibilities to perform a full risk assessment for uses resulting in direct releases to e.g. soil or surface water. PEC values were calculated within the release module but were not necessarily reflected in the output tables of the fate and distribution module or the risk assessment module.

In EUSES 2.2.0, the possibility to assess direct release was implemented in the fate and distribution and in risk characterisation modules for relevant product types. All calculation steps are shown in a similar manner as done for the release via STP in the respective result windows under "Direct releases" tab (e.g. Study> Distribution > Life cycle steps > [life cycle stage] "Local PECs" window or Study > Risk characterization > Environmental exposure > Local > Risk characterisation of [life cycle stage] "Environmental risk characterization" window).

	", IC=15/UC=39] [Serv	ice life]			_		×
Release via S <mark>TP [</mark>	irect release						
Freshwater Sedim	nent Soil Groundwa	ater					
Application & Lo	eaching (if applicatio	n is relevant)					
<u>No removal</u>							
Local PEC a	t the end of the initia	al assessment period	2.	12E-03	[mg.kgwwt-1]	0	
Local PEC a	t the end of the inte	rmediate assessment peri	od 2.	12E-03	[mg.kgwwt-1]	ο	
Local PEC a	t the end of the long	jer assessment period	2.	12E-03	[mg.kgwwt-1]	ο	
<u>With removal</u>							
Local PEC a	t the end of the initia	al assessment period	2.	12E-03	[mg.kgwwt-1]	0	
Local PEC a	t the end of the inte	rmediate assessment peri	od 2.	12E-03	[mg.kgwwt-1]	0	
Local PEC a	t the end of the long	jer assessment period	2.	11E-03	[mg.kg ww t-1]	0	
<u> P</u> rev	<u>N</u> ext	• Einish	5 <u>U</u> ndo	>	🕻 A <u>b</u> ort	<u>? н</u> е	lp
Environmental		[1 "", IC=15/UC=39] [Servic	e life]		_		×
							^
Freshwater Sedim	ent Soil						
Application & Le	eaching (if applicatio	n is relevant)					
<u>No removal</u>				2.005		_	
RCR at the	end of the initial ass	essment period		2.885		0	
RCR at the RCR at the	end of the intermedia	essment period ate assessment period		2.885	[·]	0	
RCR at the RCR at the RCR at the		essment period ate assessment period					
RCR at the RCR at the RCR at the <u>With removal</u>	end of the intermedia end of the longer as:	essment period ate assessment period sessment period		2.885 2.885	[-]	0	
RCR at the RCR at the RCR at the <u>With removal</u> RCR at the	end of the intermedia end of the longer as: end of the initial ass	essment period ate assessment period sessment period essment period		2.885 2.885 2.885			
RCR at the RCR at the RCR at the <u>With removal</u> RCR at the RCR at the	end of the intermedia end of the longer as: end of the initial ass	essment period ate assessment period sessment period essment period ate assessment period		2.885 2.885	[-]	0	

Specific implementations and workarounds regarding exposure assessment with direct release assessment are provided in the following sections.

5.2.1 Direct releases – service life assessment periods

In case of continuous direct releases to soil during service life, EUSES provides the concentrations in soil at the end of each of the assessment periods, TIME 1, TIME 2 and TIME 3. Time-weighted concentrations are not calculated by EUSES in line with the agreement of the BPC ENV WG.

5.2.2 Direct releases to surface water via rainwater sewer in PT 6, 7, 8, 9, 10 and 14

In order to assess the direct release to surface water via rainwater sewers the "Effluent discharge rate of local STP" must be equal to $6E+05 I.d^{-1}$. The default value for the "Effluent discharge rate of local STP" however is $2E+06 I.d^{-1}$, which corresponds to the effluent discharge rate of a standard wastewater sewer in relation to a local STP.

As this parameter is not editable, and while it is calculated from "Number of inhabitants feeding one STP" x "Sewage flow", one of these parameters, or both, need to be set to an appropriate value. For instance, set the "Number of inhabitants feeding one STP" to 3E+03 [eq] (edit Study > Defaults \rightarrow Sewage treatment defaults \rightarrow tab General).



Next, in the Study > Distribution > Sewage treatment > [life cycle stage] > Input and configuration > "Local STP input and configuration" window, select "Bypass STP" for the parameter "Use or bypass STP (local freshwater assessment)".

This approach is applicable e.g. in order to assess direct releases to surface water via rainwater sewers e.g. in scenarios for PT 6, 7, 8, 9, 10 or 14.1.

new open save edit search expand collapse select start print		
Study S		- □
nput STP Configuration		
Use or bypass STP (local freshwater assessment)	Bypass STP	▼ s
Use or bypass STP (local marine assessment)	Bypass STP	• d
Local emission to wastewater	1.23E+03 [kg.d-1]	(
Concentration in untreated wastewater	617 [mg.l-1]	
Local emission entering the STP	1.23E+03 [kg.d-1]	
Chemical class	Neutral	- d
Apparent Octanol-water partition coefficient of a base at actual pH	?? [-]	
	7	
pKa (acid dissociation constant)	· · ·	,
pKa (acid dissociation constant)	1.26E+03 [l.kg-1]	0
pKa (acid dissociation constant) -Partition coefficients	1.26E+03 [l.kg-1] 377.6 [l.kgdwt-1]	
pKa (acid dissociation constant) -Partition coefficients Organic carbon-water partition coefficient	[

5.2.3 Local concentrations and deposition windows

In the result window Study > Distribution > Life cycle steps > ..."Local concentrations and depositions", only the concentrations without considering removal are presented in the case of direct release to soil or surface water.

Local concentrations and depositions [1 "", IC=15/UC=39] [Service life]				×
Direct release				
Freshwater Soil				
Application				
Local concentration at the end of the day of application	0.226	[mg.kgwwt-1]	0	
Leaching				
Local concentration at the end of the initial assessment period	0.068	[mg.kgwwt-1]	0	
Local concentration at the end of the intermediate assessment period	0.033	[mg.kgwwt-1]	0	
Local concentration at the end of the longer assessment period	8.26E-03	[mg.kgwwt-1]	0	
TOTAL (Application & Leaching)				
Local concentration at the end of the initial assessment period	0.294	[mg.kgwwt-1]	0	
Local concentration at the end of the intermediate assessment period	0.259	[mg.kgwwt-1]	0	
Local concentration at the end of the longer assessment period	0.235	[mg.kgwwt-1]	0	
Prev Next Prev Dext Dex	×	A <u>b</u> ort	<u>?</u> <u>H</u> e	lp

Local (predicted environmental) concentrations, taking into account removal in the respective compartment, as well as the calculated concentrations in subsequent compartments (e.g. sediment and groundwater) are presented only in the Study > Distribution > Life cycle steps > ... "Local PECs" window, in order to prevent redundancies.

Local PECs [1 "", IC=15/UC=39] [Service life]		_		×
Direct release				
Freshwater Sediment Soil Groundwater				
Application & Leaching (if application is relevant)				
<u>No removal</u>				
Local PEC at the end of the initial assessment period	0.294	[mg.kgwwt-1]	0	
Local PEC at the end of the intermediate assessment period	0.259	[mg.kgwwt-1]	0	
Local PEC at the end of the longer assessment period	0.235	[mg.kgwwt-1]	0	
<u>With removal</u>				
Local PEC at the end of the initial assessment period	0.29	[mg.kgwwt-1]	ο	
Local PEC at the end of the intermediate assessment period	0.219	[mg.kgwwt-1]	0	
Local PEC at the end of the longer assessment period	0.096	[mg.kg ww t-1]	ο	
▲ Prev ▶ Next ▶ Finish 5 Un	do	🕻 A <u>b</u> ort	? <u>H</u> e	lp

5.2.4 Dissolved concentration in water

In case of direct release to surface water (e.g. PT 8), the dissolved concentration (i.e. taking into account dissipation from water phase to sediment) is not shown; this refinement needs to be performed outside EUSES. Only the local concentration (non-dissolved) is provided since this concentration is used for further PEC sediment calculation.

5.2.5 Release to air

For PT 8.4 indoor fumigation, calculations (as release via air from STP) run in the background, but the full STP module is not displayed since not relevant. Only the resulting PEC values are shown (see also section 4.1.4).

5.3 Implementation of SimpleTreat 4.0 in EUSES 2.2.0

EUSES 2.2.0 provides the possibility to either use SimpleTreat 3.1 or SimpleTreat 4.0 as a module to run the exposure assessment for releases via sewage treatment plant (STP). Note that for biocides, it was agreed to use only SimpleTreat 4.0 in the exposure assessment.

As default, module SimpleTreat 4.0 is set, this can be however changed in the Study > "Defaults" > "Sewage treatment defaults" > "Model version" window by actively selecting SimpleTreat 3.1.

🔛 Sewage treatment defaults			×
Model version General Raw sewage Primary settler Activated sludge tank	Solids-liquids separator		
Calculation model	SimpleTreat 3.1	▼ S	

Important note: In contrast to SimpleTreat 4.0, the temperature conversion from Kelvin to Celsius is performed in EUSES 2.2.0 by using a more precise value of 273.15 K instead of 273 K, which may lead to slightly different results in the outcome of the STP module compared to the SimpleTreat standalone version.

5.3.1 Degradation and transformation input

Following the implementation of SimpleTreat 4.0, the window under Study > Substance > Degradation and transformation rates > STP "Degradation and transformation input" has changed according to the settings in SimpleTreat 4.0. Three methods can now be chosen to include measured data, if available:

Method 1: estimated from standardised biodegradability tests (OECD 301 series, 310, 302 series). If this is chosen, the aquatic first order degradation constant (at 15°C) can be manually entered.

Degradation and transformation input				_		×
aracterization STP Water/Sediment Air Soil						
Select biodegradation test method Method 1	: estimated from standard	ized biodegradability tes	ts (OECD 301 s	eries, 310, 302 seri	es) 🔻 [s	
Percentage removal due to biodegradation			Select pe	rcentage (%)	u	
Aquatic first order degradation constant (at 15 of	3		0	[hr-1]	d	
First order degradation constant valid for combine	ed aqueous phase/sludge	(at 15 oC)	??	[hr-1]	u	
First order degradation constant valid for aqueou	s phase (at 15 oC)		??	[hr-1]	u	
Prev Next	Finish	5 Undo	×	Abort	<u>? H</u> el	lp

Method 2: chemical is biodegradable in activated sludge batch test (OECD 314 B). If this method is chosen, the first order degradation constant value for combined aqueous phase/sludge (at 15°C) can be manually entered.

haracterization STP Water/Sediment Air Soil				
Select biodegradation test method Method 2: chemical is biodegradable in act	ivated sludge batch test (OEC	D 314 B)	▼ s	
Percentage removal due to biodegradation	Select p	ercentage (%)	u	
Aquatic first order degradation constant (at 15 oC)	??	[hr-1]	u	
irst order degradation constant valid for combined aqueous phase/sludge (at 15 o	C) ??	[hr-1]	u u	
irst order degradation constant valid for aqueous phase (at 15 oC)	??	[hr-1]	u	
		1		-
	🕤 Undo 🛛 🗙 🗙	Abort	7 <u>H</u> e	h

Method 3: chemical is biodegradable in activated sludge simulation test (OECD 303 A). If this method is chosen, the first order degradation constant value for aqueous phase (at 15°C) can be manually entered.

💭 Degradation and transformation inp	ıt			_		×
Characterization STP Water/Sediment	Air Soil					
Select biodegradation test method	Method 3: chemical is biod	legradable in activated sluc	ge simulation test (OECD 3	303 A)	▼ S	
Percentage removal due to biodegra	dation		Select percent	age (%)	▼ u	
Aquatic first order degradation cons	tant (at 15 oC)		??	[hr-1]	u	
First order degradation constant val	id for combined aqueous phase	e/sludge (at 15 oC)	??	[hr-1]	u	
First order degradation constant val	id for aqueous phase (at 15 oC	;)	??	[hr-1]	u	
1	1	1	1	1	_	_
<u>Prev</u> ▶ <u>N</u> e	xt 🕨 🕨 <u>F</u> inish	5 <u>U</u> ndo	🗶 A <u>b</u> ort		? <u>H</u> elj	,

In case the EUSES study is performed using SimpleTreat 3.1, only Method 1 can be chosen, Method 2 and 3 are not displayed.

5.3.2 Local STP input and configuration

The Study > Distribution > Sewage treatment > [Industrial use] > Input and configuration > "Local STP input and configuration" window was adapted in EUSES 2.2.0 to align with the settings of SimpleTreat 4.0; different chemical classes can now be chosen under the "input" sub-header.

se or bypass STP (local freshwater assessment)	Use STP		▼ d
lse or bypass STP (local marine assessment)	Bypass STP	1	▼ d
ocal emission to wastewater	4.8	[kg.d-1]	0
oncentration in untreated wastewater	2.4	[mg.l-1]	0
ocal emission entering the STP	4.8	[kg.d-1]	o
Chemical class	Neutral		▼ S
ow (apparent octanol-water partition coefficient at actual pH)	??	[-]	0
Ka (acid dissociation constant)	7	[-]	d
Partition coefficients			
Irganic carbon-water partition coefficient	34.67	[l.kg-1]	0
olids-water partition coefficient in raw sewage sludge	10.4	[l.kgdwt-1]	0
olids-water partition coefficient in activated sewage sludge	12.83	[l.kgdwt-1]	0
IOTE: For neutral chemicals, these values are copied from the 'Partition coel	1	1 IF 4	

In the second sub-tab "STP Configuration", the STP facility type is per default set to a municipal STP, which is the standard mode to be used for the assessment of biocides. For other assessments, however, the possibility is given to choose an industrial STP.

Local STP input and configuration [1 "", IC=15/UC=39] [Industrial use]	_		×
Input STP Configuration			
Operation mode Dilution			
Facility type	Municipal	▼ S	
Type of local STP	Include primary solids removal (9-box)	▼ d	
Fraction of sewage solids removed by primary sedimentation	0.67 [-]	d	
pH	7 [-]	o	
Effluent discharge rate of this STP	2E+06 [I.d-1]	0	

5.3.3 Local STP results

The most important sub-tabs in the Study > Distribution > Sewage treatment > [Industrial use] > Output [Industrial use] "Local STP" window are:

Distribution: It provides information on the emission fractions of a substance leaving the STP to different subsequent environmental compartments (air, water, indirectly: soil via the sewage sludge) and the fraction of substance degraded in the STP.

Distribution Elimination and emission Concentrations			
Fraction of emission directed to air by STP	11.04	[%]	0
Fraction of emission directed to water by STP	3.201	[%]	0
Fraction of emission via primary settler	0.308	[%]	0
Fraction of emission via surplus sludge	5.09E-03	[%]	0
Fraction of the emission degraded in STP	85.44	[%]	0
Total of fractions	100	[%]	0

Docal STP [1 "", IC=15/UC=39] [Industrial use]				×	
Distribution Elimination and emission Concentrations					
Concentration of chemical in untreated wastewater	2.4	[mg.l-1]	0		
Concentration of chemical in air	8.91E-06	[g.m-3]	0		
Concentration of chemical in sludge					
- In primary sludge	24.54	[mg.kg-1]	0		
- In surplus sludge	1.153	[mg.kg-1]	0		
- Total concentration of chemical in combined sludge	18.46	[mg.kg-1]	0		
Concentration of chemical in mixed liquor					
- Dissolved in mixed liquor	0.089	[mg.l-1]	0		
- Associated in mixed liquor	4.63E-03	[mg.l-1]	0		
- Total concentration of chemical in mixed liquor	0.094	[mg.l-1]	0		
Concentration of chemical in the STP-effluent					
- Dissolved in the STP-effluent	0.077	[mg.l-1]	o		
- Associated in the STP-effluent	3.46E-05	[mg.l-1]	0		
- Total concentration in the STP-effluent	0.077	[mg.l-1]	0		
Concentration of chemical in solids effluent	1.153	[mg.kg-1]	0		
Concentration in effluent exceeds solubility No o					
PEC for micro-organisms in the STP	0.077	[mg.l-1]	0		
▲ Prev ▶ Next ▶ Einish 5 Undo	×	A <u>b</u> ort	? <u>H</u> el	p	

For further specific details on the background and specifications of in SimpleTreat 4.0, please refer to the SimpleTreat 4.0 user manual⁷.

³¹

⁷ <u>https://www.rivm.nl/en/soil-and-water/simpletreat</u>

Appendix 1. Emission scenarios implemented or updated in EUSES 2.2.0

(1) Human Hygiene

(2) Disinfectants

- (2.1) Sanitary sector, private and institutional areas
- (2.2.1) Medical, rooms, furniture and objects
- (2.2.2) Medical, instruments
- (2.2.3) Medical, laundry
- (2.3) Industrial areas
- (2.4.1) Air conditioning systems, shock dosing
- (2.4.2) Air conditioning systems, continuous dosing
- (2.5) Chemical toilets
- (2.6.1) Swimming pools, permanent
- (2.6.2) Swimming pools, above ground
- (2.7) Aquaria
- (2.8) Indoor fountains
- (2.9.1) Wall treatment against algae (spraying and rinsing)
- (2.9.2) Wall treatment against algae (service life)

(3) Veterinary hygiene

- (3.1) Disinfection of animal housings Not implemented
- (3.2) Disinfection of vehicles used for animal transport
- (3.3) Disinfection of veterinary hygiene: non-medicinal teat dips Not implemented
- (3.4) Disinfection of veterinary hygiene: footwear and animals' feet Not implemented
- (3.5) Disinfection in hatcheries

(4) Food and feed area

- (4.1) Food, drink and milk industries
- (4.2) Milking parlour systems and wine barrel disinfection
- (4.3) Large scale kitchens and slaughterhouses
- (4.4) Private use in food and feed areas

(5) Drinking water

- (5.1) Drinking water
- (5.2) Hospital drinking water

(6) Preservatives for products during storage

- (6.1) Detergents and cleaning fluids
- (6.2) Paints and coatings
- (6.3) Paper
- (6.4) Textile
- (6.5) Leather
- (6.6) Fuels
- (6.7) Fuels in storage tanks Not implemented

(7) Film preservatives

- (7.1) Paints
- (7.2) Polymerised materials
- (7.3) Rubber products
- (7.4) Roof membranes
- (7.5) Paper and cardboard

(8) Wood preservatives

- (8.1.1) Industrial preventive processes, Automated spraying
- (8.1.2) Industrial preventive processes, Dipping and immersion
- (8.1.3) Industrial preventive processes, Vacuum pressure and double vacuum
- (8.2) In situ treatments (curative and preventive)
- (8.3.1) Treated wood in service UC 3
- (8.3.2) Treated wood in service UC 4a
- (8.3.3) Treated wood in service UC 4b
- (8.3.4) Treated wood in service UC 5, Harbour wharf
- (8.4) Indoor fumigation
- (8.5) Injection
- (8.6) Wrapping
- (8.7) Termite control
- (8.8) In situ spraying (outdoors)
- (8.9) Railway sleepers
- (8.10) Dock and deck/fence

(9) Fibre, leather, rubber and polymerized materials preservatives

- (9.1) Textile and fabrics
- (9.2) Leather
- (9.3) Polymerised materials
- (9.4) Rubber products
- (9.5) Roof membranes
- (9.6) Paper and cardboard

(10) Construction material preservatives

- (10.1) In situ treatment with a sprayer
- (10.2) In situ treatment with a roller or brush
- (10.3) Service life house in the countryside
- (10.4) Service life city scenario

(11) Preservatives for liquid-cooling and processing

- (11.1) Once through
- (11.2) Open recirculating
- (11.3) Closed systems

(12) Slimicides

- (12.1) Paper production
- (12.2) Oil industry oil drilling processes
- (12.3) Oil industry storage, reservoir injection and closed drain systems

(13) Working or cutting fluid preservatives

(14) Rodenticides

- (14.1) Sewer systems
- (14.2) In and around buildings
- (14.3) Open areas
- (14.4) Waste dumps
- (14.5) Bank slopes

(15) Avicides

- (15.1) Baits in open rural areas
- (15.2) Egg oil-coating in open rural areas
- (15.3) Bait application in and around buildings
- (15.4) Egg oil-coating in and around buildings

(18) Insecticides, acaricides and products to control other arthropods

- (18.1) Insecticides in stables and manure Not implemented
- (18.2.1) Indoor, spray application
- (18.2.2) Indoor, gel application
- (18.2.3) Indoor, powders/dusting
- (18.2.4) Indoor, injection
- (18.2.5) Indoor, fumigant
- (18.2.6) Indoor, diffusers
- (18.3.1) Outdoor, flying insects
- (18.3.2) Outdoor, crawling insects
- (18.3.3) Outdoor, nest spraying
- (18.3.4) Outdoor, spot application

(19) Repellents and attractants

- (19.1) Insect repellents applied to human skin and garments
- (19.2) Insect repellents applied on animal skin
- (19.3) Insect repellents in the environment of humans and animals
- (19.4) Insect repellents used for factory-treated textiles

(21) Antifouling - Not implemented

(22) Embalming and taxidermist fluids

- (22.1) Taxidermy
- (22.2) Embalming

Default scenario 1

Indoor application to surface or volume

Default scenario 2

Outdoor application to surface

Appendix 2. Number of emission days

Table 2: Scenarios where the parameter number of emission days was added to the release module because is relevant to the distribution module

SCENARIO	LIFE CYCLE STAGE	ТАВ	DEFAULT VALUE
(1) Human hygiene	Industrial use	Consumption input	300
	Private use	Consumption input	365
(2.1) Sanitary sector, private and institutional areas	Industrial use	Consumption input	260
	Private use	Consumption input	365
(2.2.1) Medical, rooms, furniture and objects	Industrial use	Consumption input	300
(2.2.2) Medical, instruments	Industrial use	Input	300
(2.2.3) Medical, laundry	Industrial use	Input	300
(2.3) Industrial areas	Industrial use	Input	300
(2.5) Chemical toilets	Industrial use	Input	300
(2.6.1) Swimming pools, permanent	Private use	Chronic emissions	365
(2.6.1) Swimming pools, permanent	Private use	Peak emissions	60
(2.7) Aquaria	Private use	Input	365
(2.8) Indoor fountains	Private use	Input	365
(2.9.1) Wall treatment against algae (spraying and rinsing)	Industrial use	Input (In the city scenario)	300
(2.9.2) Wall treatment against algae (service life)	Service life	Input (In the city scenario)	365
(3.5) Disinfection in hatcheries	Industrial use	Input	365
(4.1) Food, drink and milk industries	Industrial use	Additional scenario FDM	300
(4.2) Milking parlour systems and wine barrel disinfection	Industrial use	Milking parlour systems	300
(4.2) Milking parlour systems and wine barrel disinfection	Industrial use	Wine barrel disinfection	300
(4.3) Large-scale kitchens and slaughterhouses	Industrial use	Input	300
(5.1) Drinking water	Industrial use	Input	365

SCENARIO	LIFE CYCLE STAGE	ТАВ	DEFAULT VALUE
(5.2) Hospital drinking water	Industrial use	Input	365
(6.1) Detergents and cleaning fluids	Industrial use	Washing and cleaning fluids	300
(6.1) Detergents and cleaning fluids	Private use	Human hygiene products – Consumption based	365
(6.1) Detergents and cleaning fluids	Private use	Washing and cleaning fluids	365
(6.2) Paints and coatings	Industrial use	Input	300 This parameter is enabled only when "Location of the house treated" is "In the city"
(6.2) Paints and coatings	Private use	Consumption (roller/brush) input	365 This parameter is enabled only when "Location of the house treated" is "In the city"
(6.2) Paints and coatings	Service life	City scenario	365
(6.3) Paper	Industrial use	Papermaking	300
(6.4) Textile	Industrial use	Input	300
(6.5) Leather	Industrial use	Consumption input	300
(7.3) Rubber products	Industrial use	Input	300
(7.4) Roof membranes	Service life	City scenario	365
(7.5) Paper and cardboard	Industrial use	Input	300
(8.1.1) Industrial preventive processes, automated spraying	Industrial use	Application	300
(8.1.2) Industrial preventive processes, dipping and immersion	Industrial use	Application	300
(8.1.3) Industrial preventive processes, vacuum pressure and double vacuum	Industrial use	Application	300
(8.3.1) Treated wood in service – UC3	Service life	Input	365 This parameter is enabled only for noise barrier scenario

SCENARIO	LIFE CYCLE STAGE	ТАВ	DEFAULT VALUE
(9.1) Textile and fabrics	Industrial use	Input	300
(9.2) Leather	Industrial use	Input	300
(9.4) Rubber products	Industrial use	Input	300
(9.5) Roof membranes	Service life	City scenario	365
(9.6) Paper and cardboard	Industrial use	Input	300
(10.1) In-situ treatment with a sprayer	Industrial use	Input	300 This parameter is enabled only when "Location of the house treated" is "In the city"
(10.2) In-situ treatment with a roller or brush	Industrial use	Input	300 This parameter is enabled only when "Location of the house treated" is "In the city"
(10.2) In-situ treatment with a roller or brush	Private use	Input	365 This parameter is enabled only when "Location of the house treated" is "In the city"
(10.4) Service life – city scenario	Service life	Input	365
(13) Working or cutting fluid preservatives	Industrial use	Input	300
(14.1) Sewer systems	Industrial use	Input	300
(15.1) Baits in open rural areas	Formulation	Input	300
(15.3) Baits application in and around buildings	Industrial use	Input	300
(15.4) Egg oil-coating in and around buildings	Industrial use	Input	300
(18.2.1) Indoor, spray application	Industrial use	General input	300
(18.2.1) Indoor, spray application	Private use	General input	365
(18.2.2) Indoor, gel application	Industrial use	General input	300
(18.2.2) Indoor, gel application	Private use	General input	365
(18.2.3) Indoor, powders/dusting	Industrial use	General input	300
(18.2.3) Indoor, powders/dusting	Private use	General input	365

SCENARIO	LIFE CYCLE STAGE	ТАВ	DEFAULT VALUE
(18.2.4) Indoor, injection	Industrial use	General input	300
(18.2.5) Indoor, fumigant	Industrial use	General input	300
(18.2.6) Indoor, diffusers	Private use	General input	365
(18.3.1) Outdoor, flying insects	Industrial use	General input	300 This parameter is disabled when "Location of treated surface" is "Rural area"
(18.3.2) Outdoor, crawling insects	Industrial use	General input	300 This parameter is disabled when "Location of treated surface" is "Rural area"
(18.3.2) Outdoor, crawling insects	Private use	General input	365 This parameter is disabled when "Location of treated surface" is "Rural area"
(19.1) Insect repellents applied to human skin and garments	Private use	Indoor - consumption	365
(19.2) Insect repellents applied on animal skin	Private use	Indoor – cats and dogs	365
(19.2) Insect repellents applied on animal skin	Private use	Outdoor – paved ground	365 This parameter is enabled when "Select" is "Release via STP"
(19.3) Insect repellents in the environment of humans and animals	Private use	Indoor -consumption	365
(19.3) Insect repellents in the environment of humans and animals	Private use	Outdoor – paved ground	365
(19.4) Insect repellents used for factory-treated textiles	Industrial use	Consumption based	300
(19.4) Insect repellents used for factory-treated textiles	Service life	Washing of factory treated garments and gear	365
(22.1) Taxidermy	Industrial use	Input	300
(22.2) Embalming	Industrial use	Input	300

Table 3: Scenarios where the parameter number of emission days relevant for the distribution module was already available in the release module

SCENARIO	LIFE CYCLE STAGE	ТАВ	PARAMETER IN THE RELEASE MODULE TO BE USED IN THE DISTRIBUTION MODULE
(2.4.1) Air conditioning systems, shock dosing	Industrial use	One shock dose	Number of emission days for one shock dosing
(2.4.1) Air conditioning systems, shock dosing	Industrial use	Repeated shock dosing	Number of emission days for repeated shock dosing
(2.4.2) Air conditioning systems, continuous dosing	Industrial use	Input	Number of emission days for continuous dosing
(2.6.1) Swimming pools, permanent	Industrial use	Chronic emissions	Emission period
(2.6.1) Swimming pools, permanent	Industrial use	Peak emissions	Emission period
(3.2) Disinfection of vehicles used for animal transport	Industrial use	Input	Number of emission days per year
(4.1) Food, drink and milk industries	Industrial use	CIP brewery	Number of emission days
(4.1) Food, drink and milk industries	Industrial use	General scenario FDM	Number of emission days
(6.1) Detergents and cleaning fluids	Formulation	Input	Number of emission days
(6.1) Detergents and cleaning fluids	Industrial use	Human hygiene products	Number of emission days
(6.1) Detergents and cleaning fluids	Private use	Human hygiene products – Tonnage based	Number of emission days
(6.2) Paints and coatings	Formulation	Input	Number of emission days
(6.2) Paints and coatings	Private use	Tonnage input	Number of emission days
(6.3) Paper	Formulation	Input	Number of emission days
(6.3) Paper	Industrial use	Recycling	Number of emission days
(6.4) Textile	Formulation	Input	Number of emission days
(6.5) Leather	Formulation	Input	Number of emission days
(6.5) Leather	Industrial use	Tonnage input	Number of emission days
(6.5) Fuels	Formulation	Input	Number of emission days
(7.1) Paints	Industrial use	Input	Number of emission days

SCENARIO	LIFE CYCLE STAGE	ТАВ	PARAMETER IN THE RELEASE MODULE TO BE USED IN THE DISTRIBUTION MODULE
(7.1) Paints	Private use	Input	Number of emission days
(7.2) Polymerised materials	Industrial use	General input	Number of emission days
(7.2) Polymerised materials	Service life	Input	Number of emission days
(7.5) Paper and cardboard	Waste treatment	Input	Number of emission days
(9.1) Textile and fabrics	Service life	Input	Number of emission days
(9.3) Polymerised materials	Industrial use	General input	Number of emission days
(9.3) Polymerised materials	Service life	Input	Number of emission days
(9.6) Paper and cardboard	Waste treatment	Input	Number of emission days
(11.2) Open recirculating	Industrial use	General input	Number of emission days
(11.3) Closed systems	Industrial use	General input	Number of emission days
(12.1) Paper production	Industrial use	Input for degradation	Number of emission days Only when "Select type of treatment" = "Typical case scenario" the Temission = Number of emission days
(19.1) Insect repellents applied to human skin and garments	Private use	Indoor - tonnage	Number of emission days
(19.3) Insect repellents in the environment of humans and animals	Private use	Indoor - tonnage	Number of emission days
(19.4) Insect repellents used for factory-treated textiles	Industrial use	Tonnage based	Number of emission days

Appendix 3. Scenario (3.5) Disinfection in hatcheries – model calculations

The equations implemented in EUSES for estimating the releases from this scenario are the following:

Local emission rate to water (on the day of hatching):

Elocalwater = Qaiappi * 0.001 * (F_{water_fum} * (V_{sluice} * N_{sluice} * Nappl_{sluice} + V_{hatcher} * N_{hatcher} * Nappl_{hatcher}) + F_{water_fog} * (V_{hatcher} * N_{hatcher} * Nappl_{hatcher} + V_{setter} * N_{setter} * Nappl_{setter}))

Local emission rate to air (on the day of hatching):

Elocal_{air} = Qai_{appl} * 0.001 * (F_{air_fum} * (V_{sluice} * N_{sluice} * Nappl_{sluice} + V_{hatcher} * N_{hatcher} * Nappl_{hatcher}) + F_{air_fog} * (V_{hatcher} * N_{hatcher} * Nappl_{hatcher} + V_{setter} * N_{setter} * Nappl_{setter}))

With:

Qaiappl - Quantity of disinfectant used per cubic meter

V_{sluice} - Volume of the fumigation sluice

N_{sluice} - Number of fumigation sluices

Napplsuice - Number of disinfection events in stage 1 (eggs in fumigation sluice)

V_{hatcher} - Volume of the hatcher

Nhatcher - Number of hatchers

Nappl_{hatcher} - Number of disinfection events in stage 2 (eggs in hatcher)

V_{setter} - Volume of the setter

Nsetter - Number of setters

Nappl_{hatcher} - Number of disinfection events in stage 3 (single-stage setter)

Fair_fum - Fraction released to air after fumigation

F_{water_fum} - Fraction released to wastewater after fumigation

Fair_fog - Fraction released to air after aerosol or fogging treatment

Fwater_fog - Fraction released to wastewater after aerosol or fogging treatment

EUROPEAN CHEMICALS AGENCY ANNANKATU 18, P.O. BOX 400, FI-00121 HELSINKI, FINLAND ECHA.EUROPA.EU